# DATA-DRIVEN MULTI-SCALE MODELING, ANALYSIS AND SIMULATION OF ANOMALOUS MATERIALS

By

Jorge Luis Suzuki

## A DISSERTATION

Submitted to Michigan State University in partial fulfillment of the requirements for the degree of

Mechanical Engineering – Doctor of Philosophy Computational Mathematics, Science and Engineering – Dual Major

#### ABSTRACT

# DATA-DRIVEN MULTI-SCALE MODELING, ANALYSIS AND SIMULATION OF ANOMALOUS MATERIALS

### By

#### Jorge Luis Suzuki

Anomalous rheology is a material behavior that presents the fingerprint of power-laws, arising from anomalous diffusion in microstructures, and observed in a range of complex materials. Such microstructures often display a fractal nature with sub-diffusive dynamics, *e.g.*, of entangled polymer chains, and defect interactions such as dislocation avalanches, cracks, and voids. The corresponding macroscopic non-exponential behavior makes integer-order models to lack a compact representation of the small-scale physics. Furthermore, classical linear viscoelastic models require arbitrary arrangements of Hookean/Newtonian elements, introducing a limited number of exponential relaxation modes that, at most, represent a truncated power-law approximation. While this may be satisfactory for short times at engineering accuracy, such models often yield high-dimensional parameter spaces and lack predictability for multiple time/length-scales. In this scenario, Fractional Calculus (FC) becomes an attractive modeling alternative since it naturally accounts for power-law kernels in its integro-differential operators. This allows accurate and predictive modeling of soft materials for multiple timescales, in which most standard models fail or become impractical.

In this work, a data-driven framework for efficient, multi-scale fractional modeling and failure of anomalous materials is proposed. The overarching goal is to identify/construct efficient fractional rheological models, especially for soft materials, undergoing nonlinear response and failure. To this purpose, a fractional linear and nonlinear viscoelastic existence study is developed and employed for the first time to urinary bladder tissues undergoing large strains. The framework is extended to account for power-law viscoplastic behavior, and aiming for applications to larger systems, the resulting models are solved through a new approach called fractional return-mapping algorithm, that generalizes existing predictor-corrector schemes of classical elastoplasticity. Regarding the effects of fractional constitutive laws on structural dynamics, a few developed models are incorporated

to beam and truss structures, where the effects of evolving constitutive laws on the anomalous dynamics of systems are analyzed. Although FC became an effective modeling tool in the last few decades, it requires careful considerations to satisfy basic thermodynamic conservation/dissipation laws. To this end, the thermodynamic consistency of the developed visco-elasto-plastic models with the addition of damage effects is proved. Furthermore, the associated energy release rate due to crack/void formation is consistent with the employed fractional rheological elements, which naturally introduces memory effects on damage evolution.

Fractional differential equations (FDEs) inherently carry a functional nonlocal dependency and near-singular behaviors at bounded domains, which increases the computational complexity and degenerates the global accuracy of many existing numerical schemes. Therefore, two numerical contributions are proposed in the last part of the framework. The first one is a data-driven singularity-capturing approach that automatically addresses the low solution regularity and yields high accuracy for long time-integration. In the second contribution, fast implicit-explicit (IMEX) schemes are developed for stiff/nonlinear FDEs, which are shown to have larger stability regions than existing approaches.

Copyright by JORGE LUIS SUZUKI 2021 To my wife, Letícia

#### ACKNOWLEDGEMENTS

I would like to thank my dear advisor and mentor, Dr. Mohsen Zayernouri for providing me such opportunity to join the FMATH group. His enthusiastic motivation, mentoring and support, along with his patience and constructive feedback were key elements during this PhD work. Thank you for sharing your experience and all opportunities you provided throughout this journey.

I would like to thank the respected committee members, Dr. Marta D'Elia, Dr. Tong Gao, Dr. Michael Murillo, Dr. Sara Roccabianca, and Dr. Hui-Chia Yu for all research discussions, and for providing helpful feedback and support throughout the stages of my PhD research.

Additionally, I thank my respected collaborators, Dr. Marta D'Elia, Dr. Mamikon Gulian, Dr. Sara Roccabianca and Dr. Maryam Naghibolhosseini, that contributed to fundamental aspects of fractional calculus models and experimental applications to biotissues.

I would also like to thank all current and past FMATH group members: Dr. Ehsan Kharazmi, Dr. Yongtao Zhou, Dr. Mehdi Samiee, Eduardo Moraes, Ali Akhavan-Safaei, Pegah Varghaei and Hadi Seyedi for your companionship, research discussions and collaborations.

I express my gratitude to my friends and family, especially my parents for their unconditional love and support. Most importantly, I thank my dear wife Letícia, to whom I dedicate this work. Her unconditional love, patience and emotional support were fundamental for me to overcome all challenges faced throughout these years.

This work was supported by the department of mechanical engineering and the department of computational mathematics, science and engineering at Michigan State University. The highperformance computational resources were provided by the Institute for Cyber-Enabled Research (ICER) at Michigan State University.

## **TABLE OF CONTENTS**

LIST OF	F TABLES	xii
LIST OF	F FIGURES	xiii
LIST OF	FALGORITHMS	XXV
CHAPT	ER 1 INTRODUCTION	1
1.1	Power-Law Rheology: Anomalies Across Scales	1
1.2	Definitions of fractional calculus	7
1.3	Fractional Constitutive Modeling	8
	1.3.1 Visco-Elasticity:	8
	1.3.2 Visco-Plasticity:	14
	1.3.3 Damage Mechanics:	15
	1.3.4 Key aspects in fractional models	17
1.4	Outline of this Work	18
CHAPT	ER 2 MULTI-SCALE ASPECTS: MOLECULAR DYNAMICS AND DISCRETE	
	DISLOCATION DYNAMICS	30
2.1	Introduction	30
2.2	Definitions of Dislocation Theory	31
	2.2.1 Types of Dislocations	31
	2.2.2 Burgers' vector	32
	2.2.3 Peach-Koehler forces	33
2.3	Simulations of Dislocation Motion	33
	2.3.1 Atomistic scale: molecular dynamics	33
	2.3.2 Meso-scale: discrete dislocation dynamics	35
2.4	Numerical Results	38
	2.4.1 Molecular dynamics	39
	2.4.1.1 Shear modulus	39
	2.4.1.2 Poisson ratio	40
	2.4.1.3 Edge dislocation radius and energy	40
	2.4.1.4 Dislocation mobility	41
	2.4.2 Discrete dislocation dynamics	44
CHAPT	ER 3 A DATA-DRIVEN FRACTIONAL MODELING FRAMEWORK FOR	
	ANOMALOUS RHEOLOGY: APPLICATION TO URINARY BLAD-	
	DER TISSUE	47
3.1	Background	47
3.2	Problem Setup and Methodology	50
	3.2.1 Urinary bladder experimental relaxation tests	50
	3.2.2 A Fractional Viscoelastic Modeling Framework for Anomalous Tissue	
	Rheology	53

	3.2.2.1 Fractional linear viscoelastic models	54
	3.2.2.2 Fractional quasi-linear viscoelastic modeling	57
	3.2.2.3 Numerical discretizations	58
	3.2.3 Model optimization	59
3.3	Results and Discussion	61
	3.3.1 Linear Viscoelasticity	61
	3.3.2 Nonlinear Viscoelasticity	63
	3.3.3 Discussion	66
CHAPT	ER 4 FRACTIONAL VISCO-ELASTO-PLASTIC MODELS FOR STRUC-	
	TURAL ANALYSIS	70
4.1	Background	70
4.2	Kinematics of Large Visco-Elasto-Plastic Deformations	72
4.3	Fractional-Order Visco-Elasto-Plastic Models	74
	4.3.1 Model M1	74
	4.3.2 Model M2	77
	4.3.2.1 Remark about parameter $H$	78
	4.3.2.2 Remark about visco-elastic/plastic memory effects	79
4.4	Time Integration and Discretization in Space	79
4.5	Fractional Return-Mapping Algorithms	81
	4.5.1 Algorithm for the model M1	83
	4.5.1.1 Remark	87
	4.5.2 Algorithm for the model M2	87
	4.5.3 Incremental tangent modulus	89
4.6	Results and Discussion	90
	4.6.1 Convergence analysis	90
	4.6.2 Stress vs. strain response for prescribed strains	92
	4.6.2.1 Monotonic strains	92
	4.6.2.2 Cyclic strains	94
	4.6.3 Two-member truss with snap-through effect	96
	4.6.3.1 Behavior of the models when $\beta \to 0$	96
	4.6.3.2 Variation of fractional-orders for the model M1	97
	4.6.3.3 Variation of fractional-orders for the model M2	99
CHAPT	ER 5 A THERMODYNAMICALLY CONSISTENT, FRACTIONAL VISCO-	
	ELASTO-PLASTIC MODEL WITH HISTORY-DEPENDENT DAMAGE . 1	102
5.1	Background	102
5.2	Definitions of Fractional Calculus	106
	5.2.1 Interpretation of Caputo derivatives in terms of nonlocal vector calculus 1	107
	5.2.1.1 Note on well-posedness	108
5.3	Thermodynamics of Fractional Scott-Blair Elements	108
	5.3.1 Thermodynamic principles	109
	5.3.2 Helmholtz free-energy density	109
5.4	Fractional Visco-Elasto-Plastic Model with Damage	111
	5.4.1 Thermodynamic formulation	111
	•	

		5.4.1.1 Free-energy densities
		5.4.1.2 Constitutive laws
		5.4.1.3 Evolution laws for visco-plasticity and damage
	5.4.2	Time-fractional integration
		5.4.2.1 Semi-implicit fractional return-mapping algorithm
		5.4.2.2 Numerical discretization of fractional operators
5.5	Numer	rical Tests
CHAPT	ER 6	A GENERAL RETURN-MAPPING FRAMEWORK FOR FRACTIONAL
		VISCO-ELASTO-PLASTICITY
6.1	Backg	round
6.2	Defini	tions of Fractional Calculus
6.3	Fractio	onal Visco-Elasticity
	6.3.1	Linear visco-elasticity
	6.3.2	Quasi-Linear Fractional Visco-Elasticity
6.4	Fractio	onal Visco-Elasto-Plasticity
6.5	A Clas	ss of Return-Mapping Algorithms for Fractional Visco-Elasto-Plasticity 141
	6.5.1	Time-Fractional Integration of Visco-Elastic Models
	6.5.2	Time-Fractional Integration of Visco-Plasticity
	6.5.3	Generalized fractional return-mapping algorithm
		6.5.3.1 Comparison of the return-mapping algorithm to existing approaches 147
6.6	Numer	rical Tests
CHAPT	ER 7	ANOMALOUS NONLINEAR DYNAMICS BEHAVIOR OF FRACTIONAL
		VISCOELASTIC STRUCTURES
7.1	Backg	round
7.2	Mathe	matical Formulation
	7.2.1	Nonlinear In-Plane Vibration of a Viscoelastic Cantilever Beam 160
	7.2.2	Linear Viscoelasticity: Boltzmann Superposition Principle
		7.2.2.1 Exponential Relaxation (Classical Models) vs. Power-Law
		Relaxation (Fractional Models)
		7.2.2.2 Multi-Scale Power-Laws, Distributed-Order Models 165
	7.2.3	Extended Hamilton's Principle
	7.2.4	Weak Formulation
	7.2.5	Assumed Mode: A Spectral Approximation in Space
	7.2.6	Single Mode Approximation
		7.2.6.1 Why is single-mode approximation useful?
7.3	Linear	ized Equation: Direct Numerical Time Integration
	7.3.1	Harmonic Base Excitation
	7.3.2	Free Vibration
7.4	Pertur	bation Analysis of Nonlinear Equation
	7.4.1	Method of Multiple Scales
		7.4.1.1 Case 1: No Lumped Mass At The Tip
		7.4.1.2 Case 2: Lumped Mass At The Tip

CHAPTER 8		A SELF-SINGULARITY-CAPTURING APPROACH FOR FRACTIONAL
		DIFFERENTIAL EQUATIONS
8.1	Backg	ground
8.2	Defin	itions
8.3	Two-S	Stage Time-Integration Framework    192
	8.3.1	Stage-I: Self-singularity-capturing stage
		8.3.1.1 Minimization method
		8.3.1.2 Numerical scheme for short-time integration
		8.3.1.3 Stage-I algorithm
		8.3.1.4 Computational complexity of stage-I
	8.3.2	Stage-II: Integration of FDEs with the captured singularities
8.4	Nume	rical Results
	8.4.1	Numerical behavior of correction weights
	8.4.2	Single time-step and correction term
	8.4.3	Singularity capturing for <i>M</i> correction terms
		8.4.3.1 One correction term
		8.4.3.2 Two correction terms
		8.4.3.3 Three correction terms
	8.4.4	Random singularities
		8.4.4.1 FDEs with random singularities
		8.4.4.2 Multi-term FDEs with random singularities
	8.4.5	Singular-oscillatory solutions
	8.4.6	Nonlinear FDE
CHAPT	ER 9	IMPLICIT-EXPLICIT TIME INTEGRATION SCHEMES FOR NON-
		LINEAR FRACTIONAL DIFFERENTIAL EQUATIONS 219
9.1	Backg	ground
9.2	Impli	cit-Explicit Time-Integration Methods
	9.2.1	Definitions
	9.2.2	Linear FDEs
	9.2.3	Correction terms
	9.2.4	Nonlinear FDEs
		9.2.4.1 Corrections terms for $f(t, u)$
9.3	Linea	r Stability of $IMEX(p)$ Methods
9.4	The F	ast Implementation of $IMEX(p)$ Methods
	9.4.1	Fast approximate inversion scheme
	9.4.2	Fast computation of hypergeometric functions
	9.4.3	Algorithm of $IMEX(p)$ methods
9.5	Nume	rical Tests
	CD 10	
CHAPT	EK 10	SUMMARY AND FUTURE WORKS $\dots \dots \dots$
10.1	Concl	uding Remarks
10.2	Future	e works
APPENI	DICES	

APPENDIX A	DERIVATIONS IN CHAPTER 4
APPENDIX B	DERIVATIONS IN CHAPTER 5
APPENDIX C	DERIVATIONS IN CHAPTER 6
APPENDIX D	DERIVATIONS IN CHAPTER 7
APPENDIX E	DERIVATIONS IN CHAPTER 8
APPENDIX F	DERIVATIONS IN CHAPTER 9
BIBLIOGRAPHY	

# LIST OF TABLES

Table 3.1:	Obtained material parameters for all employed linear fractional models and UB samples
Table 3.2:	Obtained material parameters for the FQLV model with all UB samples 66
Table 6.1:	Convergence behavior for the return-mapping Algorithm 6.1 obtained in this work and the original approach from [1] for an FVEP device with a SB element. 153
Table 8.1:	Influence of $\tilde{N}$ in Stage-I of the developed framework
Table 9.1:	The errors at the endpoint and convergence orders of the FAMMs for (9.63) with $p = 0$ (upper table) and $p = 1$ (lower table)
Table 9.2:	The global errors and convergence orders of the methods IMEX( <i>p</i> ) for (9.64) with $p = 0$ (upper table) and $p = 1$ (lower table) and $\alpha = 0.3$
Table 9.3:	The global errors and convergence orders of the methods IMEX( <i>p</i> ) for solving Case I) with $\alpha = 0.4$ , varying <i>h</i> and correction terms <i>M</i> with corresponding powers $\sigma_k = \delta_k = k\alpha$
Table 9.4:	The global errors and convergence orders of the methods IMEX( $p$ ) for solving Case II) with no correction term for $p = 0$ and $M = 2$ correction terms for $p = 1$ , with $\sigma = \delta = \{1 - \alpha, 1\}$
Table 9.5:	Convergence results for the IMEX(p) scheme solving Case III) without corrections for $p = 0$ and $M = 3$ correction terms for $p = 1$ , with $\sigma = \delta = \{\alpha, 2\alpha, 1 + \alpha\}$ .

# LIST OF FIGURES

Figure 1.1:	(a) Mean square displacement of single cells within an epithelial cell mono- layer under different densities. (b) Evolution of the MSD exponent over time, showing a transition of diffusive to sub-diffusive motions and transient, motion-arresting behavior at higher densities.	2
Figure 1.2:	(a) Scale-free creep behavior of embrionic stem cells nuclei under aspiration stresses. For low values of stress $\Delta P$ , the creep behavior is fit by a single power law. For larger stresses, a transition to plastic regime is observed at $\tau_{plastic} \approx 8 - 10 [s]$ , with a creep exponent $\alpha \approx 0.2$ , for all values of applied stresses. For short times, the creep exponent is higher and increases with stress, suggesting a fluid-like behavior. (b) Different stages of nucleus aspiration, showing a visco-elastic recovery (ii)-(iii), followed by irreversible plastic deformation (iv).	3
Figure 1.3:	(a) Mean squared displacement of colloidal tracer spheres with radius $a = 0.25  [\mu m]$ in F-actin networks, indicating anomalous, sub-diffusive behavior when the sphere radius $a$ is comparable in size with the mesh size $\xi$ . (b) Representative $x - y$ ( <i>left</i> ) and $y$ ( <i>right</i> ) trajectories of particles of a 0.25 $[\mu m]$ particle in F-actin ( $\xi = 0.31  [\mu m]$ ) over 600 [s].	3
Figure 1.4:	(a) Tempered power-law relaxation of polystyrene entangled ring polymers ( <i>open triangles and circles</i> ), and two power-law relaxation regimes of linear polymer chains ( <i>closed triangles and circles</i> ). (b) Creep ringing experiments demonstrating the long-time power-law behavior of acacia gum	4
Figure 1.5:	(a) Microstructures of polycrystalline ice samples with varying averaged grain sizes $\langle d \rangle$ . (Top left) 0.26 [mm], (top right) 0.87 [mm], (bottom left) 1.92 [mm], (bottom right) 5.02 [mm]. (b) Complementary cumulative prob- ability distributions for acoustic emission amplitudes $A_0$ in polycrystalline samples with different average grain sizes. (top) A tempered power-law fit in the form $P(>A_0) \approx A_0^{-\beta} \exp(-A_0/A_c)$ (black line) indicates a decrease in cutoff values $A_c$ for decreasing grain sizes, while the power-law exponent $\beta = 0.35 \pm 0.05$ is similar for all samples. (bottom) Coarse grained samples, leading to bimodel distributions for $A_1$ .	5
	Icaung to onnotal distributions for $A_0$	J

Figure 1.6:	(a) Crack propagation dynamics of heterogeneous materials. (top left) Time- series data of spatially-averaged crack front velocities, showing intermittent bursts. (top right) Distribution of normalized burst duration T, with $P(T) \propto T^{-\alpha}$ , $\alpha = 1.43$ . (bottom left) Distribution of normalized burst size S, with $P(S) \propto S^{-\tau}$ , with $\tau = 1.25$ . (bottom right) Scaling of T with respect to S, with $T \propto S^a$ and $a = 0.58$ . (b) SEM Fracture image of two different metallic glasses, showing a fractal-like formation of dimple structures		6
Figure 1.7:	Comparison between standard and fractional order models. (a) Relaxation behavior of Butyl rubber using experimental data from Scott-Blair. (b) Cole-Cole plot (G' versus G'') for the dynamic properties of acacia gum		13
Figure 1.8:	Schematics of the proposed studies in this work. Starting from physics infor- mation, <i>e.g.</i> , material design requirements and damage/failure processes, the main approaches of this thesis focus on the development and existence studies of admissible, mathematically-informed fractional models and corresponding data-driven numerical methods.		19
Figure 2.1:	Hull and Bacon [2] (a) A positive edge dislocation, denoted by line CD, after inserting an extra half-plane of atoms in ABCD. (b) A left-handed screw dislocation obtained from a displacement of faces ABCD with respect to each other along AB. (c) A Burgers' circuit enclosing an edge dislocation ( <i>left</i> ), and the same circuit in a perfect crystal ( <i>right</i> ). The required closure vector to complete the Burgers' circuit is defined as the Burgers' vector		32
Figure 2.2:	Discretization of dislocations, represented as a set of nodes connected through segments. (a) Two dislocation loops (Sills <i>et al.</i> [3]). (b) A discretized dislocation network (Bulatov <i>et al.</i> [4]).		36
Figure 2.3:	<ul> <li>(a) Orthorhombic box with an edge dislocation in the center, employed as the MD domain for the core radius, edge mobility, and shear (no dislocation) tests.</li> <li>(b) Cylindrical nano-wire domain utilized for the Poisson ratio experiment.</li> </ul>	•	39
Figure 2.4:	Block-shear stress-strain MD experiment. The linear fit over a small strain range $\gamma_{xy} < 0.05$ yielded a shear modulus $G = 73.20 [GPa]$ .	•	40
Figure 2.5:	Nanowire tensile MD experiment. <i>(left)</i> Poisson coefficient estimation $v = 0.378$ , through a linear fit over the filtered data. <i>(right)</i> Obtained stress <i>vs.</i> strain results, yielding a Young's modulus $E = 211.98 [GPa]$ .		41
Figure 2.6:	Dislocation core radius estimation through the relative difference between the potential energy of the system with a single edge dislocation $(PE_e)$ and a pure system $(PE_p)$ . The estimate $r = 2.9 [b]$ is obtained considering a moving average filter on the obtained data and a relative difference of $\approx 1.8\%$ between both systems.		42

MD domain of the dislocation mobility test. (a) $x - y$ plane, illustrating the edge dislocation core as the lattice perturbation at the center. (b) 3D view of the MD domain with the BCC lattice removed, showing the dislocation line along the <i>z</i> -axis.	43
(a) Temperature and total energy for the equilibration step, (b) Edge dislocation position $\mathbf{x}^{MD}(t)$ and (c) mobility through MD simulations for distinct values of applied shear stresses $\tau$ under $T = 750 [K]$ . We observe an overdamped motion for the applied shear stress range and a linear mobility relationship.	44
DDD tensile tests in pure iron under different strain rates. (a) Rate-dependent stress $vs$ . strain response showing visco-plastic intermittent behavior after a hardening/relaxation phase. (b) Dislocation density $vs$ . time. (c) Dislocation density $vs$ . strain, showing a ballistic behavior for lower strain-rates	45
DDD simulations of fractal dislocation network evolution at three different instants: (a) $t = 2.44 \times 10^{-12} [s]$ , (b) $t = 7.46 \times 10^{-10} [s]$ , and (c) $t = 1.90 \times 10^{-9} [s]$ . The red dots represent the dislocation arm (white lines) centroids.	45
Computation of collective dislocation velocities for the DDD tensile test with $\dot{\varepsilon} = 10^6 [s^{-1}]$ . (a) Time-series data of collective dislocation velocity, indicating the presence of intermittent, large energy bursts. (b) Acoustic energy histogram, where $P(E) \propto E^{-\delta}$ , with $\delta = 1.5$ , consistent with experimental data for dislocation avalanches.	46
(a) Dissected porcine UB showing the distinct anatomical locations from which samples were punched. (b) A diagram of the UB from the lateral view. $(c,d)$ A representative sample under clamped, uniaxial relaxation, respectively, in upper and side views, from which images are extracted for area estimation.	51
Stress relaxation data for all UB samples. $(a,b)$ - stress vs time data in linear and logarithmic scales. $(c,d)$ - successive step strain vs time data in linear and logarithmic scales. The long-term power-law behavior becomes evident especially in the first relaxation step in $(b)$ , where the slope of the black line is given by $ \beta  \approx 0.3$	52
	MD domain of the dislocation mobility test. (a) $x - y$ plane, illustrating the edge dislocation core as the lattice perturbation at the center. (b) 3D view of the MD domain with the BCC lattice removed, showing the dislocation line along the <i>z</i> -axis

Normalized relaxation moduli for each bladder specimen under distinct applied strains: (a) D, (b) L, (c) LB, (d) T, (e) V. The relaxation behavior seems to be approximately linear for most specimens in the $\varepsilon_0 \in [0.25, 0.5]$ range. All specimens clearly demonstrate a dependency of both time and applied strains for $\varepsilon_0 > 0.5$ , with largest variations observed in the LB and T samples. Furthermore, the data indicates two distinct relaxation regimes with slower ( $t < 3[s]$ ) and faster ( $t > 400[s]$ ) decays, respectively, with slopes $\beta_1$ and $\beta_2$ illustrated in (f).		53
Relaxation functions $G(t)$ for the building block models under varying frac- tional models and $\mathbb{E}_1 = 1$ , $\mathbb{E}_2 = 1$ . (a) Scott-Blair, (b) Fractional Kelvin-Voigt, and (c) Fractional Maxwell. We note the progression from a single, scale-free power-law behavior for the SB model to two dominating power-laws under small and large times for the FKV and FM models		55
Obtained linear viscoelastic fits for the fractional SB model for all bladder samples and the first strain step ( $\varepsilon_0 = 0.25$ ).		62
Obtained linear viscoelastic fits utilizing a fractional Maxwell for all bladder samples and first strain step ( $\varepsilon_0 = 0.25$ ).		63
Obtained pointwise errors for the linear SB and FM models for the first strain step: $(a)$ D, $(b)$ L, $(c)$ LB, $(d)$ T, $(e)$ V		65
Obtained fits for the fractional QLV model under all strain steps: $(a) D, (b) L$ , $(c) LB, (d) T, (e) V$ . The fit quality was very good for all bladder samples, with more significant deviations occuring on strain steps 4 and 5. The recovered fractional-orders in $(f)$ are within the $0.2 < \alpha < 0.3$ range, which is in accordance with the <i>a-priori</i> power-laws obtained from the relaxation moduli data in Fig.3.3.		65
Obtained pointwise errors for the FQLV model under all strain steps: (a) D, (b)) L, (c) LB, (d) T, (e) V. The vertical gray lines represent the step strain application instants.		66
(a) Kinematics of the truss in terms of initial and updated configurations; (b) Multiplicative decomposition of the stretch into visco-elastic and visco-plastic parts, taking place from the initial to the updated configuration.		73
Visco-elasto-plastic model M1. (a) Constitutive diagram with the rheological elements for visco-elasticity and visco-plasticity. (b) Stress versus strain response described by the yield function (Eq.4.12), showing the expansion of the visco-elastic boundary from $\partial E_{\tau}$ (point A) to $\partial E_{\tau}^*$ (point B) after exceeding the yield stress.		75
	Normalized relaxation moduli for each bladder specimen under distinct applied strains: (a) D, (b) L, (c) LB, (d) T, (e) V. The relaxation behavior seems to be approximately linear for most specimens in the $\varepsilon_0 \in [0.25, 0.5]$ range. All specimens clearly demonstrate a dependency of both time and applied strains for $\varepsilon_0 > 0.5$ , with largest variations observed in the LB and T samples. Furthermore, the data indicates two distinct relaxation regimes with slower ( $t < 3 [s]$ ) and faster ( $t > 400 [s]$ ) decays, respectively, with slopes $\beta_1$ and $\beta_2$ illustrated in ( $f$ )	Normalized relaxation moduli for each bladder specimen under distinct applied strains: (a) D, (b) L, (c) LB, (d) T, (e) V. The relaxation behavior seems to be approximately linear for most specimens in the $\varepsilon_0 \in [0.25, 0.5]$ range. All specimens clearly demonstrate a dependency of both time and applied strains for $\varepsilon_0 > 0.5$ , with largest variations observed in the LB and T samples. Furthermore, the data indicates two distinct relaxation regimes with slower ( $t < 3 [s]$ ) and faster ( $t > 400 [s]$ ) decays, respectively, with slopes $\beta_1$ and $\beta_2$ illustrated in (f)

Figure 4.3:	Visco-elasto-plastic model M2 considering visco-plastic regularization. (a) Constitutive diagram with the rheological elements for visco-elasticity and visco-plasticity. (b) Stress versus strain response: path A-B described by the yield function (Eq.4.16), which is visco-elastic perfectly plastic; path A-B' with the stress response after the visco-plastic regularization (V-P-R) procedure (Eq.4.18). The relaxation path B'-B occurs at constant strain levels and $t \rightarrow \infty$ (compared to the relaxation time of the material).		77
Figure 4.4:	Schematic of stress update in the fractional return-mapping algorithm. The trial stress $\tau_{n+1}^{trial}$ is projected to $\tau_{n+1}$ . When unloading is performed from $\tau_{n+1}$ , the new yield stress is $\tau^y$ instead of $\tau^Y$		84
Figure 4.5:	Stress versus total strain curves for the benchmark solutions. The number of data points for the model M2 is truncated for better visualization, since the results overlap with the model M1. Both models provide the same qualitative results for monotonic strains for the considered values of $\beta_E$ , $\beta_K$		91
Figure 4.6:	$L^{\infty}$ -norm errors in $\tau_{ap}$ versus time step size $\Delta t$ in both models M1 and M2, where, $\beta_E = 0.5$ .		92
Figure 4.7:	Stress versus strain responses for both models using $\beta_E = 0.01$ . We observe that both models recover the limit case of rate-independent elasto-plasticity (EP) when $\beta_K \rightarrow 0$ . However, the classical visco-plasticity of Duvaut-Lions type (EVP-DL) is not recovered for the model M1 when $\beta_K \rightarrow 1$ . An asymptotic perfect visco-plastic solution is obtained instead		93
Figure 4.8:	Stress versus strain response for both models with $\beta_E = \beta_K$ . We observe the same response for monotonic strains. The variation of the fractional-orders affects the rate-dependent behavior for both visco-elastic and visco-plastic ranges. In this case, the increase of the fractional-order led to higher stress levels in the visco-elastic range and also more hardening.		93
Figure 4.9:	Stress versus total strain curves for the model M1 with $\beta_E = \beta_K = 0.5$ , $K = 5Pa/s^{\beta_K}$ and different values of <i>H</i> . We observe less nonlinearity and more dominant linear hardening as the numerical value of <i>H</i> approaches <i>K</i> .	•	94
Figure 4.10:	Cyclic stress versus strain response for the models. We observe that due to the lack of internal hardening for the model M2, the stress amplitudes are smaller. Also, the response of the models after the first loading cycle is distinct.	•	95
Figure 4.11:	Cyclic stress versus strain response for the models considering different ratios $K/E$ , $\beta_E = 1.0 \times 10^{-3}$ , $\beta_K = 0.8$ . We observe higher stress values for the model M2 as we increase $K/E$ , which become more pronounced with higher strain rates.		95

Figure 4.12:	(a) Two-member truss. The snap-through phenomenon occurs when the vertical displacement of node 2 is $-127 mm$ . (b) Applied negative vertical force over time
Figure 4.13:	Recovery of the models to rate-independent elasto-plasticity, $\Delta t = 6.0 \times 10^{-5} s$ . The snap-through effect occurs at $t = 0.089 s$
Figure 4.14:	Results for the model M1 considering $\beta_E = 1.0 \times 10^{-4}$ and variation of $\beta_K$ . (a) Displacement vs. time. (b) Stress vs. strain. (c) Internal force vs. displacement. We observe the increased visco-plastic hardening and damping with the increase of $\beta_K$
Figure 4.15:	Displacement versus time and stress versus strain for the model M1, $T = 1 s$ , $\beta_E = 1.0 \times 10^{-4}$ and variation of $\beta_K$
Figure 4.16:	(a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M1, $\beta_E = 0.1$ and different values for $\beta_K$
Figure 4.17:	(a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M2, $\beta_E = 1.0 \times 10^{-4}$ and variation of $\beta_K$ 100
Figure 4.18:	Displacement versus time and stress versus strain for the model M2, $\beta_K = 0.1$ . 100
Figure 4.19:	(a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M2, $\beta_E = 0.1$ and different values for $\beta_K$
Figure 5.1:	( <i>left</i> ) Schematics of the SB element recovering standard limit cases. ( <i>right</i> ) The SB element seen as an infinite, hierarchical mechanical representation of canonical elements, coding an infinite number of relaxation times. The pair $(\mathbb{E}, \beta)$ represents a dynamic process of the material
Figure 5.2:	Damaged fractional visco-elasto-plastic model. (A) Constitutive diagram with visco-elastic/plastic rheological elements. (B) Stress response showing the yield surface expansion (hardening) and contraction (softening)
Figure 5.3:	Numerical results for the free-energy computation with a quadratic form for $\varepsilon(t)$ . ( <i>Left</i> ) $\psi^{\delta}$ vs strain with varying $\beta$ . ( <i>Right</i> ) Relative error vs time-step size for varying $\beta$ , with second-order accuracy
Figure 5.4:	CPU time <i>vs</i> number of time-steps of the developed time-integration schemes for the fractional Helmholtz free-energy density under monotone strains 126
Figure 5.5:	(A) Free-energy density computations for cyclic strains vs time, $N = 3200$ time-steps and $\beta = 0.5$ . (B) Convergence analysis showing second-order accuracy

Figure 5.6:	Stress vs strain for the benchmark solution with time-step size $\Delta t = 2^{-20}$ , $\beta_E = 0.5$ and different $\beta_K$ values
Figure 5.7:	Fractional visco-elasto-plastic model with damage under monotone strains. (A) First-order convergence behavior. (B) Computational time $vs$ number of time-steps, with second-order computational complexity
Figure 5.8:	Developed model under monotone strains: (A) Damage vs accumulated plastic strain, with higher damage but less plasticity for higher $\beta_K$ . (B) Damage energy release rate vs visco-elastic strains, which are both larger for higher values of fractional order $\beta_K$
Figure 5.9:	Stress hysteresis response for cyclic strains with frequencies ( <i>A</i> )-( <i>C</i> ) $\omega = 2\pi$ , ( <i>D</i> )-( <i>F</i> ) $\omega = 4\pi$ , ( <i>G</i> )-( <i>I</i> ) $\omega = 8\pi$
Figure 5.10:	Damage vs accumulated plastic strains with varying strain frequencies 130
Figure 5.11:	Damage energy release rate vs time for the total strain with varying frequency 131
Figure 6.1:	Fractional linear viscoelastic models employed in this work, constructed from serial/parallel combinations of SB elements. The SB building blocks naturally account for an infinite fractal arrangement of Hookean/Newtonian elements. The fractional quasi-linear model employed is not represented by a mechanical analogue, although the time-dependent component of the relaxation function has a SB-like representation
Figure 6.2:	Fractional visco-elasto-plastic model diagram. Here, any of the linear and quasi-linear fractional viscoelastic models can be separately coupled with a fractional viscoplastic rheological device
Figure 6.3:	Convergence analysis for the fractional visco-elastic models with known analytical solutions. ( <i>a</i> ) A stress relaxation test with non-smooth step-strains, and material parameters $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (1, 1, 1)$ and $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$ , yielding first-order convergence. ( <i>b</i> ) Convergence for the fractional QLV model with a fabricated solution of linearly increasing strains and material properties $(E, \beta, A, B) = (1, 0.3, 1, 1)$ . The slopes of the error curves are $q \approx 2 - \beta$
Figure 6.4:	Convergence analysis for all fractional visco-elastic models with $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (1, 1, 1)$ and $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$ . A cubic strain function was employed and a reference solution with time-step size $\Delta t = 2^{-17}$ Monotone loading test with convergence rates $q \approx 1.3$ for all models
Figure 6.5:	CPU times for the developed fractional return-mapping algorithm and the original one [1] for a SB visco-elastic part. The black line has slope $q = 2$ 153

Figure 6.6:	Comparison between the presented return-mapping algorithm and the reference approach from [1], under low and high frequency loading
Figure 6.7:	Convergence analysis for the fractional visco-elasto-plastic models under cyclic loads. Due to the particular choice of fractional orders (with $\beta_2 = \beta_K = 0.7$ being dominant), we observed convergence rates $q \approx 1.3$ for all models, except for the FKV. In the latter case, we observe a linear convergence to the reference solution
Figure 6.8:	Visco-elasto-plastic reference solutions for the employed models for the first 30 loading cycles. We notice a similar behavior for most models under the choice of material parameters, except for the FPT and FKV models. The FKV particularly yielded a very stiff response due to the combination of high fractional order values and high strain rates
Figure 7.1:	(a) In-plane kinematics of the cantilever beam subject to a base displacement $v_b(t)$ with respect to an inertial coordinate system $(x, y, z)$ . The terms $u(s, t)$ and $v(s, t)$ denote, respectively, the axial and vertical displacements with respect to a $(x', y', z')$ coordinate system attached to the base, and $\psi(s, t)$ is the rotation angle about the z'-axis. (b) The total deformation of an arbitrary (red) point, composed of an axial displacement $u$ and vertical displacement $v$ , as well as the displacement due to rotation $\psi$
Figure 7.2:	Deformation of an arbitrary element of the beam. The initial configuration $CD$ translates, rotates and elongates to an updated configuration $C^*D^*$ 162
Figure 7.3:	Classical viscoelastic models as a combination of spring (purely elastic) and dash-pot (purely viscous) elements. Kelvin-Voigt (top) and Maxwell (bottom) rheological models
Figure 7.4:	Lumped representation of the system as a fractional damper, with constants $E_r c_l$ and fractional order $\alpha$
Figure 7.5:	Anomalous change of the maximum amplitude vs frequency at the tip of the beam in presence of harmonic base excitation for different fractional order $\alpha$ . The solid black line represents the standard, undamped natural frequency of the system
Figure 7.6:	Anomalous linear free vibration modal displacement <i>vs.</i> time. ( <i>Left</i> ) Riemman- Liouville definition with short-time anomalies. ( <i>Right</i> ) Caputo definition with long-time anomalies
Figure 7.7:	Classical linear free vibration modal displacement $vs$ . time under varying values of $E_r$

Figure 7.8:	Nonlinear anomalous free vibration of a viscoelastic cantilever beam with no lumped mass at the tip and $E_r = 0.1$ . The rate of amplitude decay strongly depends on the fractional order $\alpha$ , where a rapid decay is observed as $\alpha$ is increased <i>(left)</i> . On the other hand, for increasing $\alpha$ , the phase lag $\varphi(\epsilon t)$ , increases in the lower range of $\alpha$ , and decreases in the higher range of $\alpha$ 178
Figure 7.9:	Anomalous super-sensitivity of the decay rate $\tau_d$ with respect to $\alpha$ under free vibration. Increasing $\alpha$ when $\alpha < \alpha_{cr}$ leads to higher dissipation and decay rate. The reverse effect is observed when $\alpha > \alpha_{cr}$ . Here, the notions of softening/hardening are associated to high/lower decay rates as $\alpha$ is increased (introducing extra viscosity)
Figure 7.10:	( <i>Left</i> ) Storage and loss moduli, and tangent loss for the fractional Kelvin-Voigt model at $\omega_0$ with varying fractional-orders and $E_r = 1$ . ( <i>Right</i> ) Stress-time response under a monotone load with constant strain rate undergoing ballistic hardening response for short-time and higher $\alpha$ , followed by a stress relaxation. 181
Figure 7.11:	Primary resonance of the viscoelastic cantilever beam with no lumped mass at the tip. Steady state amplitude ( <i>right</i> ) and its bifurcation diagram ( <i>left</i> ) by changing the detuning parameter $\Delta$ for different values of $\alpha$ and $E_r = 0.3$ , $f =$ 1
Figure 7.12:	Frequency-Response curve for the case of primary resonance in the vis- coelastic cantilever beam with no lumped mass at the tip. Each sub-figure corresponds to a fixed value of $\alpha$ and $f$ when $E_r = \{0.1, 0.2, \dots, 1\}$ . As effect of fractional element becomes more pronounced, i.e. $\alpha$ and $E_r$ in- crease, the corresponding amplitude peaks decrease and shift towards the lower frequency range
Figure 8.1:	In Stage-I, the scheme captures the singularities for the short time-domain $\tilde{\Omega}$ , given the short initial data. In Stage-II, the framework uses the singularities obtained in Stage-I for full time-integration of the FDE over $\Omega$
Figure 8.2:	(a) Condition numbers for different choices of powers $\sigma_k$ . We observe that the choice $\sigma_k = 0.1k$ for unknown regularity of $u(t)$ [5] leads to the highest condition number, where at most $M = 9$ correction terms can be used with double precision arithmetic. (b) First correction weight $W_{1,1}$ with respect to $\Delta t$
Figure 8.3:	Initial weights $W_{1,n}$ for different time-step sizes $\Delta t$ , with corrections for fractional differentiation/integration (a) $\alpha = 0.5$ (fractional differentiation), where the initial weights have a larger magnitude that quickly decreases in the first time-steps, indicating that they are most relevant near $t = 0$ . (b) $\alpha = -0.5$ (fractional integral)

Figure 8.4:	Convergence behavior with $\sigma^* = 0.5$ and initial guesses $\sigma^{(0)} = \{0.0001, 1.05\}$ and time-step size $\Delta t = 0.01$
Figure 8.5:	Convergence behavior with $\sigma^* = 0.1$ and initial guesses $\sigma^0 = \{0.0001, 1.1\}$ and time-step size $\Delta t = 0.01$
Figure 8.6:	Convergence behavior with $\sigma_1^* = 0.1$ , $\sigma_2^* = 0.2$ , initial guesses $\sigma^{(0)} = \{0.001, 0.5\}$ and time-step size $\Delta t = 0.01$ . The converged value for the singularity $\sigma \approx 0.1377$ is between $\sigma_1^*, \sigma_2^*, \ldots, \ldots, \ldots, \ldots$ 205
Figure 8.7:	Convergence behavior with $\sigma_1^* = 0.1$ , $\sigma_2^* = 0.3$ , $\sigma_3^* = 0.5$ , initial guesses $\sigma^{(0)} = \{0.001, 0.5\}$ and time-step size $\Delta t = 0.01$ . The converged value for the singularity is $\sigma \approx 0.1856$
Figure 8.8:	Converged values for the singularity $\boldsymbol{\sigma}$ vs time-step size $\Delta t$ with two choices of $\boldsymbol{\sigma}^* = \begin{bmatrix} \sigma_1^*, \ \sigma_2^*, \ \sigma_3^* \end{bmatrix}^T$
Figure 8.9:	Second-order asymptotic convergence behavior for $M = 1$ correction term, $S = 1$ singularity with value $\sigma_1^* = 0.1$ . The obtained relative error for the converged $\sigma_1$ is $E_1^{\sigma} = 2.290 \times 10^{-8}$
Figure 8.10:	Convergence behavior for $M = 1$ , $S = 2$ with $\sigma^* = [0.1, 0.3]^T$ . With the plateau in error and $\sigma$ due to gradient convergence within the tolerance $\epsilon_1$ . The scheme converges to an " <i>intermediate</i> " value $\sigma \approx 0.153$ , between the true singularities
Figure 8.11:	Convergence behavior for $M = 1$ , $S = 3$ with $\sigma^* = [0.1, 0.3, 0.5]^T$ . In for both initial guesses, the scheme converges to an " <i>intermediate</i> " value $\sigma \approx 0.184$ , which is closer to the strongest true singularity $\sigma_1^* = 0.1$ 208
Figure 8.12:	Error function $E(\sigma)$ for $M = 2$ , $S = 2$ , with $\sigma_1^* = 0.1$ , $\sigma_2^* = 0.3$ . Two minima occur at $\sigma^* = [0.1, 0.3]^T = [0.3, 0.1]^T$ , corresponding to the true singularities. We set $\sigma_1 \neq \sigma_2$ to avoid a singular matrix in linear system (8.11)
Figure 8.13:	Two correction terms $M = 2$ and two singularities $S = 2$ , with $\sigma^* = [0.1, 0.3]^T$ . The obtained converged values are $\sigma = [0.299974, 0.099990]^T$ , which correspond to component-wise relative errors $E^{\sigma} = [8.61, 9.94]^T \times 10^{-5}$ .

Figure 8.14:	Two correction terms $M = 2$ and three singularities $S = 3$ , with $\sigma^* = [0.1, 0.3]^T$ and $\epsilon_1 = 10^{-11}$ . The converged values are $\sigma = [0.112635, 0.420495]^T$ , which are closer to the stronger singularities $\sigma_1 = 0.1$ and $\sigma_3 = 0.5$ . The approximate singularities still lead to an approximation error of $1.47 \times 10^{-11}$ . 210
Figure 8.15:	Results for $M = 3$ , $S = 1$ . The obtained relative error for $\sigma_1$ is $E_1^{\sigma} = 4.869 \times 10^{-8}$ . The components $\sigma_1$ , $\sigma_2$ remained practically constant
Figure 8.16:	Results for $M = 3$ , $S = 2$ . The obtained converged values are $\sigma = [0.099997, 0.299995, 0.939015]^T$ , where $\sigma_1, \sigma_2$ captured the singularities, respectively with errors $E_1^{\sigma} = 3.07 \times 10^{-5}$ and $E_2^{\sigma} = 1.65 \times 10^{-5}$
Figure 8.17:	Results for $M = 3$ , $S = 3$ using $\epsilon = 10^{-15}$ . The converged values are $\sigma = [0.099, 0.498, 0.293]^T$ , which correspond to component-wise relative errors $E^{\sigma} = [0.014, 0.005, 0.024]^T$
Figure 8.18:	Comparison of error vs time for long time-integration between the captured singularities and $\sigma_k = 0.1k$ for different values of time-step size $\Delta t$
Figure 8.19:	Singularities $\sigma$ vs iteration number for a multi-term FDE with $N_{\alpha} = 3$ in Stage- I for each $M$ in Algorithm 8.1. (a) $M = 1$ , with error $E(\sigma) = 1.10 \times 10^{-5}$ , (b) $M = 2$ , with error $E(\sigma) = 3.83 \times 10^{-13}$ , and (c) $M = 3$ with convergence at $E(\sigma) = 2.31 \times 10^{-15}$ . The black horizontal lines correspond to the true random singularities in the solution
Figure 8.20:	(a) Convergence analysis comparing the accuracy of the captured singularities in Stage-I with <i>ad-hoc</i> choices for time-integration with $T = 1$ [s] in Stage-II. The term q denotes the convergence rate. The self-captured case uses $M = 2$ correction terms, while for $\sigma_k = 0.1k$ and $\sigma_k = \alpha k$ we use $M = 4$ . (b) Exact and approximate solutions for $u(t)$ using the captured singularities for longer time-integration over $T = 25$ [s]
Figure 8.21:	Self-captured and benchmark solutions <i>versus</i> time for full time-integration of a nonlinear FDE
Figure 9.1:	Research timeline on significant and diverse numerical schemes for time- fractional differential equations
Figure 9.2:	(a) Stability region of IMEX(0) with $\alpha = 0.2$ and $\rho = 0.5\lambda$ ; (b) Stability region of IMEX(0) with $\alpha = 0.5$ and $\rho = 0.5\lambda$ ; (c) Stability region of IMEX(0) with $\alpha = 0.8$ and $\rho = 0.5\lambda$ ; (d) Stability region of the IMEX(1) with different $\alpha$ and $\rho = 0.5\lambda$ .

Figure 9.3:	Computational time <i>versus</i> number of time steps $N$ for the original (red curves) and the developed, fast (blue curves) FAMMs
Figure 9.4:	Solution <i>versus</i> time t for Case III) using $h = 0.005$ and $M = 1$ correction term. 250
Figure 9.5:	(a) Solution versus time t for Case III) using $h = 0.005$ with $M = 1$ correction term. (b) Computational time versus number of time steps N for the developed IMEX schemes
Figure D.1:	Top: The first eigenfunctions, $X_1(s)$ , of the undamped linear counterpart of our model. It is used as the spatial functions in the single mode approximation. Bottom: The first eigenfunctions, $X_1(s)$ , of the undamped linear counterpart of our model with no lumped mass at the tip. It is used as the spatial functions in the single mode approximation

## LIST OF ALGORITHMS

Algorithm 4.1: Fractional return-mapping algorithm for the model M1
Algorithm 4.2: Fractional return-mapping algorithm for the model M2
Algorithm 5.1: Fractional return-mapping algorithm
Algorithm 5.2: Fast computation of fractional damage energy release rate
Algorithm 6.1: Fractional return-mapping algorithm
Algorithm 8.1: Stage-I Self-Singularity-Capturing Scheme for FDEs
Algorithm 8.2: Stage-I Singularity Capturing Algorithm (with <i>M</i> correction terms) 200
Algorithm 8.3: Complete solution framework for FDEs
Algorithm 9.1: Fast IMEX(0) Integration Scheme for Nonlinear FDEs

#### **CHAPTER 1**

#### INTRODUCTION

## 1.1 Power-Law Rheology: Anomalies Across Scales

Power-law rheology is a constitutive behavior observed in a wide range of complex materials. In macro-rheology experiments, such power-law materials, also termed *anomalous* materials, exhibit *memory-effects* by means of single-to-multiple power-law type of relaxation/creep in the form  $J(t) \propto t^{\alpha}$  and  $G(t) \propto t^{-\alpha}$  (in time) and also power-law dynamic storage/dissipation (in frequency) [6]. Therefore, contrary to the standard (exponential) material relaxation, the power-law scaling parameter  $\alpha$  often lies in the range  $0 < \alpha < 1$ . The mechanistic origins of macroscopic power-law behavior is due to spatial and temporal *anomalous* sub-diffusive processes [7] in the multiscale fractal-like micro-structure, where, for the temporal case, the mean squared displacement of micro-structural constituents follows a non-linear scaling in time of the form  $\langle \Delta r \rangle^2 \propto t^{\alpha}$ . Such behavior has been experimentally observed in distinct classes of materials, *i.e.*, such as bio-tissues [8–14], polymers [15–17], soft glassy materials [18] and metals.

In this chapter, we outline a number of experimental evidences of such power-law phenomena across multiple length- and time-scales, suggesting that biological and engineering materials physics can either start, or evolve into anomalous states throughout their life cycle. We then briefly introduce some definitions of fractional calculus employed in this work, followed by an introduction to fractional viscoelasticity, where a key rheological model, called *Scott-Blair* element, is widely applied as a fundamental building block for complex power-law rheology. Later on, a brief literature survey is presented on fractional modeling applications to anomalous materials, followed by the objectives and introductions to each contribution from this PhD dissertation.

**Biological Cells and Tissues:** Regarding the 'micro-rheological' evidence, the collective dynamics of MCF-10A epithelial cell monolayers was studied by Nnetu *et al.* [19] at different cell density levels. Through the evaluation of mean-squared displacements (MSD)  $\langle r^2 \rangle$  over time of single cell motions, a ballistic motion was observed at low densities, that is,  $\langle r^2 \rangle \propto t^2$  (see Fig. 1.1). As the cell density is increased, single cell motion is suppressed due to crowding effects, leading to sub-diffusive behavior. Such high cell density motion suppression is also termed *caging*, which intermittently attains critical states, followed by relaxation. The rheology of human embrionic stem cells (ESCs) under differentiation was studied by Pajerowski *et al.* [20], through aspiration experiments using micro-pipettes at different pressures. The creep behavior of the cell nucleous demonstrated distinct visco-elasto-plastic power-law scalings, where a value of  $\alpha = 0.2$  was observed for the plastic regime, independent of the applied pressure. It is discussed that such low power-law exponent arises due to the fractal arrangement of chromatin inside the cell nucleous.



Figure 1.1: (a) Mean square displacement of single cells within an epithelial cell monolayer under different densities. (b) Evolution of the MSD exponent over time, showing a transition of diffusive to sub-diffusive motions and transient, motion-arresting behavior at higher densities.

Studies on force-induced mechanical plasticity of mouse embrionic fibroblasts applied through magnetic micro-beads were performed by Bonadkar *et al.* [21]. It was found across multiple specimens that the visco-elastic relaxation and the permanent deformations followed a stochastic, normally-distributed, power-law scaling  $\beta(\omega)$ , with values ranging from  $\beta \approx 0$  to  $\beta \approx 0.6$ . The intrinsic microstructural mechanism of plastic deformation in the cytoskeleton is due to the combination of permanent stretching and buckling of actin fibers.

**Polymers and Engineering Bio-Materials:** Wong *et al.* [22] studied the thermal motion of colloidal tracer particles in entangled actin filament (F-actin) networks, under different actin con-



Figure 1.2: (a) Scale-free creep behavior of embrionic stem cells nuclei under aspiration stresses. For low values of stress  $\Delta P$ , the creep behavior is fit by a single power law. For larger stresses, a transition to plastic regime is observed at  $\tau_{plastic} \approx 8 - 10 [s]$ , with a creep exponent  $\alpha \approx 0.2$ , for all values of applied stresses. For short times, the creep exponent is higher and increases with stress, suggesting a fluid-like behavior. (b) Different stages of nucleus aspiration, showing a visco-elastic recovery (ii)-(iii), followed by irreversible plastic deformation (iv).

centrations and therefore network mesh sizes. They observed a sub-diffusive behavior of tracer particles with radius comparable to the network mesh size. Such anomalous behavior happens due to a similar caging behavior, where particles are intermittently trapped, followed by sudden jumps (*see Fig.1.3*).



Figure 1.3: (a) Mean squared displacement of colloidal tracer spheres with radius  $a = 0.25 \, [\mu m]$  in F-actin networks, indicating anomalous, sub-diffusive behavior when the sphere radius a is comparable in size with the mesh size  $\xi$ . (b) Representative x - y (*left*) and y (*right*) trajectories of particles of a 0.25 [ $\mu m$ ] particle in F-actin ( $\xi = 0.31 \, [\mu m]$ ) over 600 [s].

Regarding the influence of fractal micro-structures on the macroscopic properties of polymers,

Kapnistos *et al.* [23] found an unexpected tempered power-law relaxation behavior of entangled polystyrene ring polymers, compared to the usual relaxation plateau of linear chain polymers (*see Fig.1.4a*). Such behavior is justified through self-similar conformations of double-folded loops the in ring polymers, instead of the reptation observed in linear chains. Jaishankar and McKinley [24] studied the creep-ringing interface dynamics of acacia gum across four decades, showing the long-time power-law creep dynamics, with an excellent fit obtained through a fractional Maxwell model (*see Fig. 1.4b*).

We note that other material characteristics, such as composition/space-dependent heterogeneity can introduce distinct length-scale-dependent relaxation spectra, leading to the emergence of multiple power-law response. Stamenović [25] performed complex shear modulus  $G^*(\omega)$  measurements over six frequency decades  $\omega$  of cultured human airway smooth muscle (HASM) cells, and observed two distinct power-law regimes separated by an intermediate *plateau*.



Figure 1.4: (a) Tempered power-law relaxation of polystyrene entangled ring polymers (open triangles and circles), and two power-law relaxation regimes of linear polymer chains (closed triangles and circles). (b) Creep ringing experiments demonstrating the long-time power-law behavior of acacia gum.

**Crystalline Materials:** Richeton *et al.* [26] investigated the emergence of intermittency and dislocation avalanches in polycrystalline plasticity through acoustic emission (AE) experiments on ice under creep compression. Their findings demonstrate that different from the scale-free, close-to-critical dislocation dynamics of single crystals [27], the introduction of average grain sizes < d > from the polycrystal microstructure led to a tempered power-law distribution of avalanche

sizes. While the exponential tempering cutoff changes with the averaged microstructure grain size, the authors observed a constant power-law scaling for all samples. The evidence of such power-law distributions of dislocation avalanches indicate the presence of stochastic effects in failure initiation, which cannot be described by a single, deterministic power-law exponent throughout the material life-cycle.



Figure 1.5: (a) Microstructures of polycrystalline ice samples with varying averaged grain sizes  $\langle d \rangle$ . (Top left) 0.26 [mm], (top right) 0.87 [mm], (bottom left) 1.92 [mm], (bottom right) 5.02 [mm]. (b) Complementary cumulative probability distributions for acoustic emission amplitudes  $A_0$  in polycrystalline samples with different average grain sizes. (top) A tempered power-law fit in the form  $P(>A_0) \approx A_0^{-\beta} \exp(-A_0/A_c)$  (black line) indicates a decrease in cutoff values  $A_c$  for decreasing grain sizes, while the power-law exponent  $\beta = 0.35 \pm 0.05$  is similar for all samples. (bottom) Coarse grained samples, leading to bimodal distributions for  $A_0$ .

**Crack Formation and Propagation:** Cracking behavior of heterogeneous materials under slow loading display a stochastic nature, characterized by intermittent, jerky dynamics, with random sudden jumps spanning over a broad range of time and length scales [28]. Bonamy *et al.* [29] simulated the cracking dynamics at the interface between two brittle plates subject to slow external loads. Their approach was based on a linear elastic fracture mechanics (LEFM) model for the crack

front with added Gaussian noise to account for media heterogeneity. Their results on spatiallyaveraged crack front velocities indicate a Barkhausen-like noise indicative of intermittent, jerky dynamics with power-law stochastic nature (*see Fig.1.6a*). Through scanning electron microscopy (SEM) analysis of fractured metallic glasses (MGs), Gao *et al.* [30] reported the emergence of fractal-like dimple structures. Utilizing a box counting algorithm, the authors evaluated fractal dimensions in the range of 1.6 - 1.8 among different types of MGs. The formation of fractal structures suggests that the fracture of MGs is a far-from-equilibrium process, forming a dissipation structure due to the nonlinear, localized plastic flow dynamics at the crap tip.



Figure 1.6: (a) Crack propagation dynamics of heterogeneous materials. (top left) Time-series data of spatially-averaged crack front velocities, showing intermittent bursts. (top right) Distribution of normalized burst duration T, with  $P(T) \propto T^{-\alpha}$ ,  $\alpha = 1.43$ . (bottom left) Distribution of normalized burst size S, with  $P(S) \propto S^{-\tau}$ , with  $\tau = 1.25$ . (bottom right) Scaling of T with respect to S, with  $T \propto S^a$  and a = 0.58. (b) SEM Fracture image of two different metallic glasses, showing a fractal-like formation of dimple structures.

Given the aforementioned evidence of power-laws arising in a range of material classes, we now focus on a brief introduction to definitions of fractional calculus, followed by its applications towards constitutive modeling.

## **1.2** Definitions of fractional calculus

We start with some preliminary definitions of fractional calculus [31]. The left-sided Riemann-Liouville integrals of order  $\mu$ , when  $0 < \mu < 1$ , is defined, as

$$\binom{RL}{x_L} \mathcal{I}_x^{\mu} f(x) = \frac{1}{\Gamma(\mu)} \int_{x_L}^x \frac{f(s)}{(x-s)^{1-\mu}} \, ds, \quad x > x_L, \tag{1.1}$$

where  $x_L$  denotes the lower integration limit and  $\Gamma(\cdot)$  represents the Euler gamma function, given by:

$$\Gamma(z) = \int_0^\infty x^{z-1} \exp(-x) \, dx.$$

The corresponding inverse operator, i.e., the left-sided fractional derivatives of order  $\mu$ , is then defined based on Eq.1.1 as

$$\binom{RL}{x_L}\mathcal{D}_x^{\mu}f(x) = \frac{d}{dx}\binom{RL}{x_L}\mathcal{I}_x^{1-\mu}f(x) = \frac{1}{\Gamma(1-\mu)}\frac{d}{dx}\int_{x_L}^x \frac{f(s)}{(x-s)^{\mu}}ds, \quad x > x_L.$$
 (1.2)

Furthermore, the corresponding left-sided Caputo derivatives of order  $\mu \in (0, 1)$  is obtained as

$$\binom{C}{x_L}\mathcal{D}_x^{\mu}f(x) = \binom{RL}{x_L}I_x^{1-\mu}\frac{df}{dx}(x) = \frac{1}{\Gamma(1-\mu)}\int_{x_L}^x \frac{f'(s)}{(x-s)^{\mu}}\,ds, \quad x > x_L.$$
 (1.3)

We note that power-law convolution kernels of the presented fractional operators (1.1)-(1.3) become singular as  $x \to x_L$ . Furthermore, the definitions of Riemann-Liouville and Caputo derivatives are linked by the following relationship, which can be derived by a direct calculation

$$\binom{RL}{x_L}\mathcal{D}_x^{\mu}f(x) = \frac{f(x_L)}{\Gamma(1-\mu)(x+x_L)^{\mu}} + \binom{C}{x_L}\mathcal{D}_x^{\mu}f(x),$$
(1.4)

which denotes that the definition of the aforementioned derivatives coincide when dealing with homogeneous Dirichlet initial/boundary conditions. Finally, we introduce the two-parameter Mittag-Leffler function  $E_{a,b}(z)$ , which generalizes a number of mathematical functions and is widely present in solution of fractional differential equations [32]:

$$E_{a,b}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(ak+b)}, \quad Re(a) > 0, \quad b \in \mathbb{C}, \quad z \in \mathbb{C}.$$
 (1.5)

## 1.3 Fractional Constitutive Modeling

Fractional differential equations (FDEs) have been successfully applied to describe the anomalous rheology of distinct classes of materials, which share the fingerprint of power-laws either in their fractal-like structure and/or response. Such power-law qualities are naturally embedded in the kernel of fractional derivatives, which are integro-differential operators that interpolate between their integer-order counterparts. In the following, we classify a few models and applications of fractional calculus by material/effect type, namely, viscoelasticity, viscoplasticity and damage.

### **1.3.1** Visco-Elasticity:

The main focus of this Section is on the so-called Scott-Blair (SB) model, which is the fundamental building block of anomalous rheology, from which a number of applied models are derived in the literature. We start with the Boltzmann superposition integral for linear viscoelasticity, obtained from the linear superposition of infinitesimal step strains  $\delta \varepsilon(t)$  applied to a viscoelastic material [32]:

$$\sigma(t) = \int_{-\infty}^{t} G(t - \tau)\dot{\varepsilon}(\tau) \, d\tau, \qquad (1.6)$$

where  $\dot{\varepsilon}$  and  $\sigma(t)$  denote, respectively, the strain rate and stress. The convolution kernel G(t), is a relaxation function, directly related to stress relaxation experiments under step strains. It is traditionally modeled through combinations of Hookean springs and Newtonian dashpots, yielding a multi-exponential relaxation in the form  $G(t) = \sum_{i=1}^{N} C_i \exp(-t/\tau_i)$ . In this particular choice of kernel, (1.6) has an equivalent representation as a multi-term ordinary differential equation (ODE), where derivative operators acting on stresses/strains are of integer-order.

Relaxation experiments across multiple time- and frequency-scales indicate that anomalous materials exhibit *memory effects* in time for stress/strain responses, which translates into a single power-law scaling in the form  $G(t) \propto t^{-\alpha}$ , with  $\alpha \in (0, 1)$ . This indicates that, contrary to exponential relaxation forms, there is a spectrum of relaxation times arising from the material microstructure [24], for which standard ODE models (e.g. generalized Maxwell model in

creep/relaxation representations) would require a large number of parameters.

The fundamental Scott-Blais fractional rheological building block element is obtained by substituting the power-law kernel  $G(t) = Et^{-\alpha}/\Gamma(1-\alpha)$  into (1.6), leading to the following form:

$$\sigma(t) = {}_{-\infty}^{C} \mathcal{D}_{t}^{\alpha} \varepsilon(t) = \frac{E}{\Gamma(1-\alpha)} \int_{-\infty}^{t} (t-\tau)^{-\alpha} \dot{\varepsilon}(\tau) \, d\tau, \qquad (1.7)$$

which is equivalent to the Riemann-Liouville fractional derivative  $\frac{\text{RL}}{-\infty} \mathcal{D}_t^{\alpha} \varepsilon(t)$  if the function  $\varepsilon(t)$  is sufficiently well behaved at  $t \to -\infty$  [33]. While this equivalence is satisfied for semi-infinite domains, the choice of Riemann-Liouville and Caputo definitions matter when we introduce a causal strain history and switch the lower bound of (1.7) from  $-\infty$  to 0, which leads to two different fractional Cauchy problems. For the Caputo definition, we have [32]:

$$\sigma(t) = E_0^{C} \mathcal{D}_t^{\alpha} \varepsilon(t), \quad t > 0, \quad 0 < \alpha < 1, \quad \varepsilon(0) = \varepsilon_0.$$
(1.8)

On the other hand, when employing Riemann-Liouville derivatives, we obtain:

$$\sigma(t) = E {\mathop{\mathrm{RL}}_{0}} \mathcal{D}_{t}^{\alpha} \varepsilon(t), \quad t > 0, \quad 0 < \alpha < 1, \quad {\mathop{\mathrm{RL}}_{0}} \mathcal{D}_{t}^{\alpha - 1} \varepsilon(t)|_{t=0} = \varepsilon_{0}, \tag{1.9}$$

where we remark that problem (1.8) is more commonly adopted due to the appearance of integerorder initial conditions (ICs), while both aforementioned problems are equivalent in the presence of homogeneous ICs. The SB element provides a constitutive interpolation between a Hookean spring ( $\alpha \rightarrow 0$ ) and a Newtonian dashpot ( $\alpha \rightarrow 1$ ). The unique parameter pair ( $E [Pa.s^{\alpha}], \alpha$ ) codes snapshots of a dynamic process instead of an equilibrium state of the system [24]. Consequently these properties are only associated to equilibrium states in the limit cases for the fractional order  $\alpha$ .

**Mechanistic and thermodynamic interpretations.** Apart from the Boltzmann integral representation (1.6), characterized by an integro-differential nature, the SB element can also be obtained through a continuous arrangement of canonical, Hookean and Newtonian elements, both from their constitutive and free-energy levels [34, 35], making the notion of SB elements intrinsically incorporating an infinite number of relaxation times more evident. In [34], a hierarchical ladder-like structure of standard Maxwell viscoelastic elements was employed. This structure led to a coupled system of ODEs, which had an infinite continued fraction (a recursion of fractions) representation in terms of the Maxwell model constants in the Laplace domain. Then, applying an inverse Laplace transform, a fractional stress-strain relationship was recovered for homonegeous initial conditions, therefore equivalent to both forms (1.8) and (1.9). In [35], an isothermal Helmholtz free-energy density was derived for the SB element from the elastic energies of a discrete-to-continuum arrangement of standard Maxwell branches, obtaining the following form for the free-energy  $\psi$  as a function of the strain:

$$\psi(\varepsilon) = \frac{1}{2} \int_0^\infty \tilde{E}(z) \left[ \int_0^t \exp(-\frac{t-s}{z}) \dot{\varepsilon}(s) ds \right]^2 dz, \quad \tilde{E}(z) = \frac{E z^{-1-\alpha}}{\Gamma(\alpha) \Gamma(1-\alpha)}, \quad (1.10)$$

where  $\tilde{E}$  denotes the relaxation spectrum. Therefore, (1.10) represents the amount of available elastic energy to perform work from the SB element in the time domain, which cannot be directly inferred from (1.8) and (1.9). Naturally, the two limit cases for  $\alpha$  are  $\psi(\varepsilon) \rightarrow E\varepsilon^2/2$  when  $\alpha \rightarrow 0$ , and  $\psi(\varepsilon) \rightarrow 0$  when  $\alpha \rightarrow 1$ . Furthermore, under suitable thermodynamic constraints, it is shown that the SB element is thermodynamically admissible and that the Caputo representation of (1.9) can be derived from (1.10) under continuum mechanics arguments.

**Energy decoupling in the frequency domain.** Similar to the aforementioned representations, power-law structures also appear in viscoelastic dynamic properties and rheological experiments in the frequency domain [24], such as the complex relaxation modulus, defined as the ratio between the Fourier transform of stresses and strains:

$$G^{*}(\omega) := \frac{\mathcal{F}[\sigma](\omega)}{\mathcal{F}[\varepsilon](\omega)} = G'(\omega) + iG''(\omega), \qquad (1.11)$$

where  $\omega [s^{-1}]$  denotes the frequency. The term G' is the storage modulus, and G" denotes the loss modulus, *i.e.*, the stored and dissipated energy per cycle, respectively. Employing definition (1.11) into (1.9), the dynamic modulus of the Scott-Blair element is obtained [36]:

$$G'(\omega) = Re(G^*) = E\omega^{\alpha} \cos\left(\frac{\alpha\pi}{2}\right), \quad G''(\omega) = Im(G^*) = E\omega^{\alpha} \sin\left(\frac{\alpha\pi}{2}\right), \quad (1.12)$$

which provides a clear storage/loss decomposition, with the value of  $\alpha$  determining whether the material of interest is predominantly dissipative for certain frequency ranges.

Relationships to material microstructure and stochastic processes. The mechanistic origins of macroscopic power-law behaviors in complex materials are due to spatial-temporal *anomalous* sub-diffusive processes [7] in fractal micro-structures. We focus on the temporal case, in which the MSD of micro-structural constituents follows a nonlinear scaling in the form  $\langle \Delta x \rangle^2 \propto t^{\alpha}$ .

In [37] Bagley and Torvik provided a relationship between the complex shear modulus obtained from the Rouse theory of polymer dynamics. They started with the result of Rouse's theory for the shear modulus, i.e.

$$G'(\omega) = nkT \sum_{p=1}^{N} \frac{\omega^2 \tau_p^2}{1 + \omega^2 \tau_p^2}, \quad G''(\omega) = \omega \mu_s + nkT \sum_{p=1}^{N} \frac{\omega \tau_p}{1 + \omega^2 \tau_p^2}, \quad (1.13)$$

where *n* denotes the number of molecules per unit volume, *N* is the number of monomers in the polymer chain, *T* represents the absolute temperature, *k* is Boltzmann's constant. The term  $\tau_p$  denotes the relaxation times of the solution, which was approximated as  $\tau_p \approx \tau_1/p^2 = 6(\mu_0 - \mu_s)/(p^2\pi^2 nkT)$ , which is valid when the number of submolecules *N* is large. The terms  $\mu_0$  and  $\mu_s$  denote, respectively, the steady-flow viscosities of the solution and solvent. They further worked on Rouse's results, and by assuming the polymers chain and  $\omega \tau_1$  to be sufficiently large, obtained the following power-law form for the dynamic relaxation modulus:

$$G^*(\omega) = i\omega\mu_s + \left[\frac{3}{2}(\mu_0 - \mu_s)nkT\right]^{1/2}(i\omega)^{1/2}.$$
(1.14)

After applying the inverse Fourier transform, the above relationship leads to a Riemann-Liouville representation between stresses-strains with  $\alpha = 1/2$ . Similar observations were also reported for  $\sigma(t)$  utilizing a Zimm model, where the inclusion of hydrodynamic interactions lead to a fractional order  $\alpha = 2/3$ .

In [38] Glöckle and Nonnenmacher showed that fractional relaxation can be modeled by a special type of continuous-time random walk (CTRW) describing a trapping problem due to entanglements of polymer chains, thus slowing down the relaxation process. In their work, the random walkers, i.e.,
the particles, are considered as packages of free volume that allow conformational reorientations of chain segments, thus leading to relaxation. They obtained a waiting time distribution of such particles through a Fox function representation in the form:

$$\chi(t) \sim \frac{A}{\bar{\tau}} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(-\beta k - \beta)} \left(\frac{\bar{\tau}}{t}\right)^{\beta k + \beta + 1},\tag{1.15}$$

for which the leading term indicates that the CTRW waiting time corresponding to fractional relaxation exhibits a Lévy-type decay in the form  $\chi(t) \sim t^{-\beta-1}$ .

**Connecting dynamic viscoelasticity across scales.** A connection between power-laws propagating from micro- to macro-rheology was proposed in [39], with the use of a Generalized Stokes-Einstein Relation (GSER) for spheres undergoing generalized Langevin dynamics in a viscoelastic medium:

$$|G^*(\omega)| \approx \frac{kT}{\pi a \langle \Delta r^2(1/\omega) \rangle \Gamma[1+\alpha(\omega)]}, \quad \alpha(\omega) \equiv \frac{d \ln \langle \Delta r^2(1/\omega) \rangle}{d \ln t}|_{t=1/\omega}, \tag{1.16}$$

which is valid for spheres of radius *a* comparable to the length-scale of the embedding medium. Here, the dynamic relaxation modulus  $G^*(\omega)$  is related to a velocity memory function from Langevin dynamics. Among a variety of representations for the GSER, (1.16) assumes a power-law structure of the MSD with exponent  $\alpha$ , which approaches zero when the sphere is confined by elastic structures present in the complex fluid. Such power-law representation also reduces errors near the frequency extremes when employing Laplace and Fourier transforms.

**Physical interpretation of fractional orders.** Despite existing connections between micro- and macro-rheological properties, the physical interpretation of the emerging fractional orders has been elusive. More recently, a connection between the fractional order and the fractal dimension of the material microstructure was made by Mashayekhi *et al.* [40], where the authors extended the Zimm theory of polymer dynamics to fractal media as a bridge between the meso- and macro-scales. They showed that the fractional order is a rate-dependent material property that is strongly correlated with the fractal and spectral dimensions in fractal media.



Figure 1.7: Comparison between standard and fractional order models. (a) Relaxation behavior of Butyl rubber using experimental data from Scott-Blair. (b) Cole-Cole plot (G' versus G'') for the dynamic properties of acacia gum.

Regarding applications of fractional viscoelastic models for memory-dependent response in biological tissues, Craiem *et al.* [10] employed fractional visco-elastic models to describe the stress-relaxation response of human arteries. In [24] Jaishankar and McKinley fitted classical and fractional Maxwell models to the 4 orders-of-magnitude relaxation data for highly anomalous butyl rubber data from Scott-Blair *et al.* [41] (Fig.1.7 (a)), and observed that the three-parameter fractional Maxwell model provided an excellent fit to the experimental data, while a multi-exponential, integer-order Maxwell model required 6 parameters to provide a satisfactory fit. Moreover, using the calibrated fractional relaxation parameters they obtained an accurate prediction of the creep compliance for the same material, especially for long-time behavior. The second experiment from [24] concerns the dynamic properties of acacia gum, a commonly used food preservative. In this case, they compared a 4-parameter fractional Maxwell model with a single mode (3 parameter) standard Maxwell model (Fig.1.7(b)) and demonstrated that while the fractional Maxwell model captures a complex Cole-Cole behavior, its integer-order counterpart is unable to even estimate the qualitative response. We refer the reader to [8, 42–45] for additional applications of fractional calculus to bio-tissues and food rheology.

### **1.3.2** Visco-Plasticity:

Several efforts were done in the last decade to employ fractional calculus to take into account material heterogeneities and multi-scale effects influencing the plastic regime of distinct materials. Of particular interest are three classes of fractional models: time-fractional, space-fractional and stress-fractional.

Time-fractional approaches focus on introducing memory effects into non-equilibrium viscous variables [1, 46], and consequently modeling power-laws in both viscoelastic and visco-plastic regimes. This is of interest for polymers, cells, tissues, and metals, and this type of approach is focused in Chapters 4, 5 and 6.

A three-dimensional space-fractional approach to elastoplasticity was developed in [47] to account for spatial nonlocalities. The model is based on rate-independent elastoplasticity, and nonlocal effects are accounted for through a fractional continuum mechanics approach, where the strains are defined by a space-fractional Riesz-Caputo derivative of displacements u(x) in the form:

$${}^{\mathrm{RC}}_{a}\mathcal{D}^{\alpha}_{b} = \frac{\Gamma(2-\alpha)}{2} \left( {}^{\mathrm{C}}_{a}\mathcal{D}^{\alpha}_{x}u(x) + (-1)^{n} {}^{\mathrm{C}}_{x}\mathcal{D}^{\alpha}_{b}u(x) \right), \tag{1.17}$$

with  $n = \lceil \alpha \rceil$ .

Finally, stress-fractional models for plasticity have found applicability in soil mechanics and geomaterials that follow non-associated plastic flow [48, 49], i.e., the yield surface expansion in the stress space does not follow the usual normality rule, and may be non-convex. The work by [48] proposed a three-dimensional fractional visco-plastic model, where a fractional flow-rule with order  $0 < \alpha < 1$  in the stress domain naturally models non-associative plasticity. Interestingly, this model recovers the classical Perzyna visco-plasticity as  $\alpha \rightarrow 1$ , and the effect of the fractional flow rule can be a compact descriptor of micro-structure anisotropy. Recently, a similar stress-fractional model was developed [49], and successfully applied to soils under compression. We refer the reader to the detailed review work by [50] for a review of uses fractional calculus in plasticity.

#### **1.3.3 Damage Mechanics:**

There have also been recent efforts to include damage, ageing and failure effects into fractional calculus frameworks. Existing formulations are focused on either adding classical failure frameworks into existing fractional constitutive laws, or by developing fractional failure mechanisms. Here, we mostly focus on the latter and start with the work by [51], that developed a variable order viscoelastic model in the form:

$$\sigma(x,t) = g(\alpha(x,t))A(x)_{t_0}^C \mathcal{D}_t^{\alpha(x,t)} \varepsilon(x,t), \qquad (1.18)$$

where  $g(\alpha(x, t)) := (\alpha_C - \alpha(x, t))^2/4$  denotes a material degradation function with critical damage  $\alpha_C$ , A(x) represents a space-dependent pseudo-property, and  $0 < \alpha(x, t) < \alpha_C$  is the variable fractional order, also interpreted here as damage. Interestingly, this mixed interpretation for  $\alpha(x, t)$  makes it a multi-physics descriptor for anomalous damage, viscosity, and material ageing. The evolution of  $\alpha(x, t)$  is described by an integer-order phase-field equation, and the resulting model is proved to be thermodynamically admissible.

A key aspect to develop failure models relies on consistent forms of damage energy release rates, i.e., on obtaining the compatible operator for the loss of elastic energy, which is a nontrivial task even for the simplest fractional constitutive law (1.8). This has been achieved by employing the concept of fractional free-energy densities [35, 52, 53]. Alfano and Musto in [53] developed a cohesive zone, damaged fractional viscoelastic Kelvin-Zener model, and studied the influence of integer and fractional damage energy release rates on damage evolution. In this case, integer-order energy loss considers Hookean-type rheology to compute the damage energy release rates, which may be justified when Hookean elements are present in the viscoelastic constitutive law, but incompatible for fully fractional cases (an arrangement of Scott-Blair elements). The corresponding free-energy for the Scott-Blair element is given by:

$$\psi^{SB}(t) = \frac{E}{2\Gamma(1-\alpha)} \int_0^t \int_0^t (2t - \tau_1 - \tau_2)^{-\alpha} \dot{\varepsilon}(\tau_1) \dot{\varepsilon}(\tau_2) d\tau_1 d\tau_2, \qquad (1.19)$$

with  $0 < \alpha < 1$ , which clearly carries a power-law behavior over time. Among their findings, the authors obtained a rate-dependence of the fracture energy in terms of the fractional-order  $\alpha$ ,

opening interesting directions towards failure of anomalous viscoelastic media such as polymers. In this dissertation, fractional-order extensions to plasticity-induced damage and their thermodynamic consistency are addressed in Chapter 5. Sumelka *et al.* in [54] also developed the idea of memory-dependent damage for soft materials through a stress-driven time-fractional hyperelastic damage model, with evolution equation in the following fractional nonlinear Cauchy form:

$${}_{t-l_t}^C \mathbb{D}_t^\alpha D(x,t) = \frac{1}{T^\alpha} \Phi \langle \frac{I_D}{\tau_D} - 1 \rangle, \qquad (1.20)$$

where  $\Phi$  represents an overstress function in terms of a stress intensity  $I_D$ , threshold stress  $\tau_D$  for damage evolution, and a ramp function in Macaulay notation  $\langle . \rangle$ . The memory length is driven by a time-scale  $l_t$ , which was taken as a fraction of the total time T. This model was applied with an Ogden hyperelastic law to patient-specific three-dimensional abdominal aortic aneurysm (AA) for critical zone identification, with obtained  $\alpha = 0.75$ .

Additional work on variable-order models in the context of fractional damage, ageing and failure include the following contributions. In [55] a variable-order viscoelastic creep model was developed, where the evolution of the fractional order  $\alpha(t)$  dictates the process of concrete ageing. The variable-order viscoelastic model developed in [56] employed a piecewise constant order followed by two linear decreasing functions for  $\alpha(t)$  successfully described the initial viscoelasticity, softening and hardening of amorphous glassy polymers under compression. Finally, variable-order operators also proved to be useful mathematical tools to determine the onset of fracture. [57] employed a variable fractional order activation function for damage, where the sharp power-law activation threshold induced by the fractional operator was successfully employed to determine crack propagation and branching of brittle materials. We refer the reader to the recent review works on the use of variable-order [58] and distributed-order [59] fractional models in viscoelasticity and structural mechanics. In the distributed-order case, fractional derivatives are integrated with respect to a distribution of fractional orders within a certain range of values.

### **1.3.4** Key aspects in fractional models

Fractional models are able to code self-similar micro-structural features and therefore be applied to the complex response of power-law materials in a compact mathematical language. The significant advancement of numerical methods for FDEs since the 2000s allowed more efficient computations of the history and long-range interactions induced by the integro-differential nature of fractional operators. However, several multi-disciplinary challenges are still present when developing/employing fractional models.

When compared to their standard, integer-order counterparts, fractional models demonstrated to be highly suited, *i.e.*, for soft material rheology, demonstrating better agreement with experimental data over a wide range of time-scales without requiring the re-calibration of parameters. However, new modeling approaches require careful consideration of physical consistency, which should be properly addressed, *e.g.*, by ensuring that conservation/dissipation laws are not violated. Furthermore, it is important to determine the physical meaning of the fractional order of differentiation for distinct models and systems, and whether multiple orders of differentiation are required to account for system heterogeneity. Regarding the mathematical aspects, fractional operators do not possess all the same properties as integer-order ones, which requires careful considerations by researchers when developing new models. Furthermore, the inherent non-smoothness due to single- to multiple- singularities nearby the initial time/boundaries of fractional systems degenerates the accuracy of many existing practical numerical schemes for FDEs, and poses additional computational challenges on top of the history computations.

Given the aforementioned challenges, we aim to develop a multi-scale fractional modeling framework, which takes into account the following multi-disciplinary elements:

• **Reduced-Order Modeling:** An essential aspect is to develop fractional models that effectively incorporate the smaller scale dynamics, non-localities and memory-effects into a lumped element representation. Together with careful physical and thermodynamic considerations, this allows researchers to construct fractional models with a significantly reduced

number of material parameters.

- Machine Learning: In the development of data-infused models, machine learning tools are fundamental to learn the underlying multi-scale stochastic processes occuring in anomalous media and properly upscale such qualities in the language of the operator kernel and/or the fractional model parameters. Here, we aim to develop fundamental modeling steps of the framework, making the fractional models promptly available to be incorporated to a machine-learning-based model form selection framework for future studies. In such, material models and their most suited numerical methods for FDEs with *pragmatic accuracy*, would be determined from nature of the data or desired design.
- Numerical Schemes: Due to the nature of fractional-order operators, time integration of FDEs requires robust schemes that efficiently compute the history load and do not lose accuracy due to the power-law singularities nearby the initial time. Furthermore, solutions to stiff fractional systems undergoing non-linearities and the emergence of new operators for which no numerical schemes are available pose additional challenges and require special attention.

# **1.4 Outline of this Work**

The main objective of this research is to develop a robust, physics- and mathematically-informed multi-scale framework, where the anomalous multi-scale characteristics are incorporated in the form of physics-preserving and mathematically consistent fractional operators. Although most of the multi-scale focus in this work relates to the time-domain due to the capabilities of time-fractional derivatives, some brief developments are motivated in the context of upscaling material properties from microstructure simulations, which is of value for future studies involving fractional viscoplasticity. In this sense, we focus on developing and employing mathematically complex, yet, more compact operators that produce models with minimal number of parameters and uncertainty. Concurrently, we aim on efficiently and accurately solving the corresponding fractional multi-term

FDEs, which are determined from data-driven existence studies. The schematics of the proposed framework is illustrate in Figure 1.8. This work is comprised of nine chapters, that are summarized below.



Figure 1.8: Schematics of the proposed studies in this work. Starting from physics information, *e.g.*, material design requirements and damage/failure processes, the main approaches of this thesis focus on the development and existence studies of admissible, mathematically-informed fractional models and corresponding data-driven numerical methods.

### Chapter 2:

In this Chapter we provide some additional motivation regarding the emergence of power-laws in plasticity. The end goal is to take initial steps towards stochastic dislocation-driven plasticity and failure, to establish a bridge between molecular dynamics (MD) until reduced-order fractional models at the continuum. The MD and DDD simulations would therefore emerge as important tools for synthetic data generation to the developed stochastic models. Starting from a series of canonical numerical experiments [60] through molecular dynamics (MD) simulations using LAMMPS (https://lammps.sandia.gov) [61], we can estimate upscaled material parameters necessary for carrying discrete dislocation dynamics (DDD) simulations of pure iron crystals using ParaDis (https://ipo.llnl.gov/technologies/paradis) [62].

At the MD level (*atomistic-scale*):

- We start with two experiments on pure systems, *i.e.* a shear test on a block domain to obtain the corresponding shear modulus *G*, and a tensile test in a nanowire to obtain the Poisson ratio *v*.
- Dislocation-dependent parameters for DDD are obtained through two additional experiments: An edge dislocation core radius  $r_c$  test, obtained by analyzing influence radius of an edge dislocation's strain energy.
- The last experiment estimates the edge dislocation mobility  $M_d$ , where the dislocation glide motion is initiated through applied shear stresses, yielding the dislocation velocity and allowing us to compute the mobility as a proportionality constant in a linear shear stressvelocity relationship. The methodology employed in this experiment has been used for data generation of probabilistic surrogate models for dislocation mobility [63], which are able to propagate the mobility uncertainty for DDD approaches.

At the DDD level (meso-scale):

- After obtaining the required DDD input parameters for ParaDis, we perform strain-driven tensile simulations employing constant strain rates in a periodic Fe cubic lattice. The DDD simulations allow us to have an insight on the evolving fractal dislocation network, where we obtain time-series data of collective dislocation velocities and therefore a power-law distribution of acoustic energy.
- Finally, we obtain the homogenized stress-strain curve and dislocation density data, which indicate the presence of ballistic effects on dislocation density growth, visco-plasticity and stress intermittency. Such homogenized responses could be leveraged to identify parameters of visco-elasto-plastic models at the continuum-level.

### Chapter 3:

We introduce a data-driven fractional modeling framework for linear and nonlinear viscoelasticity of porcine bladder tissue mechanics. From consecutive uniaxial multi-step relaxation experiments (up to 200% strains) of five distinct anatomical locations of porcine bladder, we determine that the porcine urinary bladder has an anomalous relaxation character, with two power-laws dominating the short and long time responses, as well as a nonlinear response under large strains. The anomalous character is affected by intrinsic regional material composition and nonlinearities taking place due to large strains. Our developed modeling approach is as follows:

- Starting with the first relaxation step, we develop the first component of our modeling framework, which is an *existence study* to determine admissible candidate fractional linear viscoelastic models that qualitatively describe the experimental relaxation behavior. Our single relaxation results indicate that a fractional Maxwell model form with two fractional orders emerges as the most suitable candidate, being able to capture both short- and long-term behaviors and yielding the lowest fitting errors.
- For the multi-step relaxation case under large strains, we employ a four-parameter fractional quasi-linear viscoelastic model, given by a multiplicative kernel decomposition of a Scott-Blair relaxation function and an exponential elastic response of the true stress. Our obtained results demonstrate that the employed fractional quasi-linear model, with a single fractional order in the range  $\alpha = 0.25 - 0.30$  for distinct bladder samples, is suitable for the porcine urinary bladder, producing root mean squared errors below 2% without recalibration, throughout all consecutive relaxation steps.
- Our analyzes demonstrate that fractional models arise as attractive tools to capture the bladder tissue behavior under small-to-large strains and multiple time-scales, therefore being potential alternatives to describe multiple stages of bladder functionality.

#### Chapter 4:

Experimental evidence supports the emergence of power-law scalings in stress relaxation, permanent strains and dislocation avalanches of anomalous visco-elasto-plastic materials [11, 20, 21, 26, 27]. Although space-fractional visco-plastic models have been developed for non-associative

plastic flow and employed in the context of soil mechanics [64–66], time-fractional extensions accounting for memory effects in order to capture some of the aforementioned power-law features were still lacking in the literature.

In this Chapter, we make contributions in fractional rheological modeling by developing two fractional-order models for uniaxial large strains and visco-elasto-plastic behavior of materials in structural analysis. Here, the fractional operators seamlessly interpolate between the standard elasto-plastic and visco-elasto-plastic models, taking into account the history (memory) effects of the accumulated plastic strain to specify the state of stress. We summarize the contributions as follows:

- We develop two models, namely M1 and M2, corresponding to visco-elasto-plasticity considering a rate-dependent yield function and visco-plastic regularization, respectively. Specifically, we employ a fractional-order constitutive law that relates the Kirchhoff stress to the Caputo time-fractional derivative of the strain with order β ∈ (0, 1). When β → 0 the standard rate-independent elasto-plastic model with linear isotropic hardening is recovered by the models for general loading, and when β → 1, the corresponding classical visco-plastic model of Duvaut-Lions (Perzyna) type is recovered by the model M2 for monotonic loading.
- Since the material behavior is path-dependent, the evolution of the plastic strain is achieved by fractional-order time integration of the plastic strain rate with respect to time. The plastic strain rate is then obtained by means of the corresponding plastic slip and proper consistency conditions.
- Finally, we develop the so called *fractional return-mapping algorithm* for solving the nonlinear system of the equilibrium equations developed for each model. This algorithm seamlessly generalizes the standard return-mapping algorithm to its fractional counterpart.
- We test both models for convergence subject to prescribed strain rates, and subsequently we implement the models in a finite element truss code and solve for a two-dimensional snap-through instability problem. The simulation results demonstrate the flexibility of fractional-

order modeling using the Caputo derivative to account for rate-dependent hardening and viscous dissipation, and its potential to effectively describe complex constitutive laws of engineering materials and especially biological tissues.

### Chapter 5:

As observed in a series of experimental studies, material failure is an anomalous process where power-law scalings are observed in acoustic emissions experiments and self-similar fracture surfaces through SEM imaging. Motivated by previous developments on coupling continuum damage mechanics (CDM) and fractional constitutive laws [35, 53, 67–74], where damage variables were assumed to evolve in an exponential fashion, we introduce an anomalous modeling of failure to a fractional visco-elasto-plastic model [1, 75]. In order to provide a bridge between the self-similar energy loss to the continuum-level, we aim on a consistent representation of the bulk damage energy loss to be employed in a thermodynamically admissible fractional model.

The main contributions of this Chapter rely on a novel rheological development, where we present a thermodynamically consistent, fractional visco-elasto-plastic model coupled with damage for anomalous materials. The presented formulation obtains the constitutive equations from the fractional Helmholtz free-energy potentials, and also addresses the thermodynamics of the model M1 developed in Chapter 2. Furthermore, we develop a novel discretization for the free-energy potentials, which provide the corresponding damage energy release rates that drive the damage evolution. The main contributions of this Chapter are summarized as follows:

- The model utilizes Scott-Blair rheological elements for both visco- elastic/plastic parts. The constitutive equations are obtained through Helmholtz free-energy potentials for Scott-Blair elements, together with a memory-dependent fractional yield function and dissipation inequalities.
- A memory-dependent Lemaitre-type damage is introduced through fractional damage energy release rates.

- For time-fractional integration of the resulting nonlinear system of equations, we develop a first-order semi-implicit fractional return-mapping algorithm. We also develop a finitedifference discretization for the fractional damage energy release rate, which results into Hankel-type matrix-vector operations for each time-step, allowing us to reduce the computational complexity from  $O(N^3)$  to  $O(N^2)$  through the use of Fast Fourier Transforms.
- Our numerical results demonstrate that the fractional orders for visco-elasto-plasticity play a crucial role in damage evolution, due to the competition between the anomalous plastic slip and bulk damage energy release rates.

### Chapter 6:

Motivated by the existence of materials exhibiting multiple power-laws [23, 25] in the linear visco-elastic range, as well as the nonlinear visco-elasticity of bio-tissues, we aim to develop a generalized fractional visco-elasto-platic modeling framework, where, distinctively from the preceding contribution, here a number of canonical fractional visco-elastic models can be taken into account. Specifically:

- We develop a generalized, fractional return-mapping framework for power-law visco-elastoplasticity. In our approach, the fractional visco-elasticity can be accounted through canonical combinations of Scott-Blair elements to construct a series of well-known fractional linear visco-elastic models, such as Kelvin-Voigt, Maxwell, Kelvin-Zener and Poynting-Thomson. We also consider a fractional quasi-linear version of Fung's model to account for stress/strain nonlinearity.
- The fractional visco-elastic models are combined with a fractional visco-plastic device, which is currently not a trivial task in existing return-mapping approaches coupled with fractional visco-elastic models involving serial combinations of Scott-Blair elements.
- We then develop a general return-mapping procedure, which is fully implicit for linear viscoelastic models, and semi-implicit for the quasi-linear case. Interestingly, we find that, in

the correction phase, the discrete stress projection and plastic slip have the same form for all considered models, although with different property and time-step dependent projection terms.

- A series of numerical experiments is carried out with analytical and reference solutions to demonstrate the convergence and computational cost of the proposed framework, which is shown to be at least first-order accurate for general loading conditions.
- Our numerical results demonstrate that the developed framework is more flexible, preserves the numerical accuracy of existing approaches, while being more computationally tractable in the visco-plastic range due to a reduction of 50% in CPU time. Our formulation is especially suited for emerging applications of fractional calculus in bio-tissues that present the hallmark of multiple visco-elastic power-laws coupled with visco-plasticity.

### Chapter 7:

Due to key developments in fractional constitutive laws and numerical methods for FDEs, recently, a series of works analyzed the nonlinear vibration of fractional visco-elastic beams [76–80] under distinct material responses and boundary/loading conditions, where the numerical solutions were based on the strong form of the resulting FDEs. However, from the rheology standpoint, studying the effects of varying fractional orders, seen as evolving material properties, *e.g.* softening, hardening, as well as their sensitivity and effects on the response of the system are still lacking in the literature. Such view is fundamental for a model form selection of constitutive laws from the available data or desired mechanical response of the system. In this Chapter, we investigate the nonlinear vibration of a fractional viscoelastic Euler-Bernoulli cantilever beam, subject to base excitation, where:

• The viscoelasticity takes the general form of a distributed-order fractional model, and the beam curvature introduces geometric nonlinearity into the governing equation. We use Hamilton's principle to derive the governing equation of motion for specific material distribution functions that lead to fractional Kelvin-Voigt viscoelastic model.

- By spectral decomposition in space, the resulting governing time-fractional PDE reduces to a nonlinear time-fractional ODE. We use direct numerical integration in the decoupled system, in which we observe the anomalous power-law decay rate of amplitude in the linearized model.
- We further develop a semi-analytical scheme to solve the nonlinear equations, using a method of multiple scales as a perturbation technique. We replace the expensive numerical time integration with a cubic algebraic equation to solve for frequency response of the system.
- We observe the super sensitivity of response amplitude with respect to the fractional model parameters at free vibration, and bifurcation in steady-state amplitude at primary resonance.

### Chapter 8:

Solutions to fractional models inherently exhibit non-smooth behavior, which significantly deteriorates the accuracy and therefore efficiency of existing numerical methods. The basic building block of fractional visco-elastic models, the Scott-Blair element can be mathematically expressed as the following fractional nonlinear Cauchy equation:

$${}^{C}_{a}\mathcal{D}^{\alpha}_{t}u(t) = f(t, u(t)), \quad u(a) = u_{0}, \quad 0 < \alpha < 1,$$
(1.21)

which possesses single-to-multi power-law singular behavior nearby the left limit, *i.e.*,  $t \approx a$ . The nature of such singularity arises from the power-law kernel in the definition of the fractional operator, with corresponding singular powers dependent on the regularity of the solution u(t) and the nonlinear right-hand-side f(t, u(t)). Therefore, constructions of more general visco-elastic models require multi-term FDEs and consequently giving rise to multiple solution singularities. Motivated by several works on addressing singularities for FDEs [5, 81–87], we develop the idea of self-singularity-capturing methods for FDE.

In this Chapter we develop a two-stage data-infused computational framework for accurate time-integration of single- and multi-term fractional differential equations. The steps and main aspects of the framework are described as follows:

- In the first stage, we formulate a self-singularity-capturing scheme, given available data for diminutive time, experimentally obtained or sampled from an approximate numerical solution utilizing a fine grid nearby the initial time. In this approach, the fractional differential equation provides the necessary knowledge/insight on how the hidden singularity can bridge between the initial and the subsequent short-time solution data.
- We develop a new self-singularity-capturing finite-difference algorithm for automatic determination of the underlying power-law singularities nearby the initial data, employing gradient descent optimization.
- In the second stage, we can utilize the multi-singular behavior of solution in a variety of numerical methods, without resorting to making any *ad-hoc/*uneducated guesses for the solution singularities. Particularly, we employed an implicit finite-difference method, where the captured singularities, in the first stage, are taken into account through some Lubich-like correction terms, leading to an accuracy of order  $O(\Delta t^{3-\alpha})$ .
- We carry out a series of numerical tests, and our computational results demonstrate that the developed framework can either fully capture or successfully control the solution error in the time-integration of fractional differential equations, especially in the presence of strong multi-singularities.

### Chapter 9:

In addition to the near-singular behavior of FDEs nearby the initial time, requiring the development of appropriate numerical methods (*see Chapter 6*), numerical solutions to nonlinear FDEs are stiff and pose additional challenges regarding the stability of numerical methods, especially at lower fractional order values. Furthermore, efficient long-time integration of nonlinear FDEs is significantly challenging due to the integro-differential nature of the fractional operators. Since the 80's, many numerical methods were developed, such as finite-difference schemes [86, 88–93], fractional Adams schemes [82, 94], spectral methods [95–102], correction methods [86], gradedmesh approaches [83–85], fast schemes [103–107], among others. Fractional multi-step schemes such as the Adams-schemes proved to be interesting alternatives for stiff FDEs [94, 108–114].

Although a significant amount of relevant works was developed, they usually address the aforementioned singularity/performance/stability issues for stiff/nonlinear problems separately. In this regard, there is still a need for numerical schemes aimed at stiff/nonlinear FDEs that I) efficiently handle the numerical solution with low-regularity for both the solution u(t) and nonlinear term f(t, u(t)); II) present linear complexity with respect to the number of time-steps N; III) have larger stability regions compared to the existing numerical schemes; IV) mimick and generalize the structure of existing integer-order multi-step schemes, widely employed by the scientists and engineers to its fractional-order counterparts.

In this Chapter we develop two efficient first- and second-order implicit-explicit (IMEX) methods for accurate time-integration of stiff/nonlinear fractional differential equations with fractional order  $\alpha \in (0, 1]$  in the form:

$${}_{0}^{C}D_{t}^{\alpha}u(t) = \lambda u(t) + f(t,u), \ \alpha \in (0,1], \ t \in (0,T]; \ u(0) = u_{0},$$
(1.22)

where  $\lambda \in \mathbb{C}$ ,  $u_0 \in \mathbb{R}^d$ , and prove their convergence and linear stability properties. The main aspects of this work are:

- The developed methods are based on a linear multi-step fractional Adams-Moulton method (FAMM), followed by the extrapolation of the nonlinear force terms.
- In order to handle the singularities nearby the initial time, we employ Lubich-like corrections to the resulting fractional operators.
- The obtained linear stability regions of the developed IMEX methods are larger than existing IMEX methods in the literature. Furthermore, the size of the stability regions increase with the decrease of fractional order values, which is suitable for stiff problems.
- We also rewrite the resulting IMEX methods in the language of nonlinear Toeplitz systems, where we employ a fast inversion scheme to achieve a computational complexity of

 $O(N \log N)$ , where N denotes the number of time-steps.

• Our computational results demonstrate that the developed schemes can achieve global firstand second-order accuracy for highly-oscillatory stiff/nonlinear problems with singularities.

Chapter 10: We present the concluding remarks and future steps of this work.

#### **CHAPTER 2**

# MULTI-SCALE ASPECTS: MOLECULAR DYNAMICS AND DISCRETE DISLOCATION DYNAMICS

# 2.1 Introduction

Multi-scale materials modeling simulations are a rapidly growing scientific field, where it is critical to accurately and efficiently bridge/propagate the properties/uncertainties between adjacent length- and time-scales. Among several types of material imperfections that cause disturbances in crystal structures, dislocations are line defects [2] that are naturally present from manufacturing until failure of crystalline materials. Describing the small-scale buildup and dynamics of dislocations can provide an important insight on early fatigue precursors [115, 116], which are beyond the resolution of existing continuum models of fatigue damage. However, in order to accurately propagate such early statistics of failure to the continuum for large-scale applications, consistent and robust coupling frameworks between the atomistic and meso-scales are fundamental.

Molecular dynamics is a first-principle theory that explicitly describes the motion individual atoms at small scales based on Newton's second law. In the context of dislocations, MD has been employed as an effective tool for the atomistic understanding of canonical types of dislocation motion for diverse crystal structures and their corresponding mobilities [117–119], as well as the estimation of core energies, responsible for dislocation self-interactions [60, 120].

In order to describe the complex arrangements and mechanics of dislocation networks developed in larger systems (meso-scale), more computationally friendly approaches are necessary. Discrete dislocation dynamics is a framework that describes the motion of these dislocation networks in the same scale as scanning electron microscopy [4], making it a practical computational tool [62] that allowed the discovery of new physics, such as dislocation multi-junctions [121], as well as synthetic data generation.

In this work, we focus on dislocation-driven material visco-plasticity, where relevant properties

to carry out meso-scale DDD simulations are physically informed through MD simulations at the atomistic scale. Our main objective is to be able to utilize both methods in a robust way for data generation and model calibration of probabilistic surrogates [63] and advection-diffusion models of dislocation motion for future studies.

This chapter is organized as follows: In Section 2.2, we introduce some basic definitions of dislocation theory. In Section 2.3 we introduce the theories of molecular dynamics and discrete dislocation dynamics, followed by our numerical computations and results in Section 2.4.

# 2.2 Definitions of Dislocation Theory

We now present a few basic fundamental concepts and definitions of dislocation theory, which form the basis of the employed computational frameworks.

### 2.2.1 Types of Dislocations

We present two basic types of dislocations, namely *edge* and *screw* dislocations, illustrated in the cubic lattices of Figure 2.1 [2]:

- A *positive edge dislocation (see Fig.2.1a, line DC)* can be geometrically described by assuming that the bonds at surface ABCD are broken, separating the faces of the crystal, and inserting an extra half-plane of atoms. The disturbance of the crystal structure only occurs around the line DC. Conversely, a negative edge dislocation is obtained by performing the same procedure at the bottom half of the lattice.
- A *positive screw dislocation (see Fig.2.1b, line DC)* can be geometrically described by displacing both faces of ABCD relative to each other along the direction AB, which forms a spiral-like surface of atoms around line DC. Conversely, a negative screw dislocation is obtained by displacing both faces in ABCD along direction BA.

Although the aforementioned types are two canonic forms, in real crystal structures dislocations have a mixed edge/screw nature [2].



Figure 2.1: Hull and Bacon [2] (a) A positive edge dislocation, denoted by line CD, after inserting an extra half-plane of atoms in ABCD. (b) A left-handed screw dislocation obtained from a displacement of faces ABCD with respect to each other along AB. (c) A Burgers' circuit enclosing an edge dislocation (*left*), and the same circuit in a perfect crystal (*right*). The required closure vector to complete the Burgers' circuit is defined as the Burgers' vector.

### 2.2.2 Burgers' vector

An important definition in this work is the *Burgers' vector*, denoted here by  $\mathbf{b} = [b_1 \ b_2 \ b_3]$ , and defined as the closure failure between the Burgers' circuits around the dislocation line and in a perfect crystal (*see Fig.2.1c*). For edge dislocations, the orientation of  $\mathbf{b}$  is normal to the dislocation line, while for screw dislocations, such orientation is parallel to the dislocation line. For the body-centered cubic (BCC) cells, which are the crystal structures of interest, the Burgers' vector and magnitude *b* are given, respectively, by:

$$\mathbf{b} = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}, \qquad b = \frac{a\sqrt{3}}{2}, \tag{2.1}$$

where *a* denotes the inter-atomic spacing. The Burgers' vector is intrinsically related to *slip* mechanisms, *i.e.*, motion of dislocations in elastic, continuum media. More specifically, the slip direction is always parallel to **b**. Additionally, dislocation lines can end at the crystal boundaries, but never inside the crystal. Therefore, dislocations must form closed loops or branch with other dislocations inside a given crystal, which leads to the following necessary condition for n interconnected dislocation branches:

$$\sum_{i=1}^{n} \mathbf{b}_i = \mathbf{0},\tag{2.2}$$

### 2.2.3 Peach-Koehler forces

Let  $P \in \mathbb{R}^3$  be an arbitrary point on a given (straight or curved) dislocation line, under the effect of a local stress field  $\sigma$ . Furthermore, let  $\xi$  be the direction of a tangent line to the dislocation at point *P*. Then the Peach-Koehler (PK) force per unit-length acting at *P* is given by [4]:

$$\mathbf{f}^{PK} = (\boldsymbol{\sigma} \cdot \mathbf{b}) \times \boldsymbol{\xi},\tag{2.3}$$

which is fully defined by the local stress field  $\sigma$ , arising from surface traction forces, dislocation interactions, or strain-producing defects.

# 2.3 Simulations of Dislocation Motion

Having a few fundamental aspects of dislocation theory defined in the previous section, we now focus on the simulation of dislocation containing systems at the atomistic- and meso-scales. Although other methods are available for the atomistic scale, such as Monte Carlo methods, we employ Molecular Dynamics, since it allows us to simulate the real dynamics of atoms, and thus a detailed description of dislocations, while preserving the *Boltzmann* statistics at small scales [4]. At the meso-scale, we employ Discrete Dislocation Dynamics, which discretizes and explicitly describes the motion of dislocation lines and their networks in a continuum elastic medium. We remark that although DDD is regarded as the discretization of a continuum model, the associated length-scale is of order  $l \sim 10^{-7} - 10^{-5}$  [m], which can be interpreted as an *intermediate scale* that bridges between micro- and macro-scales.

### 2.3.1 Atomistic scale: molecular dynamics

Consider a Hamiltonian system composed of *N* atoms of mass *m* and with positions denoted by the set  $\{\mathbf{r}_i\} := \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N$ , velocity  $\mathbf{v}_i$  and momentum  $\mathbf{p}_i = m\mathbf{v}_i$ . The system is assumed to be at a sufficiently high temperature *T* such that quantum effects are negligible. The total energy of the system, *i.e.*, the *Hamiltonian* is given by [4]:

$$H(\{\mathbf{r}_{i}, \, \mathbf{p}_{i}\}) = \sum_{i=1}^{N} \frac{|\mathbf{p}_{i}|^{2}}{2m} + E(\{\mathbf{r}_{i}\}),$$
(2.4)

where the first term on the right-hand-side represents the total kinetic energy, and  $V({\mathbf{r}_i})$  represents the total potential energy of the system. The classical equations of motion in Hamiltonian mechanics are given by:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i},\tag{2.5}$$

$$\frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{r}_i}.$$
(2.6)

Substituting (2.4) into (2.6), we obtain the equation of motion for every atom j = 1, 2, ..., N in the MD system:

$$m\frac{d^2\mathbf{r}_j}{dt^2} = -\frac{\partial V(\{\mathbf{r}_i\})}{\partial \mathbf{r}_j},\tag{2.7}$$

which is equivalent to Newton's second law, where the interatomic force is given by:

$$\mathbf{f}_j = -\frac{\partial V(\{\mathbf{r}_i\})}{\partial \mathbf{r}_j}.$$
(2.8)

Therefore, with appropriate definitions for the potential energy and therefore computations of the interatomic force  $\mathbf{f}_i$ , MD simulations are carried out through the numerical integration of (2.7). We refer the reader to [4] for additional details regarding numerical integration algorithms. The total potential energy of the system can be written as the following atom-wise summation:

$$V(\{\mathbf{r}_i\}) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \phi(r_{ij}), \qquad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|,$$
(2.9)

where  $\phi(r_{ij})$  denotes an interatomic potential between atoms *i* and *j*. A well-known pairwise potential is the Lennard-Jones potential, which accounts for long-range attraction and short-range repulsion, given by:

$$\phi^{LJ}(r) = 4\epsilon_0 \left[ \left(\frac{\sigma_0}{r}\right)^{12} - \left(\frac{\sigma_0}{r}\right)^6 \right], \qquad (2.10)$$

where the pair  $(2^{1/6}\sigma_0, \epsilon_0)$  yields the minimum interatomic energy. Since the crystal structures in our studies involve multiple atomic bonds, their lengths and orientations, we follow [60, 122] and utilize a Ziegler-Biersack-Littmark potential that has been employed for Fe-C interactions, in the form:

$$\phi(r) = F(r)\phi^{T}(r) + \phi^{ZBL}(r)(1 - F(r)), \qquad (2.11)$$

where  $\phi^T(r)$  denotes a bond-order Tersoff potential,  $\phi^{ZBL}$  a universal repulsive Ziegler-Biersack-Littmark potential, and F(r) represents the Fermi-Dirac function given by:

$$F(r) = \frac{1}{1 + \exp\left[-b_f(r - r_f)\right]},$$
(2.12)

where  $b_f$  and  $r_f$  are fitting parameters. We observe that  $F(r) \rightarrow 1$  as r is sufficiently large in (2.11), thus making the Tersoff component of  $\phi(r)$  dominant at long-distance interactions.

#### 2.3.2 Meso-scale: discrete dislocation dynamics

We now consider the theory of discrete dislocation dynamics [4], which essentially is a segmentwise discretization of the dislocations (*see Fig.2.2*), with corresponding velocities interpolated through a set of basis functions and nodal coefficients. Here we assume that the dislocations have no mass. Therefore inertia effects are neglected and therefore the dislocation lines are in an *overdamped motion*, *i.e.*, their velocities have an instantaneous response due to applied forces. The balance between the applied and drag forces leads to a linear system of equations to be solved for the nodal velocity coefficients, where the matrix of coefficients codes the dislocation mobility in the embedding elastic medium. This allows us to compute the collective motion of dislocation networks and their associated non-Gaussian statistics due to their collective motion.

Figure 2.2 [3, 4] illustrates the segment discretizations of dislocations, assuming that each segment connects two nodes denoted by *i* and *j*, with positions  $\mathbf{r}_i$  and  $\mathbf{r}_j$  and associated Burgers' vector  $\mathbf{b}_{ij}$  with respect to the i - j direction. Therefore, the nodal positions and their segment connectivities for the entire dislocation network can be fully specified by  $\{\mathbf{r}_i, \mathbf{b}_{ij}\}$ . Also, the nodal velocities are denoted by  $\mathbf{v}_i$  and  $\mathbf{v}_j$ . The position at a given coordinate **s** defined between nodes *i* and *j* are interpolated, respectively, in the following way:

$$\mathbf{r}(\mathbf{s}) = N_i(\mathbf{s})\mathbf{r}_i + N_i(\mathbf{s})\mathbf{r}_i, \qquad (2.13)$$

where  $N_i(\mathbf{s})$  and  $N_j(\mathbf{s})$  denote two piecewise linear interpolation functions that satisfy the collocation properties at  $\mathbf{s} = \mathbf{r}_i$  and  $\mathbf{s} = \mathbf{r}_j$ . The velocity is interpolated in the same fashion as follows:

$$\mathbf{v}(\mathbf{s}) = N_i(\mathbf{s})\mathbf{v}_i + N_j(\mathbf{s})\mathbf{v}_j, \qquad (2.14)$$



Figure 2.2: Discretization of dislocations, represented as a set of nodes connected through segments. *(a)* Two dislocation loops (Sills *et al.* [3]). *(b)* A discretized dislocation network (Bulatov *et al.* [4]).

Let  $C := {\mathbf{r}_i, \mathbf{b}_{ij}}$  be defined as the set of all dislocation nodes and segment Burgers' vector of the network. The total forces acting on node *i* are defined as following:

$$\mathbf{f}_{i} = -\frac{\partial E_{tot}(\{\mathbf{r}_{i}, \mathbf{b}_{ij}\})}{\partial \mathbf{r}_{i}} = -\frac{\partial E_{tot}(C)}{\partial \mathbf{r}_{i}}.$$
(2.15)

The total energy of the network can be linearly decomposed in two parts: a *non-local* elastic component  $E_{el}(C, r_c)$  that accounts for interactions with others dislocation segments and the elastic medium, and a *local* core component  $E_c(C, r_c)$  accounting for nonlinear and singular effects due to self-interactions nearby the dislocation line:

$$E_{tot}(C) = E_{el}(C, r_c) + E_c(C, r_c), \qquad (2.16)$$

where  $r_c$  denotes the *dislocation core radius*, which acts as a cut-off parameter from linear elasticity theory to isolate the nonlinearities and singularies within the dislocation core, and can be determined from atomistic simulations. By differentiating (2.16) with respect to the position  $\mathbf{r}_i$ , we obtain the following decomposition of the nodal forces:

$$\mathbf{f}_i = \mathbf{f}_i^{el} + \mathbf{f}_i^c, \tag{2.17}$$

where  $\mathbf{f}_i^{el}$  and  $\mathbf{f}_i^c$  denote, respectively, the elastic and core forces acting on node *i*. Recall the Peach-Kohler force (2.3) acting on a given position **s** over the dislocation line connecting nodes *i* 

and j,

$$\mathbf{f}^{PK}(\mathbf{s}) = (\boldsymbol{\sigma}(\mathbf{s}) \cdot \mathbf{b}) \times \boldsymbol{\xi}(\mathbf{s}).$$
(2.18)

Although not shown here for simplicity (see [4], Section 10.1.3), the internal stress field  $\sigma$  is defined as an integral over the entire dislocation network, which takes into account two Lamé parameters, namely, the *shear modulus G* and the *Poisson ratio v*. The discrete elastic force can be computed in terms of the PK force as the following integration over all segments connected to node *i* as follows:

$$\mathbf{f}_{i}^{el} = \oint_{C} \mathbf{f}^{PK}(\mathbf{s}) N_{i}(\mathbf{s}) dL(\mathbf{s}).$$
(2.19)

The computation of core forces  $\mathbf{f}_i^c$  acting on node *i* is less trivial, and usually requires the knowledge of the core energy  $E_c$  to estimate its corresponding derivative. This is usually obtained through atomistic simulations, where the total dislocation energy is computed, and the core energy can be obtained through (2.16). Alternatively, the dislocation core radius  $r_c$  can be obtained from the total energy, and the core energy can be estimated analytically.

The last definition in order to compute the nodal dislocation velocities is the *dislocation mobility*, which we employ as a linear constitutive relationship between a drag force  $\mathbf{f}^{drag}$  (due to the motion resistance from the elastic medium) and the velocity **v**:

$$\mathbf{f}^{drag}(\mathbf{s}) = -\mathcal{B}(\boldsymbol{\xi}(\mathbf{s})) \cdot \mathbf{v}(\mathbf{s}), \tag{2.20}$$

where  $\mathcal{B}$  denotes the dislocation mobility tensor, which takes distinct forms according to the crystal structure and edge/screw dislocations under *glide* and *climb* motions. For BCC metals, we consider the following forms [62]:

$$\mathcal{B}(\boldsymbol{\xi}) = B_{\boldsymbol{\xi}}(\mathbf{I} - \boldsymbol{\xi} \otimes \boldsymbol{\xi}), \quad \text{when } \boldsymbol{\xi} \parallel \mathbf{b} \quad (\text{screw dislocation}), \tag{2.21}$$

with  $B_s$  denoting a drag coefficient for screw dislocations, and,

$$\mathcal{B}(\boldsymbol{\xi}) = B_{eg}(\mathbf{m} \otimes \mathbf{m}) + B_{eg}(\mathbf{n} \otimes \mathbf{n}) \quad \text{when } \boldsymbol{\xi} \perp \mathbf{b} \quad \text{(edge dislocation)}, \tag{2.22}$$

where  $B_{eg}$  and  $B_{ec}$  denote, respectively, the glide and climb drag coefficients for edge dislocations, and  $\mathbf{n} := \mathbf{b} \times \boldsymbol{\xi} / ||\mathbf{b} \times \boldsymbol{\xi}||, \mathbf{m} := \mathbf{n} \times \boldsymbol{\xi}$ . In our numerical experiments, we will consider the same drag coefficient for all aforementioned cases, denoted by *B*, which we obtain from an edge dislocation glide MD experiment, and relate it to an *edge dislocation glide mobility* in the form  $M_{eg} = B/b$ , which is one of the input parameters of the DDD framework.

We now let  $\mathbf{f}^{drive}(\mathbf{s})$  be the driving force, which is comprised of a summation of elastic, core and any other forces (*e.g. chemical forces due to inclusions*) acting on a point  $\mathbf{s}$  of the dislocation network. The balance of drag and driving forces is therefore given by:

$$\mathbf{f}^{drag}(\mathbf{x}) + \mathbf{f}^{drive}(\mathbf{x}) = \mathbf{0},\tag{2.23}$$

and therefore, using (2.20),

$$\mathcal{B}(\boldsymbol{\xi}(\mathbf{s})) \cdot \mathbf{v}(\mathbf{s}) = \mathbf{f}^{drive}(\mathbf{x}).$$
(2.24)

The above equation is posed in weak form, by multiplying both sides by a test function  $N_i(\mathbf{s})$  and integrating with respect to the entire length of the dislocation network, leading to the following equation to be solved for the velocity vector of each node *i* of the newtork:

$$\sum_{j} \mathbf{B}_{ij} \, \mathbf{v_j} = \mathbf{f}_i, \tag{2.25}$$

where the mobility matrix is given by:

$$\mathbf{B}_{ij} = \oint_C N_i(\mathbf{s}) \mathcal{B}(\boldsymbol{\xi}(\mathbf{s})) N_j(\mathbf{s}) \, dL(\mathbf{s}).$$
(2.26)

# 2.4 Numerical Results

Following the studies from Lehtinen *et al.* [60], we perform a series of numerical experiments using LAMMPS to estimate intrinsic BCC iron (Fe) material parameters required for DDD ParaDis simulations, namely, shear modulus G, Poisson ratio v, dislocation core radius  $r_c$  and edge glide dislocation mobility  $M_{eg}$ . Other required parameters like the Burgers' vector magnitude b and dislocation core energy  $E_c$  are computed through theoretical estimates.

### 2.4.1 Molecular dynamics

Figure 2.3 presents the employed MD systems for pure Fe-Fe interactions. An orthorhombic box is employed for shear, mobility and core radius experiments (*see Fig.2.3a*), while a cylindrical nano-wire is utilized for the Poisson ratio test (*see Fig.2.3b*). For all analyses, we equilibrated the system in consideration to a reference temperature T = 750 [K]. We utilize the ZBL interatomic potential (2.11) with the fitted parameters provided by Henriksson et al. [122]. The Burgers' vector magnitude *b* can be determined theoretically using (2.1) as  $b = \frac{\sqrt{3}a}{2} = 0.2501 [nm]$ , from an inter-atomic spacing a = 0.2889 [nm]. We present the procedure for the remaining material parameters below.



Figure 2.3: (*a*) Orthorhombic box with an edge dislocation in the center, employed as the MD domain for the core radius, edge mobility, and shear (no dislocation) tests. (*b*) Cylindrical nanowire domain utilized for the Poisson ratio experiment.

#### 2.4.1.1 Shear modulus

The shear modulus *G* is a property of the elastic medium required to compute the stress tensor  $\sigma$  in DDD frameworks. Therefore, we consider the system in Fig.2.3a in the absence of the edge dislocation. The top and bottom layers of atoms are fixed in the *y*-direction, and a constant velocity of  $v_x = 0.2 [nm/ps]$  is imposed on the top layer. The corresponding force acting on the top layer

and the shear strains  $\gamma_{xy}$  are computed, allowing us to estimate the shear modulus G = 73.20 [GPa] through the slope of a linear fit of the small-strain region in Figure 2.4.



Figure 2.4: Block-shear stress-strain MD experiment. The linear fit over a small strain range  $\gamma_{xy} < 0.05$  yielded a shear modulus G = 73.20 [GPa].

### 2.4.1.2 Poisson ratio

Figure 2.3b illustrates the MD domain for this experiment. The orientation of the BCC crystals is [110] along the nano-wire's axis. The initial length  $L_0$  of the wire is taken as  $L_0 = 4D_0$ , where  $D_0$  denotes the initial diameter. The bottom layer of atoms in the nano-wire is fixed in all directions. The wires were initially relaxed for t = 20 [ps] at T = 750 [K] using a Berendsen-type temperature control. After the temperature equilibration step, we impose a constant axial strain rate  $\dot{\varepsilon}_x = 0.001 [ps]$ . The engineering strains at the boundaries of the wire in the axial and radial directions are defined, respectively, as  $\Delta \varepsilon_x = \Delta L/L_0$  and  $\Delta \varepsilon_r = \Delta R/R_0$ . The Poisson ratio is then computed as  $v = -\frac{\Delta \varepsilon_x}{\Delta \varepsilon_r}$ , by employing a moving average filter with N = 25 points on the raw data and a linear fit over the small strain range. Figure 2.5 presents the obtained results, with an estimated value of v = 0.378.

#### 2.4.1.3 Edge dislocation radius and energy

The edge dislocation core radius  $r_c$  around an infinite edge dislocation is defined as the distance beyond which the dislocation-induced potential energy becomes sufficiently close to the total



Figure 2.5: Nanowire tensile MD experiment. (*left*) Poisson coefficient estimation v = 0.378, through a linear fit over the filtered data. (*right*) Obtained stress vs. strain results, yielding a Young's modulus E = 211.98 [GPa].

potential energy V of a corresponding perfect lattice [123]. Therefore, we perform a minimization on the system illustrated in Fig.2.3a with and without the edge dislocation and computed the corresponding potential energies of atoms within a varying cylinder of radius r, centered at the dislocation core (blue line). Figure 2.6 illustrates the obtained results, where we obtain a dislocation core radius  $r_c \approx 2.9 [b]$  with a relative error of less than 2% between the computed potential energies. The dislocation core energy  $E_c$  is later estimated using ParaDis' defaults from the estimated  $r_c$ .

#### 2.4.1.4 Dislocation mobility

Following body-centered-cubic Fe-C simulations from [60], we generate synthetic dislocation motion data in a pure Fe system and estimate the edge mobility property through MD simulations utilizing the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [61]. All the MD simulations in this work are run in 80 Intel Xeon Gold 6148 CPUs with 2.40GHz.

The MD system under consideration is illustrated in Fig. 2.7, consisting of a simulation box of  $61 \times 40 \times 20 \alpha$ -Fe unit cells with dimensions  $25.14 \times 26.96 \times 24.06 [nm]$  in the *x*, *y*, *z* directions.



Figure 2.6: Dislocation core radius estimation through the relative difference between the potential energy of the system with a single edge dislocation  $(PE_e)$  and a pure system  $(PE_p)$ . The estimate r = 2.9 [b] is obtained considering a moving average filter on the obtained data and a relative difference of  $\approx 1.8\%$  between both systems.

A straight edge dislocation with Burgers' vector  $\mathbf{b} = \frac{1}{2}[1, 1, 1]$  is generated by removing a (1, 1, 1) half-plane of atoms from the center of the box. The MD domain consists of 1 353 132 atoms with periodic boundary conditions applied in the *x* and *z* directions, and shrink-wrapped boundary conditions applied to the unit cells in the top- and bottom-planes along the *y*-direction. We perform an NVE time-integration, where the system's temperature is relaxed to T = 750 [K] through velocity-rescaling for 100 [ps] (see Fig.2.8a). We utilize a combined Tersoff bond-order and repulsive Ziegler-Biersack-Littmark (ZBL) interatomic potential, with corresponding parameters from [122].

We apply shear stress values in the range  $\tau \in [15, 100] MPa$  to the top layer in Fig. 2.7a, parallel to **b**, which induces a glide motion in the *x*-direction on the (1, 1, 0) plane. No temperature control is enforced in this stage and we run the simulation over 1 [ns] with time-step size  $\Delta t^{MD} = 2 [fs]$ . The MD time-series data is saved every 100 time-steps and the atom positions are post-processed utilizing the Polyhedral Template Matching (PTM) method [124] implemented in OVITO (https: //www.ovito.org/) [125], which allows us to detect and track the lattice disturbance. We define the dislocation position as the average of all *x*-coordinates of atoms belonging to the disturbed region (dislocation core) in Fig.2.7a. Therefore, for every applied shear stress  $\tau$ , we obtain a position vector  $\mathbf{x}^{MD}(t)$  with 5000 data-points (*see Fig. 2.8b*) of size  $\Delta t^{MD} = 2 [fs]$ , from which



Figure 2.7: MD domain of the dislocation mobility test. (a) x - y plane, illustrating the edge dislocation core as the lattice perturbation at the center. (b) 3D view of the MD domain with the BCC lattice removed, showing the dislocation line along the *z*-axis.

we compute the corresponding velocity  $v^{MD}$  through a linear fit. The obtained velocity from the post-processed MD simulation can be related to the one-dimensional solution from dislocation dynamics denoted by  $v_x$ , and given by the following relationship:

$$v_x = M \cdot b \cdot \tau. \tag{2.27}$$

where *M* denotes the edge dislocation mobility, and  $b = \sqrt{3}a/2$  represents the magnitude of **b**. Equation (2.27) is obtained from the balance between the applied Peach-Kohler force induced by the shear stress  $\tau$  and the dislocation drag force. Therefore, setting  $v^{MD} = v_x$  and from the slope  $m = M \cdot b$  of the velocity *versus* stress curve in Fig. 2.8c, we estimate the edge dislocation glide mobility as  $M = m/b \approx 5931.3 [(Pa.s)^{-1}]$ , which is in good quantitative agreement (1.73% difference) compared to the results obtained by Lehtinen et al.[60].

The presented dislocation mobility results obtained from MD simulations here were employed for data generation for a graph-based coarse grained probabilistic surrogate model developed in [63].



Figure 2.8: (a) Temperature and total energy for the equilibration step, (b) Edge dislocation position  $\mathbf{x}^{MD}(t)$  and (c) mobility through MD simulations for distinct values of applied shear stresses  $\tau$  under T = 750 [K]. We observe an overdamped motion for the applied shear stress range and a linear mobility relationship.

### 2.4.2 Discrete dislocation dynamics

Following the studies by Lehtinen *et al.* [120], we utilize the estimated parameters from the MD experiments as inputs for 3D simulations in ParaDis. We assume the mobility of screw dislocations  $M_s = M_{eg} \approx 5931.3 [1/(Pa.s)]$ . The domain consists of a BCC iron cube with length  $L = 0.75 [\mu m]$  periodic boundary conditions and temperature T = 750 [K]. An initial random configuration with 24 straight screw dislocations in the  $\frac{1}{2}\langle 111\rangle [110]$  slip system. The initial dislocation density is  $7.38 \times 10^{13} [m^2]$ . We impose distinct values of uniaxial strain rates  $\dot{\varepsilon}$ , and illustrate the obtained results in Figure 2.9. We observe the a rate-dependent plastic behavior, with a relaxation observed for all strain rates, followed by intermittent hardening, with the yield recovery occurring at larger strains as the strain rate is increased. The dislocation density *vs.* total strain plot indicates that the earlier onset of strain hardening for  $\dot{\varepsilon} = 10^6 [s^{-1}]$  seems to be connected by a ballistic dislocation density evolution, compared to higher strain-rates. Such results suggest that dislocation interactions are quickly resolved at lower strain rates, leading to a faster relaxation process, while an early arresting mechanism is more pronounced at higher strain rates.

Figure 2.10 illustrates three snapshots of the dislocation network formations at different timesteps of the DDD simulations for  $\dot{\varepsilon} = 10^7 [s^{-1}]$ , from which we observe the evolution of the fractal dislocation microstructure.



Figure 2.9: DDD tensile tests in pure iron under different strain rates. (*a*) Rate-dependent stress *vs.* strain response showing visco-plastic intermittent behavior after a hardening/relaxation phase. (*b*) Dislocation density *vs.* time. (*c*) Dislocation density *vs.* strain, showing a ballistic behavior for lower strain-rates.

We also compute the average dislocation arm centroid velocity V(t) time-series for the case  $\dot{\varepsilon} = 10^6 [s^{-1}]$ , as well as the instantaneous acoustic energy  $E(t) = V(t)^2$  distribution, and present the obtained results in Figure 2.11. We observe typical *self-similar* behavior of plasticity in singlecrystals, with intermittent avalanche energy bursts, given by the larger acoustic energy events. We note that the notion of intermittency here relates to the rare events involving high velocity gradients, which deviate from Gaussian statistics, and therefore leading to an acoustic energy distribution in the form  $P(E) \propto E^{-\delta}$ , with observed power-law scaling  $\delta = 1.5$ .



Figure 2.10: DDD simulations of fractal dislocation network evolution at three different instants: (a)  $t = 2.44 \times 10^{-12} [s]$ , (b)  $t = 7.46 \times 10^{-10} [s]$ , and (c)  $t = 1.90 \times 10^{-9} [s]$ . The red dots represent the dislocation arm (white lines) centroids.



Figure 2.11: Computation of collective dislocation velocities for the DDD tensile test with  $\dot{\varepsilon} = 10^6 [s^{-1}]$ . (a) Time-series data of collective dislocation velocity, indicating the presence of intermittent, large energy bursts. (b) Acoustic energy histogram, where  $P(E) \propto E^{-\delta}$ , with  $\delta = 1.5$ , consistent with experimental data for dislocation avalanches.

#### **CHAPTER 3**

## A DATA-DRIVEN FRACTIONAL MODELING FRAMEWORK FOR ANOMALOUS RHEOLOGY: APPLICATION TO URINARY BLADDER TISSUE

# 3.1 Background

Bio-tissues are complex and multi-functional materials, optimized for their specific host organisms, and constrained by limited set of building blocks and available resources [126]. While the mechanical behavior of a number of standard engineering materials (*e.g.*, metals, polymers, rubbers) is quite well-understood, there is still a significant effort towards bio-materials, where microstructure heterogeneities, randomness and small scale physical mechanisms lead to non-standard and at times counter-intuitive responses. Power-law rheology is a complex response observed in many bio-tissues such as arteries [8], cartilage [9, 10], lungs [11], smooth muscle [12], liver and kidneys [13], red blood cell membranes [14], and other materials like cross-linked polymers [15], gels [16, 17], soft glassy materials [18]. These power-law materials, also termed *anomalous*, exhibit power-law scaling for creep/relaxation in the form  $J(t) \propto t^{\beta}$  and  $G(t) \propto t^{-\beta}$  and also for dynamic storage/dissipation in the frequency domain [6]. The origin of this power-law behavior at the continuum level is due to (non-Fickian) sub-diffusive processes [7] in the corresponding fractal-like micro-structures[127, 128].

The aforementioned anomalous non-exponential behavior usually requires a significant number of material parameters when employing standard viscoelastic models. These consist of mechanical arrangements of linear springs and Newtonian dashpots, which induces a finite number of relaxation modes, which may lack predictability when performing outside the experimental time scales [9, 24]. In this regard, fractional models become attractive alternatives, since their integro-differential operators naturally utilize power-law convolution kernels, coding self-similar microstructural features in a reduced-order mathematical language with smaller parameter spaces. Therefore, they have been employed as compact and predictive models for a number of anomalous systems, such as biological
materials [9–13], fluid turbulence [129–132], and instabilities [133]. We particularly note that such predictability has been shown to extend across different experiments (relaxation/creep) in certain cases [24]. Additionally, calibrating experimental data with a set of existing rheological models leads to a material model selection problem, which is inherently ill-conditioned, since multiple models can pragmatically yield similar errors when confronted to experiment. In this work, we attempt to reduce this implicit ill-posedness by introducing fractional-order models as attractive alternatives to their integer-order counterparts, and employed to urinary bladder (UB) tissue modeling. Our fractional modeling framework aims to obtain compact mathematical models with a reduced number of material model parameters, while introducing a minimal, but sufficient number of fractional rheological elements that capture the qualitative response of multiple power laws and minimizes the errors, also rigorously taking into account the corresponding power-law memory effects.

The lower urinary tract, and especially the urinary bladder, is a highly dynamic organ system. To ensure its proper function, the bladder needs to be able to significantly increase in size while maintaining a low internal pressure, and this ability is dictated by the mechanics of the bladder wall. Specifically, during filling, the bladder tissue must leverage its viscoelastic characteristics to accommodate for large deformations without resulting in significant increase the luminal pressure. When this behavior is compromise due to disease, the resulting increase in pressure might generate a high-pressure urine reflux from the bladder to the kidneys, resulting in renal failure [134, 135]. To increase the complexity of the organ mechanics, the characteristics of the bladder differ between different anatomical locations (i.e., dorsal, ventral, lateral, lower-body, trigone) [136, 137] and orientations (i.e., longitudinal/apex-to-base and circumferential/transverse) [136–144]. To describe the mechanical behavior of bladder tissue both hyperelastic [139, 140, 143–152] and viscoelastic [141, 142, 153–166] models have been used in the literature. But due to the differences in mechanical testing protocols as well as modeling, most of the results cannot be compared with one another and often results in contradicting conclusions. While several pathologies of the lower urinary tract are associated with dramatic changes of the mechanical behavior of the bladder time chanical behavior of the bladder time changes of the mechanical behavior of the bladder time conclusions. While several pathologies of the lower uninary tract are associated with dramatic changes of the mechanical behavior of the bladder time changes of the mechanical behavior of the bladder to bladder to bladder to the approximate testing protocols as well as modeling.

[167], still much is unknown about the mechanisms that affect this organ, not just in diseased states but in healthy as well. In this study, we focus on the healthy behavior of the porcine urinary bladder, which a present work suggested is a good model for the human urinary bladder.

Although linear fractional visco-elasticity has been succesfully employed in a number of biomechanical applications, additional modeling considerations are necessary when dealing with other material nonlinearities, such as large strains. This would imply that the material relaxation behavior becomes strain dependent, and needs additional modeling considerations. For that purpose, a well-known model is Fung's quasi-linear-viscoelastic (QLV) theory[168], which considers a multiplicative coupling between a linear visco-elastic relaxation and a nonlinear elasticity term. Fractional extensions of Fung's QLV theory have been developed and employed for modeling the response of aortic valve cusp[169] and arterial walls[10].

To the authors' best understanding, although existing studies have addressed the hyper-viscoelastic behavior of urinary bladders, there are no studies in the literature confronting their powerlaw response with fractional viscoelastic models. In this work we develop a data-driven fractional modeling framework for linear and quasi-linear viscoelasticity to account for anomalous powerlaw relaxation and large strains. We validate the developed framework for the first time in the uniaxial relaxation of porcine urinary bladder (UB) tissue for a wide range of applied strains. The characteristics of our experimental procedure are:

- We obtain the porcine urinary bladder uniaxial relaxation data from small-to-large strains of five distinct anatomical locations.
- Our relaxation experiments are performed under increasingly larger strains, without intermediate unloading steps or tissue preconditioning.
- The mechanical response of the UB indicates nonlinear visco-elastic behavior with power-law relaxation, characterizing an anomalous behavior.

Given the anomalous response of the urinary bladder tissue, we employ our anomalous modeling framework as follows:

- Our *existence* study considers a set of fractional building block models (Scott-Blair, fractional Kelvin-Voigt, fractional Maxwell), which are selected according to the power-law nature of the relaxation data.
- The fractional linear visco-elastic models provide sufficiently accurate fits for single-relaxation steps under smaller strain levels, where the fractional Maxwell model with two fractional orders is the most suited for the UB.
- For large strains under multiple applied strain steps, we employ a fractional quasi-linear visco-elastic (FQLV) model based on Fung's QLV theory, which is able to capture the entire experimental range over four decades in time, with the presence of power-law relaxation and strain-induced material nonlinearity.

The rest of the paper is organized as follows. In Section 3.2 we present the problem setup and methodology, with the uniaxial UB stress relaxation data and our proposed fractional modeling framework for biotissues, comprised of linear and quasi-linear fractional models. In Section 3.3, we present our obtained linear viscoelasticity results for the UB relaxation under the first strain step, and the fractional quasi-linear viscoelastic model for all consecutive strain steps, followed by the discussions and potential improvements of the work.

# 3.2 Problem Setup and Methodology

### 3.2.1 Urinary bladder experimental relaxation tests

We utilize existing stress relaxation data from Dr. Roccabianca's lab at at Michigan State University, obtained from five samples of a single porcine UB, extracted from distinct anatomical locations as shown in Fig.3.1(a). The locations are dorsal (D), lateral (L), lower body (LB), trigone (T), and ventral (V). The samples were punched out with a  $1 \times 3$  [*cm*] leather punch in the apex-to-base direction as shown in Fig.3.1 (b). Each sample was clamped and subjected to five consecutive stress relaxation stages, under prescribed step strains  $\varepsilon_0 = \{0.25, 0.50, 1.00, 1.50, 2.00\}$  for 30, 45, 45, 45, and 45 minutes, respectively, as illustrated in Figs.3.1(c) and (d). Besides the strain

inputs, the force denoted by *F* is measured by a 10 [*lb*] load cell throughout the duration of the test. The cross-sectional area of each sample is calculated by taking top and side view pictures of the sample at each strain level right after each strain applications. The pictures are converted to binary images, which are processed in MATLAB to determine an approximate width *b* and thickness *h* and thickness of each sample, at each strain level. The updated cross-sectional area is assumed to remain constant throughout the relaxation at each strain level, and is evaluated as  $A^{data} = bh$ . Given force and area time-series, the true strain is evaluated as  $\sigma^{data}(t) = F^{data}(t)/A^{data}(t)$ .



Figure 3.1: (*a*) Dissected porcine UB showing the distinct anatomical locations from which samples were punched. (*b*) A diagram of the UB from the lateral view. (*c*,*d*) A representative sample under clamped, uniaxial relaxation, respectively, in upper and side views, from which images are extracted for area estimation.

Once the stress and strain time-series are obtained, we filter the data through a moving average filter with a time-window of thirty neighbor data points. Figure 3.2 illustrates the relaxation curves for all samples in linear and log-log scales. We observe a characteristic power-law scaling for long-time behavior, which is evident in Fig.3.2 (b). As will be shown later through fractional model fits, the relatively low scaling coefficient  $\beta$  indicates an anomalous behavior of predominantly elastic nature, where the relaxation behaviors has a faster decay at lower time-scales, followed by a plateau with low decay rates  $\sigma \sim t^{-\beta}$  at larger time-scales (*i.e.*, t > 400 [s]). We also note that the trigone and lower body specimens yielded higher stress levels, particularly at very high strains, while the dorsal specimen yielded lower overall values. This is in accordance to stress-strain results obtained by Korossis [136], that indicated statistically significant, higher collagen phase slopes for the lower

body and trigone regions.



Figure 3.2: Stress relaxation data for all UB samples. (a,b) - stress vs time data in linear and logarithmic scales. (c,d) - successive step strain vs time data in linear and logarithmic scales. The long-term power-law behavior becomes evident especially in the first relaxation step in (b), where the slope of the black line is given by  $|\beta| \approx 0.3$ .

We analyze the presence of strain dependency on the UB relaxation behavior, in order to determine if the visco-elasticity is of non-linear nature. Therefore, we employ the definition of linear relaxation modulus G(t)[Pa], applied for each fixed strain application from experimental data [170]:

$$G^{data}(t) := \sigma^{data}(t) / \varepsilon_0.$$

Figure 3.3 illustrates the obtained relaxation moduli for all samples and relaxation steps. We observe that although the relaxation moduli data for each sample collapse into a single curve for  $\varepsilon_0 = \{0.25, 0.50\}$  (except for the trigone sample), the behavior of *G* is clearly not only timebut also strain-dependent. Furthermore, the degree of nonlinearity is more pronounced for the lower body and trigone samples, and less pronounced for the dorsal sample. Interestingly, we notice two limiting power-law behaviors for short and long times. The short time behavior has a power law of smaller magnitude  $\beta_1$ , while the long time behavior is associated with a power-law of larger magnitude  $\beta_2$  (see Fig.3.3(f)). Larger standard deviations for the long time power-law were observed for the trigone region due to its distinct response for  $\varepsilon_0 = 0.25$ . We remark that this analysis is just performed to infer the nonlinear relaxation quality the data, and we do not intend to construct a master curve for each bladder sample.



Figure 3.3: Normalized relaxation moduli for each bladder specimen under distinct applied strains: (a) D, (b) L, (c) LB, (d) T, (e) V. The relaxation behavior seems to be approximately linear for most specimens in the  $\varepsilon_0 \in [0.25, 0.5]$  range. All specimens clearly demonstrate a dependency of both time and applied strains for  $\varepsilon_0 > 0.5$ , with largest variations observed in the LB and T samples. Furthermore, the data indicates two distinct relaxation regimes with slower (t < 3[s]) and faster (t > 400[s]) decays, respectively, with slopes  $\beta_1$  and  $\beta_2$  illustrated in (f).

## 3.2.2 A Fractional Viscoelastic Modeling Framework for Anomalous Tissue Rheology

We develop an *existence* study to identify the admissible set of anomalous constitutive laws that satisfy the quality of the experimental relaxation behavior, while shedding light on the corresponding microstructural constituents associated to anomalous behavior. Starting with the Scott-Blair (SB) model as the fundamental building block, we construct building block models through parallel and serial combinations to obtain the fractional Kelvin-Voigt (FKV) and fractional Maxwell (FM) models. In our approach, we take into account the anomalous qualities present in the experimental

relaxation data and compare them with each of the candidate building block models. Each of the models exhibit distinguished material complexities, such as distinct asymptotic behaviors of relaxation G(t), multiple power-law regimes, slower/faster relaxation at the asymptotic stages [36, 171] and presence of material nonlinearities. In the last part of the existence study we classify the candidate models in a "table of anomalous qualities", which together with obtained fitting errors make part of the model selection procedure.

#### **3.2.2.1** Fractional linear viscoelastic models

Given the experimental data presented in Section 3.2.1, we focus on the first relaxation step ( $\varepsilon_0 = 0.25$ ) of Figs.3.2 and 3.3 for our data-driven, linear visco-elastic framework. Our objective is to demonstrate how fractional visco-elastic models are able to capture the UB relaxation with simplistic mechanical arrangements and a small number of material parameters.

The rheological *building block* for our framework is the fractional *Scott-Blair* (SB) visco-elastic element, which compactly represents an anomalous visco-elastic constitutive law connecting the stresses and strains:

$$\sigma(t) = \mathbb{E} {}_{0}^{C} \mathcal{D}_{t}^{\alpha} \varepsilon(t), \quad t > 0, \quad \varepsilon(0) = 0,$$
(3.1)

with constant fractional order in the range  $0 < \alpha < 1$ , which provides a material interpolation between Hookean ( $\alpha \rightarrow 0$ ) and Newtonian ( $\alpha \rightarrow 1$ ) elements. The operator  ${}_{0}^{C}\mathcal{D}_{t}^{\alpha 1}(\cdot)$  represents the time-fractional Caputo derivative given by:

$${}_{0}^{C}\mathcal{D}_{t}^{\alpha}u(t) \coloneqq \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{u'(s)}{(t-s)^{\alpha}} \, ds, \qquad (3.2)$$

where  $\Gamma(\cdot)$  represents the Euler-gamma function[32]. The pair  $(\alpha, \mathbb{E})$  uniquely represent the SB constants, where the *pseudo-constant*  $\mathbb{E}[Pa.s^{\alpha}]$  compactly describes textural properties, such as the firmness of the material [24, 172]. In this sense  $\mathbb{E}$  is interpreted as describing a snapshot of a non-equilibrium dynamic process instead of an equilibrium state. The corresponding rheological symbol for the SB model represents a fractal-like arrangement of springs and dashpots [6, 34], which we interpret as a compact, upscaled representation of a fractal-like microstructure. Regarding the

thermodynamic admissibility, we refer the reader to Lion[35] for the SB model, and Suzuki *et al.*[75] for the combination of the SB element with more complex mechanisms of visco-plasticity and damage. The relaxation function G(t)[Pa] for the SB model is given by the following inverse power-law form:

$$G^{SB}(t) := \frac{\mathbb{E}}{\Gamma(1-\alpha)} t^{-\alpha}, \tag{3.3}$$

which is the convolution kernel of the integro-differential form in (3.2). Figure 3.4(*a*) illustrates the behavior of  $G^{SB}(t)$ , which is *scale-free*, *i.e.*, a single power-law is present for all t > 0. We note that although this relaxation response may seem to be oversimplified, it provides a flexible constitutive interpolation able to, at the very least, take into account the long-term anomalous dynamics of materials, such as the power-law  $\beta_2$  in Fig.3.3. This also allows the SB element to capture, in limited time-scales, power-law behaviors induced by predominantly elastic microstructures, such as collagen networks[169] with small  $\alpha$ -values.



Figure 3.4: Relaxation functions G(t) for the building block models under varying fractional models and  $\mathbb{E}_1 = 1$ ,  $\mathbb{E}_2 = 1$ . (a) Scott-Blair, (b) Fractional Kelvin-Voigt, and (c) Fractional Maxwell. We note the progression from a single, scale-free power-law behavior for the SB model to two dominating power-laws under small and large times for the FKV and FM models.

We utilize the SB model as our rheological building block, and define a set of "building block models", which introduce a higher degree of material complexity through multiple law behaviors for relaxation and therefore distinct anomalous regimes for small and large time-scales. This multi-fractal type of behavior is characteristic of cells[25] and biological tissues[173], due to their complex, hierarchical and heterogeneous microstructure. Here we consider only two canonical

combinations of SB elements. Through a parallel combination, we obtain the fractional Kelvin-Voigt (FKV) model, which has the following stress-strain relationship [34]:

$$\sigma(t) = \mathbb{E}_1 \ {}_0^C \mathcal{D}_t^{\alpha_1} \varepsilon(t) + \mathbb{E}_2 \ {}_0^C \mathcal{D}_t^{\alpha_2} \varepsilon(t), \tag{3.4}$$

with t > 0,  $\varepsilon(0) = 0$ , and fractional orders  $0 < \alpha_1, \alpha_2 < 1$  and associated pseudo-constants  $\mathbb{E}_1[Pa.s^{\alpha_1}]$  and  $\mathbb{E}_2[Pa.s^{\alpha_2}]$ . The corresponding relaxation modulus G(t)[Pa], is also an additive form of two SB elements:

$$G^{FKV}(t) := \frac{\mathbb{E}_1}{\Gamma(1-\alpha_1)} t^{-\alpha_1} + \frac{\mathbb{E}_2}{\Gamma(1-\alpha_2)} t^{-\alpha_2}.$$
(3.5)

Figure 3.4(*b*) illustrates the relaxation function  $G^{FKV}$  for varying fractional orders. We notice a response characterized by two power-law regimes, with a transition from faster to slower relaxation slopes. The asymptotic responses for small and large time-scales are given by  $G^{FKV} \sim t^{-\alpha_2}$  as  $t \to 0$  and  $G^{FKV} \sim t^{-\alpha_1}$  as  $t \to \infty$ . We note that this quality allows the FKV model to describe materials that reach an equilibrium behavior for large times when  $\alpha_1 \to 0$ , which is intuitive from the mechanistic standpoint as one of the SB elements becomes a Hookean spring.

Finally, through a serial combination of SB elements, we obtain the fractional Maxwell (FM) model[24], given by:

$$\sigma(t) + \left(\mathbb{E}_2/\mathbb{E}_1\right) {}_0^C \mathcal{D}_t^{\alpha_2 - \alpha_1} \sigma(t) = \mathbb{E}_2 {}_0^C \mathcal{D}_t^{\alpha_2} \varepsilon(t), \quad t > 0,$$
(3.6)

with  $0 < \alpha_1 < \alpha_2 < 1$ , and two sets of initial conditions for strains  $\varepsilon(0) = 0$ , and stresses  $\sigma(0) = 0$ . We note that in the case of non-homogeneous ICs, there needs to be a compatibility conditions[32] between stresses and strains at t = 0. The corresponding relaxation function for this building block model assumes a more complex, Miller-Ross form[24]:

$$G^{FM}(t) := \mathbb{E}_1 t^{-\alpha_1} E_{\alpha_2 - \alpha_1, 1 - \alpha_1} \left( -\frac{\mathbb{E}_1}{\mathbb{E}_2} t^{\alpha_2 - \alpha_1} \right), \tag{3.7}$$

where  $E_{a,b}(z)$  denotes the two-parameter Mittag-Leffler function, defined as [32]:

$$E_{a,b}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(ak+b)}, \quad Re(a) > 0, \quad b \in \mathbb{C}, \quad z \in \mathbb{C}.$$
(3.8)

Interestingly, the presence of a Mittag-Leffler function in (3.7) lead to a stretched exponential relaxation for smaller times and a power-law behavior for longer times, as illustrated in Fig.3.4. We also observe that the limit cases are given by  $G^{FM} \sim t^{-\alpha_1}$  as  $t \rightarrow 0$  and  $G^{FM} \sim t^{-\alpha_2}$  as  $t \rightarrow \infty$ , indicating that the FM model provides a behavior transitioning from slower-to-faster relaxation. We refer the reader to the work by Bonfanti *et al.*[174] for a number of applications of the aforementioned models. We notice that both FKV and FM models are able to recover the SB element with a convenient set of pseudo-constants. Furthermore, we also outline more complex building block models that yield more flexible responses, including three to four fractional orders, such as the fractional Kelvin-Zener (FKZ), fractional Poynting-Thomson (FPT), and fractional Burgers (FB), which in turn are able to recover the FKV and FM models. We refer the reader to the works [34, 174, 175] for more details on such models.

#### 3.2.2.2 Fractional quasi-linear viscoelastic modeling

The presented models in Section 3.2.2.1 provide candidates for power-law relaxation functions that describe the anomalous visco-elastic dynamics of biotissues, however, in biological tissues the stress-strain relationship usually becomes nonlinear as collagen fibers transition from entangled to aligned with the applied load direction. Therefore, the visco-elastic behavior itself becomes nonlinear and the relaxation function has an intrinsic dependency on the strain levels, as observed in Fig.3.3 under successive large step-strain applications. To incorporate this additional effect to our modeling framework, we follow [10, 168], and employ the following quasi-linear, fractional visco-elastic model (FQLV):

$$\sigma(t,\varepsilon) = \int_0^t G(t-s) \frac{\partial \sigma^e(\varepsilon)}{\partial \varepsilon} \dot{\varepsilon} \, ds, \qquad (3.9)$$

where the convolution kernel is given by a multiplicative decomposition of a reduced relaxation function G(t) and an instantaneous, nonlinear elastic tangent response with stress  $\sigma^e$ . In the work by Craiem *et al.*[10], the reduced relaxation function has a fractional Kelvin-Voigt-like form with one of the SB replaced with a Hookean element. Here, we assume a simpler rheology and adopt a Scott-Blair-like reduced relaxation in the form:

$$G(t) = Et^{-\alpha} / \Gamma(1 - \alpha), \qquad (3.10)$$

with the pseudo-constant *E* with units  $[s^{\alpha}]$ . We adopt the same, two-parameter, exponential nonlinear elastic part as in[10]:

$$\sigma^{e}(\varepsilon) = A\left(e^{B\varepsilon} - 1\right),\tag{3.11}$$

with A having units of [Pa]. Substituting Equations 3.10 and 3.11 into Eq.3.9, we obtain:

$$\sigma(t,\varepsilon) = \frac{EAB}{\Gamma(1-\alpha)} \int_0^t \frac{e^{B\varepsilon(s)}\dot{\varepsilon}(s)}{(t-s)^{\alpha}} \, ds, \qquad (3.12)$$

which differs slightly from the linear SB model (3.1) in the sense that an additional exponential factor multiplies the function being convoluted.

### 3.2.2.3 Numerical discretizations

We discretize the fractional Caputo derivatives in Equations 3.1-3.6 through an implicit L1 finitedifference scheme[176]. Therefore, we consider a uniform time-grid with N time-steps of size  $\Delta t$ , such that  $t_n = n\Delta t$ , with n = 0, 1, ..., N. We remark that although the equations for each of the building block models could be discretized utilizing fast schemes[106] and singularity capturing approaches[177], the number of utilized data-points is not large, with  $N^{data} \approx 3\,000$  for the first relaxation and  $N^{data} \approx 25\,000$  for all steps. Also, we avoid the singularity nearby  $t \approx 0$  since the first relaxation step is applied at approximately 80 seconds. Nevertheless, the non-smooth nature of the loading would degenerate most of the existing numerical methods for FDEs, and we found that the employed method in this work with the  $\Delta t$  described in Section 3.3 is sufficient for the accuracy to reach the plateau of the experimental data, such that model error is dominant.

In the following, we present the discretized forms for each of our employed linear fractional viscoelastic models. For more details on the step-by-step discretization of the presented and more complex models (including plasticity), we refer the reader to the work by Suzuki and Zayernouri[175]. Therefore, we have the following stresses for the SB model at  $t = t_{n+1}$ :

$$\sigma_{n+1} = C_1 \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\alpha_1} \varepsilon \right], \qquad (3.13)$$

with constant  $C_1 = \mathbb{E}/(\Gamma(2 - \alpha)\Delta t^{\alpha})$ . For the KV model, we obtain:

$$\sigma_{n+1} = C_1 \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\alpha_1} \varepsilon \right] + C_2 \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\alpha_2} \varepsilon \right], \qquad (3.14)$$

with constants  $C_1 = \mathbb{E}_1/(\Gamma(2 - \alpha_1)\Delta t^{\alpha_1})$  and  $C_2 = \mathbb{E}_2(\Gamma(2 - \alpha_2)\Delta t^{\alpha_2})$ . Finally, for the FM model, we have:

$$\sigma_{n+1} = \frac{C_1 \left[\varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\alpha_1} \varepsilon\right] + C_2 \left[\sigma_n - \mathcal{H}^{\alpha_1 - \alpha_2} \sigma\right]}{1 + C_2},$$
(3.15)

with constants  $C_1 = \mathbb{E}_1/(\Gamma(2 - \alpha_1)\Delta t^{\alpha_1})$  and  $C_2 = (\mathbb{E}_1/\mathbb{E}_2)/(\Gamma(2 - \alpha_1 + \alpha_2)\Delta t^{\alpha_1 - \alpha_2})$ . The history terms  $\mathcal{H}^{\nu}u$  in the above equations are given by the following form:

$$\mathcal{H}^{\nu}u = \sum_{j=1}^{n} b_j \left[ u_{n+1-j} - u_{n-j} \right],$$

with weights  $b_j := (j+1)^{1-\nu} - j^{1-\nu}$ . In the following, we present the nonlinear modeling approach for multiple relaxation steps.

The discretization for the FQLV model (3.12) employed in this work is shown in[175], which is a straightforward, fully-implicit, L1 finite-difference approach with a trapezoidal rule employed on the additional exponential factor. Therefore, the discretized stresses for the FQLV model are given by:

$$\sigma_{n+1} = C_1 \left[ \exp(B\varepsilon_{n+\frac{1}{2}}) \left( \varepsilon_{n+1} - \varepsilon_n \right) + \mathcal{H}^{\alpha} \left( \varepsilon, \frac{\partial \sigma^e}{\partial \varepsilon} \right) \right], \tag{3.16}$$

with constant  $C_1 = EAB/(\Delta t^{\alpha} \Gamma(2 - \alpha))$ . The discretized history load in this case is given by:

$$\mathcal{H}^{\alpha}\left(\varepsilon, \frac{\partial \sigma^{e}}{\partial \varepsilon}\right) = \sum_{k=1}^{n} \exp(B\varepsilon_{n-k+\frac{1}{2}}) \left(\varepsilon_{n-k+1} - \varepsilon_{n-k}\right) b_{k}, \tag{3.17}$$

with  $b_k = (k+1)^{1-\alpha} - k^{1-\alpha}$  and  $\varepsilon_{i+\frac{1}{2}} = (\varepsilon_i + \varepsilon_{i+1})/2$ . The presented discretization has an accuracy of  $O(\Delta t^{2-\alpha})$ , and we refer the reader to [175] for simulations of numerical convergence.

#### 3.2.3 Model optimization

We perform the model fits through a particle-swarm optimization (PSO) algorithm[178], which was implemented in MATLAB. The adopted PSO parameters are a population  $N_{pop} = 30$  and  $N_{it} = 1000$  iterations for the linear cases and  $N_{it} = 100$  iterations for the nonlinear cases. For the linear viscoelastic fits, we set the initial material pseudo-parameter in the  $0 \le \mathbb{E} \le 10^8 [Pa.s^{\alpha}]$ , and the fractional orders are constrained in the 0.0001  $\le \alpha \le 0.9999$  range, to ensure that the employed fractional models are able to recover simpler fractional counterparts and also standard rheological elements, if required by the experimental data. For nonlinear cases, we estimate ranges for parameters *A* and *B* of the FQLV model by fitting the instantaneous stress response (3.11) to each stress peak in every step-strain application of Fig.3.2. From this preliminary estimate, we have obtained parameters in the ranges  $10^4 \le A \le 10^5 [Pa]$  and  $0 \le B \le 2$ , which are taken as input parameter ranges for the PSO algorithm. For the relaxation parameters of the FQLV, as in[10], we note that the nature of the power-law relaxation kernel, it is nontrivial to obtain a normalized  $G(0^+) = 1$ . Nevertheless, for the pseudo-constant we set the range  $0 \le E \le 1$  and for the fractional order  $\alpha$  we employ the same range as the linear case.

Since the stresses  $\sigma^{data}(i)$  and strains  $\varepsilon^{data}(i)$  from the relaxation dataset are non-uniform in time, we perform a linear (first-order accurate) interpolation of the strains  $\varepsilon^{data}(i)$  to an uniform grid. We then utilize the input strains and compute the global best solution for stress for every PSO iteration through (3.13), (3.14), (3.15), or (3.16). Then, we linearly interpolate the stress back to the nonuniform grid to obtain  $\sigma^{model}$ . The time-step size for the uniform grid solution is set to  $\Delta t = 0.495 [s]$ , which is the minimum time interval between two consecutive data-points. We verification purposes, we tested smaller step-sizes ( $\Delta t = 0.0495$ ) and did not obtain improved results. The cost function is defined as:

$$Cost := \sum_{i=0}^{N_{data}} \left( \sigma_i^{data} - \sigma_i^{model} \right)^2.$$
(3.18)

The adopted error measures in this work are the normalized least-squares error (LSE) and root mean squared error (RMSE) between the experimental and mapped simulated stresses, which are

respectively given by:

$$LSE := \frac{\sqrt{\sum_{i=1}^{N_{data}} \left(\sigma_i^{data} - \sigma_i^{model}\right)^2}}{\sqrt{\sum_{i=1}^{N_{data}} \left(\sigma_i^{data}\right)^2}} \times 100\%,$$
$$RMSE := \frac{1}{\max(\sigma^{data})} \sqrt{\frac{\sum_{i=1}^{N_{data}} \left(\sigma_i^{data} - \sigma_i^{model}\right)^2}{N_{data}}} \times 100\%$$

Finally, all numerical simulations were run in a computer system with Intel Xeon Gold 6148 CPUs with 2.40GHz.

# **3.3 Results and Discussion**

#### 3.3.1 Linear Viscoelasticity

Figure 3.5 illustrates the obtained fits for all bladder samples utilizing an SB model, for the first strain step ( $\varepsilon_0 = 0.25$ ). We observe very good fits for most samples, especially at larger time scales, with an exception for the trigone (T) sample due to a sudden stress drop in the experimental data. The fitting quality decreases for all samples at the early relaxation dynamics (nearby the step-strain application), with the SB model underestimating the maximum values of stress peaks. The obtained fractional orders lie in the 0.2 - 0.3 range (*see Table 3.1*), which are similar to the observed long-term power law from the estimated experimental relaxation functions in Fig.3.3. Furthermore, the least-squared errors lie in the 2% - 11% range, while the RMS errors are within the 2% - 4% range. The higher values of the pseudo-constant and fractional order for the trigone sample are likely due to the SB model accounting for both instantaneous and long-term response over its limited set of two parameters. We also note that the FKV model pragmatically recovered the SB model in all instances, where the PSO algorithm obtained optimal values for the fractional orders that are close to the SB model. In addition, the optimal values for one pseudo-constant is either set to zero, or the summation of  $\mathbb{E}_1$  and  $\mathbb{E}_2$  recovers the value of  $\mathbb{E}$  for the SB model. This

indicates the a FKV model does not improve the bladder fit quality, and one would rather employ a SB model with half the amount of material parameters under the same error levels.



Figure 3.5: Obtained linear viscoelastic fits for the fractional SB model for all bladder samples and the first strain step ( $\varepsilon_0 = 0.25$ ).

Figure 3.6 illustrates the obtained fits for the FM model, where the added flexibility of the underlying power-law/Mittag-Leffler relaxation response improves the fitting quality for both short and long time-scales, yielding least squares errors as low as 2.08 %. The obtained parameters in Table 3.1 indicate the presence of a predominantly elastic power-law  $\alpha_1$  in the 0.17 – 0.19 range, and a predominantly viscous  $\alpha_2$  in the 0.74 – 0.99 range. Particularly, the FM model fit for the trigone specimen indicates the recovery of a dashpot element, and thus the corresponding SB element could be replace by a Newton element. Regarding pseudo-constant values, we note that  $\mathbb{E}_1$  values have variations that qualitatively agree with the intensity of stress peaks, but  $\mathbb{E}_2$  values can vary in several orders of magnitude, which could be due to the presence of multiple local minima or the discrepancy between obtained fractional orders  $\alpha_2$ . In general, the dorsal and ventral samples seem to be the most anomalous, as they present both fractional order values sufficiently far from standard elements.

Figure 3.7 illustrates the pointwise relative errors between the SB and FM models and the



Figure 3.6: Obtained linear viscoelastic fits utilizing a fractional Maxwell for all bladder samples and first strain step ( $\varepsilon_0 = 0.25$ ).

experimental data for the first strain step. We notice that the SB element has similar errors as the FM model in the 800 < t < 1200 [s] range and larger errors for longer times for most samples. For shorter time ranges, the SB model has larger errors (up to 1 order of magnitude) for all samples. This reinforces the fact that the FM model is more descriptive of both early and long-term dynamics of bladder relaxation, as the qualitative analysis and estimated experimental relaxation moduli suggest. Furthermore, we also note that the better performance of the FM model is also attributed to better approximating the loading ramp and the peak stress preceding the relaxation behavior.

We also employed more complex fractional linear viscoelastic models, such as fractional Kelvin-Zener, Poynting-Thomson and Burgers' (*see [175] for the models and their corresponding discretizations*). From our employed fitting procedure, all models either recovered or had the same performance as the FM model.

#### 3.3.2 Nonlinear Viscoelasticity

Figure 3.8 illustrates the obtained fits for the fractional QLV model under all consecutive strain steps, where we observe a very good agreement with the experimental data. Except for the trigone

Model	Parameters					Error %		Sample
	$\mathbb{E}_1[kPa.s^{\alpha_1}]$	$\alpha_1$	$\mathbb{E}_2[kPa.s^{\alpha_2}]$	α2	L	S	RMS	2ump10
SB	18.1901	0.226	_	_	4.3	32	1.72	
FKV	15.6574	0.225	2.42019	0.229	4.3	32	1.72	D
FM	14.7616	0.171	3976.90	0.743	2.2	29	0.91	
SB	31.3077	0.219	_	_	3.4	17	1.42	
FKV	31.3462	0.220	0	0.503	3.4	17	1.41	L
FM	26.9311	0.186	48826.1	0.932	2.0	)8	0.82	
SB	41.6335	0.236	_	_	5.3	33	1.98	
FKV	33.2005	0.232	7.95429	0.252	5.3	84	1.99	LB
FM	33.0853	0.183	37339.9	0.935	3.2	23	1.20	
SB	66.7689	0.278	_	_	11	.1	3.82	
FKV	66.4714	0.278	0	0.907	11	.1	3.83	Т
FM	42.4338	0.170	36938.7	0.999	4.0	)5	1.37	
SB	34.9254	0.220	_	_	3.2	21	1.24	
FKV	34.9254	0.220	0	0.579	3.2	21	1.25	V
FM	30.7605	0.188	19799.5	0.797	2.1	9	0.84	

Table 3.1: Obtained material parameters for all employed linear fractional models and UB samples.

sample, all cases had higher deviations towards the final strain steps. Nevertheless, we note that the error levels are below 6% (LSE) and 2% (RMSE) for the entire dataset, under 4 material parameters, which are listed in Table 3.2. Furthermore, the obtained fractional-orders lie in the range 0.24 - 0.3 which are in accordance with the estimated power-laws in our *a-priori* analysis presented in Fig.3.3. Particularly, the lowest fractional order was obtained for the trigone specimen, and highest for the dorsal one. A slightly higher degree of nonlinearity is also recovered for the trigone and lower-body samples due to the larger values of *B*.

Finally, Figure 3.9 illustrates the pointwise relative errors for the FQLV model under all bladder samples and strain steps. We observe a similar error behavior as the SB model in Fig.3.7, particularly for larger applied strains.



Figure 3.7: Obtained pointwise errors for the linear SB and FM models for the first strain step: (*a*) D, (*b*)) L, (*c*) LB, (*d*) T, (*e*) V.



Figure 3.8: Obtained fits for the fractional QLV model under all strain steps: (*a*) D, (*b*)) L, (*c*) LB, (*d*) T, (*e*) V. The fit quality was very good for all bladder samples, with more significant deviations occuring on strain steps 4 and 5. The recovered fractional-orders in (*f*) are within the  $0.2 < \alpha < 0.3$  range, which is in accordance with the *a-priori* power-laws obtained from the relaxation moduli data in Fig.3.3.

Sample		Err	Error %			
Sumpre	A[kPa]	В	$E[s^{\alpha}]$	α	LSE	RMSE
D	53.8823	0.7803	0.7298	0.2928	4.85	1.11
L	79.1646	0.8823	0.5677	0.2673	4.08	1.00
LB	74.5369	1.2192	0.3463	0.2510	4.17	1.00
Т	63.4435	1.2642	0.3590	0.2419	5.61	1.44
V	59.3282	0.9449	0.6704	0.2732	4.74	1.16

Table 3.2: Obtained material parameters for the FQLV model with all UB samples.



Figure 3.9: Obtained pointwise errors for the FQLV model under all strain steps: (a) D, (b)) L, (c) LB, (d) T, (e) V. The vertical gray lines represent the step strain application instants.

## 3.3.3 Discussion

To our best understanding, this was the first work in the literature addressing fractional visco-elastic modeling to bladder tissues. From the results obtained for our building block models, the overall lower range of fractional orders obtained for all linear/nonlinear models is 0.17 - 0.3, indicating a predominantly elastic yet highly anomalous behavior with smaller decay rates at long times, *i.e.*, the presence of far-from-equilibrium dynamics. A similar parametric range was obtained in other anomalous systems such as arterial wall relaxation[10], aortic valve tissue[169], 1D and 3D brain

artery walls under fluid-structure interactions[179, 180], canine and bovine liver tissue[181, 182], and lung tissue[11]. As suggested by Doehring *et al.* [169], small  $\alpha$ -values can be indications of strong fractality in bio-tissue microstructure such as collagen fibers, which are vastly present in the UB, and particularly with a larger network in the trigone region. The larger values of fractional orders  $\alpha_2$  in the 0.74 – 0.99 range obtained by the fractional Maxwell model is similar to those obtained for brain tissue relaxation[183] and human ear[184]. This indicates a significantly more dissipative behavior, possibly compensating the highly-anomalous behavior provided by the smaller fractional order  $\alpha_1$  for short time-scales, and thus better fitting the slower relaxation nearby the load application. The transitional behavior from slower-to-faster relaxation slopes observed from the UB specimens and captured by the FM model were also noticed in bio-tissues composed of weakly cross-linked collagen networks [173]. We note that although the captured fractional orders  $\alpha_1$ ,  $\alpha_2$  for the FM model on the UB relaxation do not quantitatively match the slopes  $\beta_1$ ,  $\beta_2$  for  $G^{data}(t)$  in Fig.3.3, these fractional orders refer to the asymptotic behaviors at  $t \to 0$  and  $t \to \infty$ , as illustrated in our existence study in Fig.3.4, and it is likely that relaxation experiments under a larger range of time-scales would yield a better quantitative agreement. For the purpose of our existence study, we consider a qualitative agreement and small error levels to be sufficient to select a valid candidate building block model.

The nonlinear visco-elastic behavior was well approximated by the employed FQLV model, which decomposes the relaxation kernel in a multiplicative fashion into a power-law reduced relaxation function and a tangent elastic stiffness described by an exponential elastic stress form. This allowed the nonlinear part of our existence study to capture the complex rheology of the UB with large applied strains (up to 200%) and RMS errors as low as 1%. In fact, Jokandan *et al.*[185] observed an exponential-like stress-strain response in quasi-static tensile testing of porcine bladder samples. Specifically, under relaxed states, the entangled configuration of collagen fibers yield a linear stress strain relationship, but a nonlinear regime with much higher stress levels is attained once the fibers align with the load direction and store most of the strain energy in the system. Korossis *et al.*[136] attributed the linear region to be predominantly driven by elastin, and the

nonlinear phase by collagen.

Our pointwise relative error analysis reinforced the idea that the FM model is more descriptive of both slower early dynamics of the porcine bladder, but also the faster dynamics observed at longer time-scales in the estimated experimental relaxation modulus. In our error analysis for the nonlinear case, Fig.3.9 indicates a similar qualitative error behavior between the FQLV model and the linear SB element in Fig.3.7, especially towards the larger strain regime, with higher errors in the small and large times after the step-strain applications. This suggests that coupling a fractional Maxwell-type reduced relaxation function to the existing framework would very likely improve our results for the nonlinear case as it did in the linear one.

Regarding our developed framework, the existence study proved to be interesting to identify the most proper fractional linear visco-elastic model for stress relaxation, which can later inform the fractional quasi-linear viscoelastic model on the proper form of the reduced relaxation function. For the UB, we conclude that while the SB, FKV and FM models yield errors in the same order of magnitude, the FM model better captures the two power-law qualitative behavior of the data, which is fundamental for both short- and long-term predictions of tissue response. Nevertheless, the SB model provided satisfactory results for the observed experimental time-scale, and the FKV model proved to be redundant and a source of ill-posedness in a model selection framework, since it obtained the same performance as the SB model with twice as many parameters. Although we cannot guarantee that the obtained model parameters provide a global minimum for the cost function (3.18), we find our obtained fitting errors, increased number of material parameters, and diverging qualitative behaviors between the experimental data in Fig.3.3 and the FKV relaxation behavior from Fig.3.4 to be sufficient to exclude the FKV as a viable candidate for the UB. The same analysis applies to other tested models not shown here, such as fractional Kelvin-Zener, fractional Poynting-Thomson and fractional Burgers' models[175], which consistently recovered the FM model.

Regarding potential improvements, anisotropy of bladder samples has been observed in existing studies[137], and therefore an interesting step would be to map the variation of fractional-orders for

distinct sample orientations. Based on the obtained linear and nonlinear results, another interesting aspect would be to incorporate a fractional Maxwell-type relaxation function to the fractional QLV framework, similar to Doehring *et al.*[169] to better describe the initial relaxation process in each strain step. However, due to the larger number of time-steps required by our dataset, an efficient numerical method would be required to handle the resulting differ-integral with a Miller-Ross relaxation kernel, or the FQLV framework would need to be developed in differential form, likely as a system of equations comprised of an FDE solving for elastic stresses and a separate equation for nonlinear elasticity. Finally, biaxial tests and models would give insight in the effects of shear stress to the tissue behavior, and confronting creep predictions with experiments would allow one to verify the consistency of the obtained parameters, as already succesfully done with other anomalous materials[24].

#### **CHAPTER 4**

### FRACTIONAL VISCO-ELASTO-PLASTIC MODELS FOR STRUCTURAL ANALYSIS

## 4.1 Background

Fractional differential operators appear in many systems in science and engineering such as visco-elastic materials [171, 186, 187], electrochemical processes [188] and porous or fractured media [189]. For instance, it has been found that the transport dynamics in complex and/or disordered systems is governed by non-exponential relaxation patterns [7, 190]. For such processes, a time-fractional equation, in which the time-derivative emerges as  $\mathcal{D}_t^{\gamma} u(t)$ , appears in the continuous limit. One interesting application of fractional calculus is to model complex elasto-plastic behavior of engineering materials (e.g. [191, 192]). Recently, fractional calculus has been employed as an effective tool for modelling materials accounting for heterogeneity/multi-scale effects to the constitutive model [64–66], where the fractional visco-plasticity was introduced as a generalization of classical visco-plasticity of Perzyna type [193]. The fundamental role of the formulation is the definition of the flow rule by introducing a fractional gradient of the yield function. Also, a constitutive model for rate-independent plasticity based on a fractional continuum mechanics framework accounting for nonlocality in space was developed in [194].

Formulating fast and accurate numerical methods for solving the resulting system of fractional ODEs/PDEs in such problems is the key to incorporating such nonlocal/history-dependent models in engineering applications. Efficient discretization of the fractional operators is crucial. Lubich [86, 88] pioneered the idea of *discretized fractional calculus* within the spirit of finite difference method (FDM). Later, Sanz-Serna [195] adopted the idea of Lubich and presented a temporal semi-discrete algorithm for partial integro-differential equations, which was first order accurate. Sugimoto [196] also employed a FDM for approximating the fractional derivative emerging in Burgers' equation. Later on, Gorenflo et. al. [197] adopted a finite-difference scheme by which they could generate discrete models of random walk in such anomalous diffusion. Diethelm et

al. proposed a predictor-corrector scheme in addition to a fractional Adams method [94, 108]. After that, Langlands and Henry [198] considered the fractional diffusion equation, and analyzed the  $L^1$  scheme for the time-fractional derivative. Sun and Wu [199] also constructed a difference scheme with  $L^{\infty}$  approximation of the time-fractional derivative. Of particular interest, Lin and Xu [91] analyzed a FDM for the discretization of the time-fractional diffusion equation with order  $(2 - \alpha)$ . However, there are other classes of global methods (spectral and spectral element methods) for discretizing fractional ODEs/PDEs (e.g., [95–97, 200]), which are efficient for low-to-high dimensional problems. Furthermore, Zayernouri and Matzavinos developed a fractional family of schemes, called *fractional Adams-Bashforth and fractional Adams-Moulton* method for high-order explicit and implicit treatment of nonlinear problems [201]. There were recent developments on meshless approaches applied to fractional-diffusion and space-fractional advection-dispersion problems [202, 203]. Also, Chen [204] developed a new definition of fractional Laplacian and applied to three-dimensional, nonlocal heat conduction.

The main contribution of the present work is to propose and solve two fractional-order models, namely M1 and M2, for uniaxial large strains and visco-elasto-plastic behavior of materials. Both models account for fractional visco-elastic modeling by defining a stress-strain relationship involving the Caputo time derivative of fractional-order, but have distinct formulations to model the fractional visco-plasticity. For the model M1, visco-plasticity is achieved by including history effects in time for the internal hardening parameter in the yield function, making it rate-dependent. Differently from some works found in the literature [64–66], we do not modify the flow rule. The model M2 accounts for a rate-independent yield function without an internal hardening parameter, and the visco-plastic effect is achieved based on the approach of *visco-plastic regularization* used in the classical visco-plastic model of Duvaut-Lions type (which is equivalent to Perzyna's model). Furthermore, the models consider different memory effects for visco-elasticity and visco-plasticity. Both models are used within the framework of a time-fractional backward-Euler integration procedure with a *fractional return-mapping algorithm*, based on the classical models in the literature [191, 192]. The developed algorithm seamlessly generalizes the standard return-mapping algorithm to its fractional counterpart, making it amenable for path-dependent visco-elasto-plastic analyses in engineering and bio-engineering applications. We also present the standard nonlinear finite element formulation for trusses and show that the only required modifications are in the stress update procedure, which will be described in constitutive boxes for each model.

Several numerical analyses are performed to investigate the behavior of the models. We test the algorithms presented in terms of convergence using a benchmark solution, then we perform tests with cyclic strains to account for hysteresis behavior. Both models are implemented in the context of finite element method (FEM) using an updated Lagrangean approach to solve a two-bar snap-through problem. Because no analytical solutions are derived, we implemented the classical one-dimensional models for elasto-plasticity with linear hardening and visco-plasticity of Duvaut-Lions type, and we recover these limit cases for verification. We verify that both fractional-order models recover the classical rate-independent elasto-plastic behavior with the variation of the fractional-order parameters. The obtained results show the flexibility of the fractional-order models to describe the rate-dependent hardening and viscous dissipation. This motivates the application of the models developed in this work to identify material parameters of complex constitutive laws of engineering materials and biological tissues.

# 4.2 Kinematics of Large Visco-Elasto-Plastic Deformations

Consider the truss element with nodes 1, 2 illustrated in Figure 4.1a for the initial configuration at time t = 0, with coordinates vectors  $\mathbf{X}_1$ ,  $\mathbf{X}_2$ , length L, area A and volume V. The updated configuration at time t is denoted with the current coordinates  $\mathbf{x}_1$ ,  $\mathbf{x}_2$ , area a, volume v and normal vector  $\mathbf{n}$ . The terms  $\mathbf{u}_1$ ,  $\mathbf{u}_2$  represent the nodal displacement vectors from the updated configuration at time t to a new configuration taking place at time t + dt. Figure 4.1b shows the multiplicative decomposition of the stretch  $\lambda$  into visco-elastic  $\lambda^{ve}$  and visco-plastic  $\lambda^{vp}$  parts, with the latter accounting for a visco-plastic updated length  $l^{vp}$ .



Figure 4.1: (a) Kinematics of the truss in terms of initial and updated configurations; (b) Multiplicative decomposition of the stretch into visco-elastic and visco-plastic parts, taking place from the initial to the updated configuration.

The updated length l and normal unit vector **n** are given by [205]

$$l = \sqrt{(\mathbf{x}_2 - \mathbf{x}_1) \cdot (\mathbf{x}_2 - \mathbf{x}_1)}, \quad \mathbf{n} = \frac{\mathbf{x}_2 - \mathbf{x}_1}{l},$$
 (4.1)

where the updated coordinates of the element nodes are denoted as

$$\mathbf{x}_1 = \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}, \quad \mathbf{x}_2 = \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}. \tag{4.2}$$

We consider the decomposition of the stretch illustrated in Figure 4.1b for the truss element when subject to a change in configuration. The visco-elastic and visco-plastic stretches are given by

$$\lambda^{ve} = \frac{l}{l^{vp}}, \quad \lambda^{vp} = \frac{l^{vp}}{L}.$$
(4.3)

The total stretch is given by

$$\lambda = \lambda^{\nu e} \lambda^{\nu p} = \frac{l}{L}.$$
(4.4)

Applying the natural logarithm to the above equation, we obtain an additive decomposition given by [191]

$$\ln(\lambda) = \ln(\lambda^{\nu e}) + \ln(\lambda^{\nu p}), \tag{4.5}$$

which is called logarithmic strain and is usually denoted as

$$\varepsilon = \varepsilon^{\nu e} + \varepsilon^{\nu p}. \tag{4.6}$$

The logarithmic strain measure defined in Eq.4.5 is thermodynamically conjugate to the Kirchhoff stress  $\tau$  [191], which will be addressed in the next section, along with the constitutive equations for the visco-elasto-plastic models.

# 4.3 Fractional-Order Visco-Elasto-Plastic Models

We consider two visco-elasto-plastic models, called M1 and M2. The developed framework for both models incorporates memory effects for the evaluation of visco-elasto-plastic large strains. We present the mathematical formulation for each model and an efficient algorithm to solve the nonlinear system of fractional-order differential equations, and remark on how the models recover the classical local models.

To account for the memory effects in time, we modify the classical models presented in the literature [191, 192]. The model M1 is a modification of classical elasto-plasticity with linear hardening and the model M2 is a modification of visco-plasticity of Duvaut-Lions type. For this purpose, we introduce Scott-Blair elements with fractional-order  $\beta$ , which interpolate between linear spring when  $\beta \rightarrow 0$  and viscous Newton element when  $\beta \rightarrow 1$  [171].

The memory effects for both models will be presented in the stress-strain relationship regarding the visco-elastic part, which is evaluated for the entire time domain. To account for memory effects in visco-plasticity, we will consider the Caputo time-fractional derivative in the yield function for the model M1, while for the model M2 we will incorporate the memory effects via a separate equation that describes the *visco-plastic regularization*. The memory for the fractional derivatives describing visco-plasticity will be considered starting from the last attained yield stress.

#### 4.3.1 Model M1

The model M1 is illustrated in Figure 4.2a, consisting of a Scott-Blair element with constant  $E[Pa.s^{\beta E}]$  and a fractional-order  $\beta_E$  for the visco-elastic part with corresponding visco-elastic

strain  $\varepsilon^{ve}$ . The visco-plastic device consists of a parallel combination of a Coulomb frictional element with yield stress  $\tau^{Y}[Pa]$ , a linear hardening spring with constant H[Pa], a Scott-Blair element with constant  $K[Pa.s^{\beta K}]$  and fractional-order  $\beta_{K}$ . The corresponding visco-plastic strain is denoted by  $\varepsilon^{vp}$ . The term  $\tau[Pa]$  stands for the Kirchhoff stress. We start by rewriting Eq.4.6 in



Figure 4.2: Visco-elasto-plastic model M1. (a) Constitutive diagram with the rheological elements for visco-elasticity and visco-plasticity. (b) Stress versus strain response described by the yield function (Eq.4.12), showing the expansion of the visco-elastic boundary from  $\partial E_{\tau}$  (point A) to  $\partial E_{\tau}^{*}$  (point B) after exceeding the yield stress.

terms of the visco-elastic strain component:

$$\varepsilon^{ve} = \varepsilon - \varepsilon^{vp}. \tag{4.7}$$

The history-dependent constitutive law for this model is assumed to be of the form:

$$\tau = E \ {}_{0}^{C} \mathcal{D}_{t}^{\beta E}(\varepsilon^{\nu e}) = E \ {}_{0}^{C} \mathcal{D}_{t}^{\beta E}(\varepsilon - \varepsilon^{\nu p}), \qquad 0 < \beta_{E} < 1.$$
(4.8)

To satisfy the homogeneous initial conditions for the Caputo time derivative, we assume the given point of the material to have no initial strains, that is,  $\varepsilon(t = 0) = \varepsilon^{ve}(t = 0) = \varepsilon^{vp}(t = 0) = 0$ . In this sense, we observe that the Riemann-Liouville definition (Eq.1.2) could also be employed, since we consider homogeneous initial conditions. To designate a set of admissible stresses, we define the following closed convex stress space:

$$\mathbb{E}_{\tau} = \{ \tau \in \mathbb{R} \mid f(\tau, \alpha) \le 0 \}, \tag{4.9}$$

where  $f : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$  represents the yield condition, defined by

$$f(\tau, \alpha) := |\tau| - \left[\tau^{y'} + H\alpha\right],\tag{4.10}$$

where

$$\tau^{y\prime} = \tau^{y} + K {}^{C}_{tp} \mathcal{D}^{\beta_K}_t(\alpha), \qquad 0 < \beta_K < 1,$$

$$(4.11)$$

with  $\alpha$  representing an internal hardening variable with initial condition  $\alpha(t = 0) = 0$ , that is, we assume no initial hardening. The term  $\tau^y$  denotes a yield stress which is updated according to unloading conditions ( $\tau^y = \tau^Y$  in the beginning of the process) and  $t_p$  denotes the time of onset of plasticity. The term  $\tau^{y'}$  in Eq.4.11 can be interpreted as an updated yield stress accounting for memory effects in visco-plasticity, while the term  $H\alpha$  represents a local hardening parameter.

The time  $t_p$  for plasticity is reset when we unload the material from a visco-plastic state, and the yield stress is updated to a new value  $\tau^{y'}$ . Substituting Eq.4.11 into Eq.4.10, we obtain

$$f(\tau,\alpha) := |\tau| - \left[\tau^{y} + K {}_{tp}^{C} \mathcal{D}_{t}^{\beta K}(\alpha) + H\alpha\right].$$
(4.12)

We do not consider different time derivative limits for Eq.4.8 because plastic strains inevitably take place in the visco-elastic range. Notice that we included the Caputo derivative of order  $\beta_K$ inside  $f(\tau, \alpha)$ , thus making the yield condition rate-dependent. The corresponding boundary of  $\mathbb{E}_{\tau}$ is the convex set denoted by  $\partial \mathbb{E}_{\tau}$ , given as

$$\partial \mathbb{E}_{\tau} = \{ \tau \in \mathbb{R} \mid f(\tau, \alpha) = 0 \}, \tag{4.13}$$

where  $f(\tau, \alpha) = 0$  is the so-called *consistency condition* in the classical elasto-plastic models. In the present model, we assume that the hardening is isotropic in the sense that at any state of loading the center of  $\mathbb{E}_{\tau}$  remains at the origin of the stress-strain domain. The expected stress versus strain response based on Eqs.4.12 and 4.13 is presented in Figure 4.2b. The consistency condition (Eq.4.13) will be addressed in incremental form in time to derive the visco-plastic solutions. Moreover, similar to classical elasto-plasticity, the evolution of hardening is assumed to be linear in terms of the visco-plastic strain rate. Therefore

$$\dot{\alpha} = |\dot{\varepsilon}^{\nu p}|,\tag{4.14}$$

and the flow rule is not modified, and is given by

$$\dot{\varepsilon}^{vp} = \gamma \operatorname{sign}(\tau), \tag{4.15}$$

where  $\gamma$  denotes the amount of plastic slip, also with initial condition  $\gamma(t = 0) = 0$ , and the term  $\operatorname{sign}(\tau)$  represents the direction of the plastic flow. Recalling Eq.4.12 and the definition of the fractional derivative, when  $\beta_K \to 0$ , we recover the limit case without rate effects (spring) and the constant *K* accounts for the standard plastic modulus of rate-independent plasticity, with units of [*Pa*]. On the other hand, if  $\beta_K \to 1$  we recover the limit case of a local integer-order derivative (dashpot), where *K* would be equivalent to the material viscosity  $\eta$ , with corresponding units of [*Pa.s*].

### 4.3.2 Model M2

The schematic diagram of the model M2 is illustrated in Figure 4.3a, which consists of the same elements as the model M1, except that we remove the linear hardening spring with constant H in the visco-plastic part.



Figure 4.3: Visco-elasto-plastic model M2 considering visco-plastic regularization. (a) Constitutive diagram with the rheological elements for visco-elasticity and visco-plasticity. (b) Stress versus strain response: path A-B described by the yield function (Eq.4.16), which is visco-elastic perfectly plastic; path A-B' with the stress response after the visco-plastic regularization (V-P-R) procedure (Eq.4.18). The relaxation path B'-B occurs at constant strain levels and  $t \rightarrow \infty$  (compared to the relaxation time of the material).

The stress-strain relation for this model is the same as Eq.4.8. We consider the yield function of perfect plasticity given by

$$f(\tau) := |\tau| - \tau^{y'},$$
 (4.16)

where we consider the yield stress  $\tau^{y'} = \tau^{Y}$  when t = 0 and update it when the material is unloaded from visco-plastic behavior (more details will be addressed in Section 4.5). Because the model is based on visco-plasticity of Duvaut-Lions type, we use the idea of *visco-plastic regularization* in [192] to take into account the memory effect of the visco-plastic strain  $\varepsilon^{vp}$  when we obtain an over-stressed level  $f(\tau) > 0$ :

$$K {}_{tp}^{C} \mathcal{D}_{t}^{\beta K}(\varepsilon^{\nu p}) = \tau - \tau_{\infty}, \qquad (4.17)$$

where  $\tau_{\infty}$  is the relaxed stress when  $t \to \infty$  (compared to the natural relaxation time of the material). Substituting the stress-strain relation from Eq.4.8 into Eq.4.17, and rearranging the visco-plastic strains to the left-hand-side, we obtain

$$E {}^{C}_{0}\mathcal{D}^{\beta E}_{t}(\varepsilon^{\nu p}) + K {}^{C}_{tp}\mathcal{D}^{\beta K}_{t}(\varepsilon^{\nu p}) = E {}^{C}_{0}\mathcal{D}^{\beta E}_{t}(\varepsilon) - \tau_{\infty}.$$
(4.18)

The solution for this model involves determination of the rate-independent stress  $\tau_{\infty}$  by applying the consistency condition to Eq.4.16 and substituting the result into Eq.4.18 to determine the viscoplastic strains  $\varepsilon^{\nu p}$ . After that, the time-dependent stress can be determined from the constitutive relation (Eq.4.8). Figure 4.3b presents the stress versus strain response in the relaxed state (path O-A-B) described by the yield function (Eq.4.16) and the regularized state (path O-A-B') achieved with Eq.4.18. More details about this procedure will be presented after the time discretization scheme. We note that when  $\beta_K \rightarrow 1$  in Eq.4.18 we recover the local first-order derivatives and therefore the classical Duvaut-Lions formulation.

#### **4.3.2.1** Remark about parameter *H*

We note that when we set the linear hardening parameter H = 0 in the model M1, we obtain the same diagram for both models. However, the approaches are still different, since the model M1 considers the Caputo-time fractional derivative in the yield function (Eq.4.12) while the model M2 uses a yield function of visco-elastic perfectly plastic behavior and accounts for visco-plastic regularization with relaxation effects described by Eq.4.17.

#### 4.3.2.2 Remark about visco-elastic/plastic memory effects

The initial study of the presented models considered the entire time domain for the visco-plastic equations (4.12, 4.18) without updating the yield stress  $\tau^y$ . However, for model M1 it was observed that due to long memory effects and no update in the yield stress, the visco-elastic range did not expand in a isotropic way when cyclic loads were applied. Furthermore, for the model M2, we obtained non-physical results for the visco-plastic part without updating the yield stress  $\tau^{y'}$  due to lack of internal hardening combined with long memory on visco-plastic strains.

We consider the distinction between "visco-elastic time" and "visco-plastic time" a more natural way of treating the memory effects, since in a general problem the material will not be in a visco-plastic state (Eqs.4.13 and 4.18) at all times. On the other hand, the stress-strain relation (Eq.4.8) is used regardless of the stress state.

# 4.4 Time Integration and Discretization in Space

For notation purposes, we denote variables at times  $t_n$ ,  $t_{n+1}$  by the lower-scripts n, n+1, respectively. The governing equations on the equilibrium of a truss are discretized in time and space to obtain (e.g., see [206])

$$\psi_{n+1} = \mathbf{M} \left[ b_1 \left( \mathbf{u}_{n+1} - \mathbf{u}_n \right) - b_2 \mathbf{v}_n - b_3 \mathbf{a}_n \right] + \mathbf{R}_{n+1} - \mathbf{P}_{n+1} = \mathbf{0}, \tag{4.19}$$

where we denote  $\psi_{n+1}$  as the residual force vector, **M** as the global mass matrix for all nodes,  $\mathbf{R}_{n+1}$  as the global internal force vector dependent of the updated configuration with coordinates  $\mathbf{x}_{n+1}$ , which in turn depend on the displacements  $\mathbf{u}_{n+1}$ . The term  $\mathbf{P}_{n+1}$  represents the global external nodal force vector. The terms  $\mathbf{a}_n$  and  $\mathbf{v}_n$ , respectively, denote the global acceleration and velocity vectors. More details regarding the Newmark scheme are presented in A.2 with the description of the approximation coefficients  $b_i$ . We do not consider a linear damping matrix in Eq.4.19 because the constitutive law will naturally introduce damping effects for both visco-elastic/plastic contributions.

We note that our approach can be employed in the context of any standard numerical method

e.g., finite element method (FEM), spectral element methods, etc. This is particularly true because our history-dependent modeling results in a system of time-fractional equations. Hence, the spatial domain can be always treated using available standard discretizations. However, the computation of the incremental stresses needs special care as shown in the sequel.

The equilibrium system (Eq.4.19) is linearized by employing Newton's method using incremental global displacements, defined as

$$\mathbf{u}_{n+1}^{k+1} = \mathbf{u}_{n+1}^{k} + \Delta \mathbf{u}.$$
 (4.20)

Accordingly, the updated global coordinates are given by

$$\mathbf{x}_{n+1}^{k+1} = \mathbf{x}_n + \mathbf{u}_{n+1}^{k+1}, \tag{4.21}$$

where the superscript k + 1 refers to the current iteration of the Newton's method. The linearized form of Eq.4.19 in the direction of a displacement increment  $\Delta \mathbf{u}$  is given by the following system of equations:

$$\left[b_1\mathbf{M} + \mathbf{K}_{T_{n+1}}^k\right]\Delta \mathbf{u} = -\mathbf{M}\left[b_1(\mathbf{u}_{n+1}^k - \mathbf{u}_n) - b_2\mathbf{v}_n - b_3\mathbf{a}_n\right] - \mathbf{R}_{n+1}^k + \mathbf{P}_{n+1}.$$
(4.22)

The terms  $\mathbf{u}_n$ ,  $\mathbf{v}_n$ ,  $\mathbf{a}_n$  are obtained from the last converged time step *n*. The term  $\mathbf{K}_T$  is the *tangent stiffness matrix* and is updated at each iteration *k* along with the internal force vector. In the linear finite element spatial discretization, the element tangent stiffness for the current formulation is given by (see [191])

$$\mathbf{K}_{T}^{(e)} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix},$$
(4.23)

with,

$$\mathbf{K}_{11} = \frac{K_C}{l^3} \begin{bmatrix} (x_2 - x_1)^2 & (x_2 - x_1)(y_2 - y_1) \\ (x_2 - x_1)(y_2 - y_1) & (y_2 - y_1)^2 \end{bmatrix} + \frac{a\sigma}{l} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$
(4.24)

where the superscript <sup>(e)</sup> denotes the local elemental operation associated with the *e*-th element, and  $\mathbf{K}_{22} = \mathbf{K}_{11}, \quad \mathbf{K}_{12} = \mathbf{K}_{21} = -\mathbf{K}_{11}.$  The term *l* denotes the current element length,  $x_1, x_2, y_1, y_2$  denote the element updated coordinates,  $\sigma$  denotes the Cauchy stress at the element, and  $K_C$  is given by

$$K_C = a \frac{V}{v} \frac{\partial \tau}{\partial \varepsilon} - 2a\sigma.$$
(4.25)

The relation between the Kirchhoff and Cauchy stresses is given by  $\tau = \frac{v}{V}\sigma$ . We note that there is no assumption in the constitutive behavior, therefore the formulation presented in this section is general. The local stress derivative in terms of strain in Eq.4.25 is known as *tangent modulus*, and its computation will be addressed in the next section. Notice that this derivative is local in nature, and comes from the linearized kinematics of the problem. The elemental internal force vector and the corresponding mass matrix are given by

$$\mathbf{R}^{(e)} = \frac{a\sigma}{l} \begin{vmatrix} x_2 - x_1 \\ y_2 - y_1 \\ x_1 - x_2 \\ y_1 - y_2 \end{vmatrix}, \quad \mathbf{M}^{(e)} = \frac{\rho AL}{6} \begin{vmatrix} 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \end{vmatrix},$$
(4.26)

where  $\rho$  is the material density. In the next section we determine the current stress  $\tau_{n+1}$  and tangent modulus  $\left(\frac{\partial \tau}{\partial \varepsilon}\right)_{n+1}$  for the fractional-order models.

# 4.5 Fractional Return-Mapping Algorithms

We present the time-fractional backward-Euler integration procedure for both fractional models, where a trial state is defined by freezing the internal variables and a fractional return-mapping algorithm is obtained enforcing the proper conditions. For the model M1, the solution for the plastic slip is given by a fractional-order differential equation. For the model M2 we solve a fractional-order differential equation for the visco-plastic strain instead, using the idea of visco-plastic regularization.

The backward-Euler procedure is implicit in time, unconditionally stable and is first-order accurate. We assume that at time  $t_{n+1}$ , with  $t \in [0, T]$  all variables for the previous time step  $t_n$ are known. We consider a strain increment  $\Delta \varepsilon_n$ , which in the context of the standard finite element method, can be obtained using Eqs.4.4 and 4.5 from an increase in element length  $\Delta l$ , calculated from the displacement increments  $\Delta \mathbf{u}$  (Eq.4.22). From the constitutive model point of view, we just consider this increment to be known, regardless of being prescribed or obtained by the equilibrium of the system. The strain for time  $t_{n+1}$  is given by

$$\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_n. \tag{4.27}$$

The stress-strain relation is given by

$$\tau_{n+1} = E \left. {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \left( \varepsilon - \varepsilon^{v p} \right) \right|_{t=t_{n+1}}.$$
(4.28)

The incremental flow rule and evolution of the hardening parameter are, respectively, given by

$$\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \Delta\gamma \operatorname{sign}\left(\tau_{n+1}\right), \qquad (4.29)$$

$$\alpha_{n+1} = \alpha_n + \Delta \gamma, \tag{4.30}$$

where  $\Delta \gamma$  denotes the plastic slip for the time interval  $[t_n, t_{n+1}]$  under consideration. In our fractional return-mapping algorithm, we make use of the so called *trial state*, where we freeze the internal variables of the model at time  $t_{n+1}$  in the following way:

$$\varepsilon_{n+1}^{vp^{trial}} = \varepsilon_n^{vp}, \quad \alpha_{n+1}^{trial} = \alpha_n.$$
(4.31)

Having the trial visco-plastic strain defined, we perform a trial visco-elastic stress given by

$$\tau_{n+1}^{trial} = E \left[ {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \left( \varepsilon - \varepsilon^{v p^{trial}} \right) \right|_{t=t_{n+1}},$$
(4.32)

where we will keep the term  $\varepsilon^{vp}^{trial}$  instead of  $\varepsilon_n^{vp}$  for notation purposes, since the time-fractional Caputo derivative is evaluated at time  $t_{n+1}$ . The trial state defined in Eq.4.31 will be substituted in the discrete form of the fractional Caputo derivatives, which is presented in Section 4.5.1. The result of Eq.4.32 is applied in a trial yield function  $f_{n+1}^{trial}$  in order to check if the stress state lies within the visco-elastic or over the visco-plastic ranges, and perform the return-mapping procedure if necessary.

The current visco-plastic reference time is denoted here as  $t_{p_{n+1}}$ , and is updated when a new yield stress is achieved from cyclic behavior. We introduce an auxiliary notation to track this

visco-plastic time by using an incremental variable  $p_{n+1}$ . The initial value is considered to be  $p_0 = 0$ . In the incremental procedure, we account for the current time step  $p_{n+1} = 0$  if the state is visco-elastic. The value  $p_{n+1} = n + 1$  is set when the stress state exceeds the yield stress, coming from a visco-elastic state. When the stress state is an increasing visco-plastic state (without change of load direction), the visco-plastic time reference is the same as the previous step, that is,  $p_{n+1} = p_n$ .

## 4.5.1 Algorithm for the model M1

The yield function (Eq.4.12) at time  $t_{n+1}$  is given by

$$f_{n+1} = |\tau_{n+1}| - \left[\tau^{y} + H\alpha_{n+1} + K {}_{tp}{}_{n+1}^{C} \mathcal{D}_{t}^{\beta K}(\alpha) \Big|_{t=t_{n+1}}\right].$$
(4.33)

Considering the definition of the trial state, we obtain

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - \left[\tau^{y} + H\alpha_{n} + K_{tp_{n}}^{C} \mathcal{D}_{t}^{\beta_{K}}\left(\alpha^{trial}\right)\Big|_{t=t_{n+1}}\right], \tag{4.34}$$

where the Caputo time-fractional derivative of  $\alpha^{trial}$  is taken starting from time  $t_{pn}$ , because it is the available information about the last known yield stress  $\tau^y$ . If  $f_{n+1}^{trial} \leq 0$  we are within the visco-elastic range. Otherwise, we have an inadmissible stress indicating the onset of viscoplasticity. We enforce the discrete consistency condition  $f_{n+1} = 0$  to obtain the solution for  $\Delta \gamma$  and then to perform a projection of the trial stress onto the yield surface, as illustrated in Figure 4.4. Substituting Eq.4.29 into Eq.4.28, and recalling Eq.4.32, we obtain

$$\tau_{n+1} = \tau_{n+1}^{trial} - E \left[ {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \left( \Delta \gamma \right) \right|_{t=t_{n+1}} \operatorname{sign} \left( \tau_{n+1} \right).$$
(4.35)

We can rewrite the above equation as

$$|\tau_{n+1}| \operatorname{sign}(\tau_{n+1}) = |\tau_{n+1}^{trial}| \operatorname{sign}(\tau_{n+1}^{trial}) - E \left[ {}^{C}_{0} \mathcal{D}_{t}^{\beta E} \left( \Delta \gamma \right) \right|_{t=t_{n+1}} \operatorname{sign}\left(\tau_{n+1}\right),$$
(4.36)

hence,

$$\left[\left|\tau_{n+1}\right| + E \mathop{}_{0}^{C} \mathcal{D}_{t}^{\beta E}\left(\Delta\gamma\right)\Big|_{t=t_{n+1}}\right] \operatorname{sign}(\tau_{n+1}) = \left|\tau_{n+1}^{trial}\right| \operatorname{sign}(\tau_{n+1}^{trial}).$$
(4.37)
The terms inside the brackets must be positive since  $\Delta \gamma > 0$  and E > 0, and therefore

$$\operatorname{sign}(\tau_{n+1}) = \operatorname{sign}(\tau_{n+1}^{trial}). \tag{4.38}$$

Substituting Eqs. 4.35 and 4.30 into Eq.4.33 and recalling Eqs. 4.34 and 4.38, yields

$$f_{n+1} = f_{n+1}^{trial} - H\Delta\gamma - E {}_{0}^{C} \mathcal{D}_{t}^{\beta E} (\Delta\gamma) \Big|_{t=t_{n+1}} - K {}_{tp_{n+1}}^{C} \mathcal{D}_{t}^{\beta K} (\Delta\gamma) \Big|_{t=t_{n+1}}.$$
(4.39)

Applying the discrete consistency condition ( $f_{n+1} = 0$ ), we obtain the following fractional-order differential equation for  $\Delta \gamma$ 

$$E_{0}^{C}\mathcal{D}_{t}^{\beta E}\left(\Delta\gamma\right)\Big|_{t=t_{n+1}} + K_{t_{p_{n+1}}}^{C}\mathcal{D}_{t}^{\beta K}\left(\Delta\gamma\right)\Big|_{t=t_{n+1}} + H\Delta\gamma = f_{n+1}^{trial}, \tag{4.40}$$

which is a Volterra integral equation of second kind. The fractional return-mapping algorithm is summarized in Box 4.1 for this model.



Figure 4.4: Schematic of stress update in the fractional return-mapping algorithm. The trial stress  $\tau_{n+1}^{trial}$  is projected to  $\tau_{n+1}$ . When unloading is performed from  $\tau_{n+1}$ , the new yield stress is  $\tau^{y}$  instead of  $\tau^{Y}$ .

Algorithm 4.1: Fractional return-mapping algorithm for the model M1.

1: Database at  $x \in \Omega$ : { $\varepsilon$ ,  $\varepsilon^{\nu p}$ ,  $\alpha$ ,  $\Delta \gamma$ ,  $\tau^{y}$ ,  $\tau^{y'}$ ,  $p_n$ }. 2: Enforce a strain increment  $\Delta \varepsilon_n$ : 3:  $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_n$ 4: Trial state (freezing the visco-plastic state): 5:  $\tau_{n+1}^{trial} = E \begin{bmatrix} C \\ 0 \end{bmatrix} D_t^{\beta E} \left( \varepsilon - \varepsilon^{v p^{trial}} \right) \Big|_{t=t_{n+1}}$ 6: **if**  $p_n > 0$  (last step was visco-plastic) **then** 7:  $\tau^{y'} = \tau^y + K {}_{tp_n}^C \mathcal{D}_t^{\beta K} \left( \alpha^{trial} \right) \Big|_{t=t_{n+1}}$ 8: end if 9:  $f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - [\tau^{y'} + H\alpha_n]$ 10: **if**  $f_{n+1}^{trial} \le 0 \text{ (visco-elastic step)$ **then** $}$ 11:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp}, \quad \alpha_{n+1} = \alpha_n, \quad \tau_{n+1} = \tau_{n+1}^{trial}, \quad p_{n+1} = 0$ 12: else if  $p_n > 0$  (increasing visco-plasticity) then 13: 14:  $p_{n+1} = p_n$ 15: else  $\tau^y = \tau^{y'}$ 16: 17:  $p_{n+1} = n+1$ end if 18: Solve for  $\Delta \gamma$ : 19:  $E \stackrel{C}{}_{0} \mathcal{D}_{t}^{\beta E} (\Delta \gamma) \Big|_{t=t_{n+1}} + K \stackrel{C}{}_{tp_{n+1}} \mathcal{D}_{t}^{\beta K} (\Delta \gamma) \Big|_{t=t_{n+1}} + H \Delta \gamma = f_{n+1}^{trial}$  $\tau_{n+1} = \tau_{n+1}^{trial} - E \stackrel{C}{}_{0} \mathcal{D}_{t}^{\beta E} (\Delta \gamma) \Big|_{t=t_{n+1}} \operatorname{sign} \left(\tau_{n+1}^{trial}\right).$ 20: 21:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \Delta \gamma \operatorname{sign}\left(\tau_{n+1}^{trial}\right)$ 22: 23:  $\alpha_{n+1} = \alpha_n + \Delta \gamma$ 24: end if

The fractional derivatives present in the fractional return-mapping procedure are computed implicitly using the finite difference method (FDM) developed in [91], where  ${}_{0}\mathcal{D}_{t}^{\nu}u(t)$  is discretized as

$$_{0}\mathcal{D}_{t}^{\nu}\left(u(t)\right)\Big|_{t=t_{n+1}} = \frac{1}{\Gamma(2-\nu)}\sum_{j=0}^{n}b_{j}\frac{u(t_{n+1-j}) - u(t_{n-j})}{(\Delta t)^{\nu}} + r_{\Delta t}^{n+1},$$
(4.41)

where  $r_{\Delta t}^{n+1} \leq C_u(\Delta t)^{2-\nu}$  and  $b_j := (j+1)^{1-\nu} - j^{1-\nu}, j = 0, 1, \dots, n$ . The term  $\Delta t$  denotes the time increment size  $\Delta t = T/N$ , where T represents the total time and N denotes the number of increments. Taking the first term j = 0 outside of the sum sign, we obtain

$${}_{0}\mathcal{D}_{t}^{\nu}\left(u(t)\right)\Big|_{t=t_{n+1}} = \frac{1}{(\Delta t)^{\nu}\Gamma(2-\nu)}\left[u(t_{n+1}) - u(t_{n}) + \mathcal{H}^{\nu}u\right],\tag{4.42}$$

where

$$\mathcal{H}^{\nu} u = \sum_{j=1}^{n} b_j \left[ u(t_{n+1-j}) - u(t_{n-j}) \right].$$
(4.43)

Therefore, the use of the above equations allows us to write explicit expressions for  $u(t_{n+1})$ . The use of this scheme does not cause any loss of accuracy for this framework, because the backward-Euler procedure is already first-order accurate. The discretization for the variables subject to the trial state  $u^{trial}(t_{n+1})$  is given by

$${}_{0}\mathcal{D}_{t}^{\nu}\left(u^{trial}(t)\right)\Big|_{t=t_{n+1}} = \frac{1}{(\Delta t)^{\nu}\Gamma(2-\nu)}\left[u^{trial}(t_{n+1}) - u(t_{n}) + \mathcal{H}^{\nu}u\right],\tag{4.44}$$

recalling that  $u^{trial}(t_{n+1}) = u(t_n)$ , we obtain

$$_{0}\mathcal{D}_{t}^{\nu}\left(u^{trial}(t)\right)\Big|_{t=t_{n+1}} = \frac{\mathcal{H}^{\nu}u}{(\Delta t)^{\nu}\Gamma(2-\nu)}.$$
(4.45)

Therefore, only the history term  $\mathcal{H}^{\nu}u$  is taken into account. For the time-fractional derivatives in the visco-plastic time reference, we consider

$$t_{p_{n+1}} \mathcal{D}_t^{\nu} \left( u(t) \right) \Big|_{t=t_{n+1}} = \frac{1}{(\Delta t)^{\nu} \Gamma(2-\nu)} \left[ u(t_{n+1}) - u(t_n) + \mathcal{H}_{t_{p_{n+1}}}^{\nu} u \right],$$
(4.46)

with

$$\mathcal{H}_{tp_{n+1}}^{\nu} u = \sum_{j=1}^{n-p_{n+1}} b_j \left[ u(t_{n+1-j}) - u(t_{n-j}) \right], \tag{4.47}$$

where only the  $n - p_{n+1}$  terms from the beginning of the current visco-plastic time reference are taken into consideration. The trial state for this derivative is considered with the visco-plastic time reference from the last configuration  $p_n$ , and is denoted by

$$_{tp_n} \mathcal{D}_t^{\nu} \Big( u^{trial}(t) \Big) \Big|_{t=t_{n+1}} = \frac{\mathcal{H}_{tp_n}^{\nu} u}{(\Delta t)^{\nu} \Gamma(2-\nu)}.$$
(4.48)

with

$$\mathcal{H}_{tp_n}^{\nu} u = \sum_{j=1}^{n-p_n} b_j \left[ u(t_{n+1-j}) - u(t_{n-j}) \right], \tag{4.49}$$

leading to a complexity of mathematical operations of  $O(N^2)$ .

## 4.5.1.1 Remark

Although Eq.4.12 indicates that when  $\beta_K \rightarrow 1$  we recover a local derivative operator, this is not what happens due to the adopted algorithmic procedure. Applying Eq.4.48 for the trial state of the internal hardening parameter, we obtain

$$_{tp_n} \mathcal{D}_t^{\beta_K} \left( \alpha^{trial} \right) \Big|_{t=t_{n+1}} = \frac{\mathcal{H}_{tp_n}^{\beta_K} \alpha}{(\Delta t)^{\beta_K} \Gamma(2 - \beta_K)}.$$
(4.50)

Recalling Eq.4.47, when the fractional-order  $v \to 1$ , the associated weights  $b_j \to 0$ , and therefore the above equation for the fractional derivative of  $\alpha_n$  vanishes. This asymptotic case, in fact, leads to the following trial yield function:

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - [\tau^{y} + H\alpha_{n}].$$
(4.51)

Therefore, the only remaining hardening effect relies on the rate-independent linear hardening term  $H\alpha_n$ . If we combine both effects  $\beta_K \rightarrow 1$  and H = 0, we obtain a limit case of *asymptotic perfect visco-plasticity*, which will be observed in results of Section 4.6.2.

The above discussion shows that due to the employment of a trial state, there is no reason in using a local first order derivative of the hardening parameter  $\alpha$  in the definition of  $f(\tau, \alpha)$ , since the term would vanish regardless of the material parameters. However, the inclusion of a fractional derivative introduces memory effects that do not vanish, except when  $\beta_K \rightarrow 1$ .

## 4.5.2 Algorithm for the model M2

We consider the same stress-strain relationship as the model M1, given by Eq.4.28. The incremental yield function is given by

$$f_{n+1} = |\tau_{n+1}| - \tau^{y'}, \tag{4.52}$$

with the corresponding trial function

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - \tau^{y'}.$$
(4.53)

Substituting Eq.4.28 into Eq.4.52, and recalling Eqs.4.29 and 4.53, we obtain

$$f_{n+1} = f_{n+1}^{trial} - E {}_{0}^{C} \mathcal{D}_{t}^{\beta E} (\Delta \gamma) \Big|_{t=t_{n+1}}.$$
(4.54)

With the discrete consistency condition  $(f_{n+1} = 0)$ , we obtain the following fractional-order differential equation:

$$E_{0}^{C}\mathcal{D}_{t}^{\beta E}\left(\Delta\gamma\right)\Big|_{t=t_{n+1}} = f_{n+1}^{trial}.$$
(4.55)

To calculate the rate-independent solution for stress, we use Eq.4.35 replacing  $\tau_{n+1}$  with  $\tau_{\infty}$ :

$$\tau_{\infty} = \tau_{n+1}^{trial} - E {}^{C}_{0} \mathcal{D}^{\beta E}_{t} \left( \Delta \gamma \right) \Big|_{t=t_{n+1}} \operatorname{sign} \left( \tau_{n+1}^{trial} \right).$$
(4.56)

Comparing Eqs.4.56 and 4.55, we can rewrite Eq.4.56 as

$$\tau_{\infty} = \tau_{n+1}^{trial} - \operatorname{sign}(\tau_{n+1}^{trial}) f_{n+1}^{trial} = \operatorname{sign}(\tau_{n+1}^{trial}) \tau^{y'}.$$
(4.57)

Therefore, the expression for  $\tau_{\infty}$  is given in a closed form. The algorithm to be used is of same type as the model M1, but we consider an additional equation when solving for the visco-plastic step, which is the incremental form of Eq.4.18, given by

$$E_{0}^{C}\mathcal{D}_{t}^{\beta_{E}}\left(\varepsilon^{\nu p}\right)\Big|_{t=t_{n+1}} + K_{t_{p_{n+1}}}^{C}\mathcal{D}_{t}^{\beta_{K}}\left(\varepsilon^{\nu p}\right)\Big|_{t=t_{n+1}} = E_{0}^{C}\mathcal{D}_{t}^{\beta_{E}}\left(\varepsilon\right)\Big|_{t=t_{n+1}} - \operatorname{sign}(\tau_{n+1}^{trial})\tau^{\gamma'}.$$

$$(4.58)$$

Also, we use an auxiliary incremental loading function denoted by  $f_{n+1}^*$  to check for unloading conditions in the visco-plastic range, in order to perform an update in the yield stress in case of unloading:

$$f_{n+1}^* = |\tau_{n+1}^{trial}| - \tau_n, \tag{4.59}$$

where  $\tau_n$  is the stress from the previous time step *n*. The fractional return-mapping algorithm for the model M2 is summarized in Box 4.2, and the solution for the incremental fractional-order equations for both models are presented in A.1.

Algorithm 4.2: Fractional return-mapping algorithm with for the model M2.

1: Database at  $x \in \Omega$ : { $\varepsilon$ ,  $\varepsilon^{vp}$ ,  $\tau^{y}$ ,  $\tau^{y'}$ ,  $\tau_n$ ,  $p_n$ }. 2: Enforce a strain increment  $\Delta \varepsilon_n$ : 3:  $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_n$ 4: Trial state (freezing the visco-plastic state): 5:  $\tau_{n+1}^{trial} = E \begin{bmatrix} C \\ 0 \end{bmatrix} \mathcal{D}_t^{\beta E} \left[ \varepsilon - \varepsilon^{v p^{trial}} \right]_{t=t_{n+1}}$ 6:  $f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - \tau^{y'}$ 7: **if**  $f_{n+1}^{trial} \le 0$  (visco-elastic step) **then** 8:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp}$ ,  $\tau_{n+1} = \tau_{n+1}^{trial}$   $p_{n+1} = 0$ 9: else if  $p_n > 0$  (increasing visco-plasticity) then 10: 11:  $p_{n+1} = p_n$ 12: else  $p_{n+1} = n+1$ 13: 14: end if  $f_{n+1}^* = |\tau_{n+1}^{trial}| - \tau_n$ if  $f^* < 0$  (unloading during visco-plastic step) then 15: 16:  $\tau^{y'} = |\tau_n|$ 17: end if 18: Perform visco-plastic regularization. Solve for  $\varepsilon_{n+1}^{vp}$ : 19: 20:  $E {}^{C}_{0}\mathcal{D}^{\beta E}_{t}\left(\varepsilon^{vp}\right) \Big|_{t=t_{n+1}} + K {}^{C}_{tp_{n+1}}\mathcal{D}^{\beta K}_{t}\left(\varepsilon^{vp}\right) \Big|_{t=t_{n+1}} = E {}^{C}_{0}\mathcal{D}^{\beta E}_{t}\left(\varepsilon\right) \Big|_{t=t_{n+1}} - \operatorname{sign}(\tau^{trial}_{n+1})\tau^{y}$  $\tau_{n+1} = E \left[ {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \left( \varepsilon - \varepsilon^{vp} \right) \right]_{t=t_{n+1}}.$ 21: 22: end if

# 4.5.3 Incremental tangent modulus

The computation of the tangent modulus present in the tangent stiffness matrix shown in Eq.4.25 is fundamental to achieve quadratic convergence for Newton's method. In classical local models it is obtained by differentiating the incremental equations of Boxes 4.1 and 4.2 in terms of  $\varepsilon_{n+1}$  to achieve an expression in closed form [192]. However, we did not obtain explicit expressions for such derivatives of the fractional-order equations presented for the models. Moreover, the tangent modulus is local in nature, and therefore we compute it using a simple backward finite-difference

procedure given by

$$\left(\frac{\partial \tau}{\partial \varepsilon}\right)_{n+1} = \frac{\tau_{n+1} - \tau_n}{\varepsilon_{n+1} - \varepsilon_n},\tag{4.60}$$

where  $\tau_{n+1}$  is obtained from the fractional return-mapping procedure of Boxes 4.1 and 4.2. We note that the first-order accuracy of such finite-difference approximation does not affect the overall accuracy since our algorithm, in which the backward-Euler method is employed, is also first-order accurate.

Regarding the stability of the proposed algorithms, we have employed an unconditionally stable finite-difference method, developed in [91], for the discretization of time-fractional ODEs in the fractional return-mapping algorithms. Moreover, the governing equations of motion are integrated using a stable Newmark scheme, where the tangent modulus is computed using an implicit backward-Euler method, see e.g., [192].

# 4.6 **Results and Discussion**

Three different analyses were performed to examine the developed models and algorithms. The first one consists of a convergence analysis using a benchmark solution, since there exist no available analytical solutions. The second test investigates the stress versus strain response of the models for prescribed monotonic and cyclic strains at constant rates. The last one solves a two-member truss with a snap-through instability with large strains and high strain rates.

## 4.6.1 Convergence analysis

A convergence analysis is performed for both models considering a reference benchmark solution for the stress, denoted by  $\tau_b$ . We consider the solution of Boxes 4.1 and 4.2 using prescribed strains. The error for the approximate solution denoted by  $\tau_{ap}$  is calculated using the  $L^{\infty}$  norm as

$$E_{L^{\infty}} = \frac{||\tau_{ap} - \tau_{b}||_{L^{\infty}}}{||\tau_{b}||_{L^{\infty}}}.$$
(4.61)

The material properties used are  $E = 50 Pa.s^{\beta E}$ ,  $K = 50 Pa.s^{\beta K}$ ,  $\beta_E = 0.5$ ,  $\beta_K = \{0.3, 0.7\}$ , H = 0 Pa and  $\tau^Y = 1 Pa$ . The material parameters are chosen to give a nonlinear response

for both visco-elastic/plastic ranges for the given strain rate, as shown in Figure 4.5. The final time considered is T = 0.08 s with total monotonic strain  $\varepsilon = 0.015$ , which gives a strain rate of  $\dot{\varepsilon} = 0.1875 s^{-1}$ . The benchmark solution uses N = 40960 time steps, which is equivalent to a time increment size  $\Delta t = 1.95 \times 10^{-6} s$ .



Figure 4.5: Stress versus total strain curves for the benchmark solutions. The number of data points for the model M2 is truncated for better visualization, since the results overlap with the model M1. Both models provide the same qualitative results for monotonic strains for the considered values of  $\beta_E$ ,  $\beta_K$ .

Figure 4.6 shows the  $L^{\infty}$ -norm error of the approximate stress versus the time increment size  $\Delta t$ . The error levels obtained for the model M2 are significantly smaller because this model does not account for the integration of the internal variables  $\alpha$  and  $\Delta \gamma$ , as presented in Box 4.2. This also impacts the convergence rate, which is approximately linear for the model M1 but with slightly higher rate for the model M2.



Figure 4.6:  $L^{\infty}$ -norm errors in  $\tau_{ap}$  versus time step size  $\Delta t$  in both models M1 and M2, where,  $\beta_E = 0.5$ .

## 4.6.2 Stress vs. strain response for prescribed strains

In order to show the influence of the fractional-order parameters  $\beta_E$  and  $\beta_K$  over the stress response, we performed monotonic and cyclic tests for both models. The purpose is to show the rate-dependency of the models according to the choice of the fractional-order parameters. For validation purposes, we also show the expected recovery to the limit case of rate-independent linear elasto-plasticity when  $\beta_E$  and  $\beta_K$  are close to zero (e.g.  $\beta = \beta_E = \beta_K = 0.01$ ), as well as the behavior when  $\beta \rightarrow 1$ .

## 4.6.2.1 Monotonic strains

The first step of this test consists of showing the recovery of the classical models of linear elastoplasticity and visco-plasticity of Duvaut-Lions type. We consider the application of strain increments up to  $\varepsilon = 0.4$  with rate  $\dot{\varepsilon} = 0.05 \, s^{-1}$ , where  $T = 8 \, s$ , and N = 500. The material properties used are  $E = 50 \, Pa.s^{\beta E}$ ,  $K = 5 \, Pa.s^{\beta K}$ . For classical linear elasto-plasticity we use  $H = 5 \, Pa$  and for the classical Duvaut-Lions model we use  $\eta = 5Pa.s$ . Figure 4.7 shows the obtained results. We observe that the classical elasto-plasticity with linear hardening is recovered when  $\beta_E$ ,  $\beta_K \rightarrow 0$ . The consideration of  $\beta_K \rightarrow 1$  did not recover the classical visco-plasticity for the model M1, as expected from the algorithmic discussion presented in Section 4.5.1.1.



Figure 4.7: Stress versus strain responses for both models using  $\beta_E = 0.01$ . We observe that both models recover the limit case of rate-independent elasto-plasticity (EP) when  $\beta_K \rightarrow 0$ . However, the classical visco-plasticity of Duvaut-Lions type (EVP-DL) is not recovered for the model M1 when  $\beta_K \rightarrow 1$ . An asymptotic perfect visco-plastic solution is obtained instead.



The results for intermediate values of the fractional derivatives are shown in Figure 4.8.

Figure 4.8: Stress versus strain response for both models with  $\beta_E = \beta_K$ . We observe the same response for monotonic strains. The variation of the fractional-orders affects the rate-dependent behavior for both visco-elastic and visco-plastic ranges. In this case, the increase of the fractional-order led to higher stress levels in the visco-elastic range and also more hardening.

The effect of the linear hardening parameter *H* for constant values of *K*,  $\beta_K$  is presented in Figure 4.9 for the model M1. Generally, this parameter *H* contributes to less nonlinearity in this

example, but may be used in conjunction with higher values of  $\beta_K$  to provide more hardening when convenient.



Figure 4.9: Stress versus total strain curves for the model M1 with  $\beta_E = \beta_K = 0.5$ ,  $K = 5Pa/s^{\beta_K}$  and different values of *H*. We observe less nonlinearity and more dominant linear hardening as the numerical value of *H* approaches *K*.

# 4.6.2.2 Cyclic strains

To compute the loading/unloading response of the models and analyse the cyclic hardening behavior, we performed a cyclic test comprising three loading cycles. We start with a traction cycle from  $\varepsilon = 0$  to  $\varepsilon = 0.4$ , followed by unloading and compression cycle until  $\varepsilon = -0.4$ , from where we increment the strains again up to  $\varepsilon = 0.4$ . We consider the material parameters  $E = 100 Pa.s^{\beta E}$ ,  $K = 50 Pa.s^{\beta K}$ , H = 0 Pa. The prescribed strain rate is  $\dot{\varepsilon} = 0.005 s^{-1}$ , with time parameters T = 400 s and N = 10000.

The results for the cyclic tests are presented in Figure 4.10. We observe that both models give the same qualitative results for the entire process for the considered material properties and strain rate.



Figure 4.10: Cyclic stress versus strain response for the models. We observe that due to the lack of internal hardening for the model M2, the stress amplitudes are smaller. Also, the response of the models after the first loading cycle is distinct.

Figure 4.11 shows the cyclic stress response considering two different relaxation times by setting different ratios E/K,  $\beta_K = 0.8$  and distinct strain rates. We observe that the stress response becomes more different between the models as we increase the ratio E/K and strain rate as well. This distinct behavior is expected since for the model M1 we enforce the consistency condition  $f_{n+1} = 0$ , which provides a fast visco-plastic relaxation for the time interval  $[t_n, t_{n+1}]$ . On the other hand, the visco-plastic regularization procedure of the model M2 considers relaxation effects that depend on the natural relaxation time of the material under consideration.



Figure 4.11: Cyclic stress versus strain response for the models considering different ratios K/E,  $\beta_E = 1.0 \times 10^{-3}$ ,  $\beta_K = 0.8$ . We observe higher stress values for the model M2 as we increase K/E, which become more pronounced with higher strain rates.

## 4.6.3 Two-member truss with snap-through effect

We consider the solution of the two-member truss presented in Figure 4.12a. The material properties are  $E = 2.1 \times 10^{11} Pa.s^{\beta}E$ ,  $K = 1.0 \times 10^{11} Pa.s^{\beta}K$ ,  $\tau^{Y} = 7.0 \times 10^{8} Pa$ ,  $\rho = 7.85 \times 10^{-6} kg/mm^{3}$ ,  $\nu = 0.5$  and  $A = 7.0 mm^{2}$ . A vertical force P(t) is applied at node 2, with the behavior over time illustrated in Figure 4.12b. We consider total time  $T = \{0.3, 1.0\} s$  and we analyze the recovery of classical elasto-plasticity for the models. Then, we will present the behavior for both models considering the variation of intermediate values of the fractional-orders.



Figure 4.12: (a) Two-member truss. The snap-through phenomenon occurs when the vertical displacement of node 2 is -127 mm. (b) Applied negative vertical force over time.

## **4.6.3.1** Behavior of the models when $\beta \rightarrow 0$

Figure 4.13 shows the recovery of rate-independent elasto-plasticity with linear hardening for the models, by setting small values of  $\beta_E = 1.0 \times 10^{-5}$  and  $\beta_K = 1.0 \times 10^{-4}$ , so that both Scott-Blair elements in the visco-elastic/plastic devices recover linear springs. We do not try the recovery of Duvaut-Lions elasto-visco-plasticity in this test for the models because of the previous observations in Section 4.5.1.1, when  $\beta_K \rightarrow 1$  for the model M1, and the fact that the model M2 only recovers the classical model for monotonic loading (because of the update of the yield stress when unloading).



Figure 4.13: Recovery of the models to rate-independent elasto-plasticity,  $\Delta t = 6.0 \times 10^{-5} s$ . The snap-through effect occurs at t = 0.089 s.

## 4.6.3.2 Variation of fractional-orders for the model M1

We consider a constant value of  $\beta_E = 1.0 \times 10^{-4}$  with variations of  $\beta_K$  (fractional elasto-viscoplasticity order) to investigate the strain-herdening effect due to the Scott-Blair element in the visco-plastic device. Figure 4.14 shows the results for displacement, stress and internal force. The increasing hardening with the increase of  $\beta_K$  is observed from Figure 4.14a with the late occurrence of the snap-through for  $\beta_K = 0.9$  and larger amplitudes in displacement. The late snap-through can be justified by the higher peak in the internal force in Figure 4.14c at approximately 60 mm of vertical displacement. The hardening is also seen in Figure 4.14b with the larger visco-elastic range.



Figure 4.14: Results for the model M1 considering  $\beta_E = 1.0 \times 10^{-4}$  and variation of  $\beta_K$ . (a) Displacement vs. time. (b) Stress vs. strain. (c) Internal force vs. displacement. We observe the increased visco-plastic hardening and damping with the increase of  $\beta_K$ .

The results for longer time integration T = 1 s using  $\beta_E = 1.0 \times 10^{-4}$  and time increment  $\Delta t = 1.0 \times 10^{-4} s$  are presented in Figure 4.15. We observe that due to the high strain rates, the elastic domain expands significantly more with higher values of  $\beta_K$ , and no dissipation is observed for the oscillations because the value of  $\beta_E$  is sufficiently small.



Figure 4.15: Displacement versus time and stress versus strain for the model M1, T = 1 s,  $\beta_E = 1.0 \times 10^{-4}$  and variation of  $\beta_K$ .

We also considered the use of  $\beta_E = 0.1$  to account for visco-elastic dissipation, with  $\Delta t = 1.0 \times 10^{-5} s$ . Figure 4.16a shows a very significant reduction in the displacement amplitudes for the short time interval, where increasing the value of  $\beta_K$  led to more hardening. However, the use of a fractional-order value  $\beta_E = 0.1$  is high enough to suppress the oscillations for the considered time

domain. Figures 4.16b and 4.16c also show a more pronounced visco-elastic relaxation behavior for  $\beta_K = 0.5, 0.9$ .



Figure 4.16: (a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M1,  $\beta_E = 0.1$  and different values for  $\beta_K$ .

## 4.6.3.3 Variation of fractional-orders for the model M2

In the same way as the previous section, we tested the response of the truss for the model M2 using variation of the fractional-order parameters. Figure 4.17 shows the results obtained for  $\beta_E = 1.0 \times 10^{-4}$  and variation of  $\beta_K$ . We observe the same strain-hardening behavior as in the model M1 before the snap-through. Moreover, the snap-through phenomenon for  $\beta_K = 0.9$  occurs at  $t \approx 0.2 \, s$ , which is later than observed for the model M1 (Figure 4.14a). This is compatible with the cyclic results presented in Section 4.6.2.2 with more rate-dependent hardening for the model M2 when using higher relaxation times and strain rates combined with higher values for  $\beta_K$ .



Figure 4.17: (a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M2,  $\beta_E = 1.0 \times 10^{-4}$  and variation of  $\beta_K$ .

The behavior for T = 1 s with  $\Delta t = 1.0 \times 10^{-4} s$  is shown in Figure 4.18, which is qualitatively similar to the model M1, except for  $\beta_K = 0.9$ , where more hardening is observed for this case.



Figure 4.18: Displacement versus time and stress versus strain for the model M2,  $\beta_K = 0.1$ .

Figure 4.19 shows that the use of a fractional-order  $\beta_E = 0.1$  increased the visco-elastic dissipation similarly to the model M1. The time increment considered for this test was  $\Delta t = 1.0 \times 10^{-4} s$ . We observe that the combination of this fractional-order for visco-elasticity with  $\beta_K = 0.9$  for the model M2 increased even more the hardening before the snap-through, occurring at  $t \approx 0.23 s$  (Figure 4.19a), compared to  $t \approx 0.2 s$  (Figure 4.16a) for the model M1.

The behavior of the presented models for the snap-through problem is qualitatively similar to another application in the literature for integer order visco-elasto-plastic formulation [207]. Also,

the frequency response of the structure observed in Figures 4.14a and 4.17a due to higher effective stiffness when using lower fractional-order  $\beta$  (Scott-Blair element with lower viscosity) is also observed for linear single and multiple degree-of-freedom oscillators using fractional derivatives [208–210].



Figure 4.19: (a) Displacement vs. time, (b) stress vs. strain, and (c) internal force vs. displacement for the model M2,  $\beta_E = 0.1$  and different values for  $\beta_K$ .

#### **CHAPTER 5**

# A THERMODYNAMICALLY CONSISTENT, FRACTIONAL VISCO-ELASTO-PLASTIC MODEL WITH HISTORY-DEPENDENT DAMAGE

# 5.1 Background

Accurate and predictive modeling of material damage and failure for a wide range of materials poses multi-disciplinary challenges on experimental detection, consistent physics-informed models and efficient algorithms. Material failure arises in mechanical and biological systems as a consequence of internal damage, characterized in the micro-scale by the presence and growth of discontinuities e.g., microvoids, microcracks and bond breakage. Continuum Damage Mechanics (CDM) treats such effects in the macroscale through a representative volume element (RVE) [211]. When loading plastic crystalline materials, an initial hardening stage is observed from motion, arresting and network formation of dislocations, which is later overwhelmed by damage mechanisms, e.g. multiplication of micro-cracks/voids, followed by their growth and coalescing, releasing bulk energy from the RVE. Classical CDM models were proposed and validated in the past decades to describe the mechanical degradation, *e.g.*, of ductile, brittle, and hyperelastic materials [212, 213]. Particularly, Lemaitre's ductile damage model [211, 213] has been extensively employed for plasticity and visco-plasticity modeling of ductile materials. In such models, developing proper damage potentials driven by the so-called damage energy release rate [211] is a critical step. More recently, phase-field damage and failure models have been successfully applied in the context of brittle and ductile failure of materials [214–218].

Modeling the standard-to-anomalous damage evolution for power-law materials has additional challenges due to the non-Gaussian processes occurring on fractal-like media. Fractional constitutive laws utilize Scott-Blair (SB) elements [172, 219] as rheological building blocks that model the soft material response as a power-law memory-dependent device, interpolating between purely elastic/viscous behavior. A mechanical representation of the SB element was developed by Schies-

sel [34], as a hierarchical, continuous "ladder-like" arrangement of canonical Hookean/Newtonian elements (*see Figure 5.1*). Later on, Schiessel [36] generalized several standard visco-elastic models (Kelvin-Voigt, Maxwell, Kelvin-Zener, Poynting-Thompson) to their fractional counterparts by fully replacing the canonical elements with SB elements. Of particular interest, Lion [35] proved the thermodynamic consistency of the SB element from a mechanically-based fractional Helmholtz free-energy density.

With particular arrangements of SB and standard elements, fractional models were applied, *e.g.*, to describe the *far from equilibrium* power-law dynamics of multi-fractional visco-elastic [8, 24, 43, 187, 220, 221], distributed visco-elastic [222] and visco-elasto-plastic [1, 46, 48, 49, 223] complex materials. Concurrently, significant advances in numerical methods allowed numerical solutions to time- and space- fractional partial differential equations (FPDEs) for smooth/non-smooth solutions, such as finite-difference (FD) schemes [86, 91], fractional Adams methods [94, 112], implicit-explicit (IMEX) schemes [113, 224], spectral methods [99, 100], fractional subgrid-scale modeling [225], fractional sensitivity equations [101], operator-based uncertainty quantification [226] and self-singularity-capturing approaches [177].

Despite the significant contributions on fractional constitutive laws, few works incorporated damage mechanisms. Zhang *et al.* [67] developed a nonlinear, visco-elasto-plastic creep damage model for concrete, where the damage evolution was defined through an exponential function of time. A similar model was proposed by Kang *et al.* [68] and applied to coal creep. Caputo and Fabrizio [69] developed a variable order visco-elastic model, where the variable order was regarded as a phase-field driven damage. Alfano and Musto [53] developed a cohesive zone, damaged fractional Kelvin-Zener model, and studied the influence of Hooke/SB damage energy release rates on damage evolution, motivating further studies on crack propagation mechanisms in visco-elastic media. Tang *et al.* [70] developed a variable order rock creep model, with damage evolution as an exponential function of time. Recently, Giraldo-Londoño *et al.* [71] developed a two-parameter, two-dimensional (2-D) rate-dependent cohesive fracture model.

A key aspect to develop failure models relies on consistent forms of damage energy release

rates, usually appearing in the material-specific form of Helmholtz free-energy densities. For standard materials, direct summations of elastic/hyperelastic free-energies of the system are used. However, such process is non-trivial when modeling anomalous materials, due to the intrinsic mixed elasticity/viscosity of SB elements. Fabrizio [72] introduced a Graffi-Volterra free-energy for fractional models, but defined it without sufficient physical justification. Deseri *et al.* [73] developed free-energies for fractional hereditary materials, with the notion of order-dependent *elasto-viscous* and *visco-elastic* behaviors. Lion [35] derived the isothermal Helmholtz free-energy density for SB elements using a discrete-to-continuum arrangement of standard Maxwell branches, and employed it in the Clausius-Duhem inequality to obtain the stress-strain relationship. Later on, Adolfsson *et al.* [74] employed Lion's approach to prove the thermodynamic admissibility of the SB constitutive law written as a Volterra integral equation of first kind.

To the authors' best knowledge, only Alfano and Musto [53] coupled the fractional freeenergy density to a damage evolution equation in viscoelasticity, but fractional extensions of (nonexponential) damage for visco-elasto-plastic materials are still lacking. In addition, for damage models, efficient numerical methods for fractional free-energy computations are also virtually nonexistent in the literature. A numerical approximation was done by Burlon *et al.* [227], through a finite summation of free-energies from Hookean elements, which is a truncation of the infinite number of relaxation modes carried by the fractional operators. Alfano and Musto [53] briefly described how to discretize the SB free-energy using a midpoint finite-difference scheme. A few numerical results were presented for damage evolution, but the authors did not describe the discretizations and no accuracy is investigated for the numerical scheme.

In this work we develop a thermodynamically consistent, one-dimensional (1-D) fractional visco-elasto-plastic model with memory-dependent damage in the context of CDM. The main characteristics of the model follow:

• We employ SB elements in both visco-elastic and visco-plastic parts, respectively, with orders  $\beta_E, \beta_K \in (0, 1)$ , leading to power-law effects in both ranges.

- The damage reduces the total free-energy of the model, while constitutive laws are obtained through the Clausius-Duhem inequality.
- The yield function is time-fractional rate-dependent, while the damage potential is Lemaitrelike. The damage energy release rate is taken as the SB Helmholtz free-energy density to describe the anomalous bulk energy loss.
- We prove the positive dissipation, and therefore the thermodynamic consistency of the developed model (*see Theorem 5.4.4*).

Since obtaining analytical solutions for the resulting nonlinear system of multi-term viscoelasto-plastic fractional differential equations (FDEs) coupled with damage is cumbersome or even impossible, we performed an efficient time-integration framework as follows:

- We develop a first-order, semi-implicit fractional return-mapping algorithm, with explicit evaluation of damage in the stress-strain relationship and yield function. An implicit FD scheme is employed to the ODEs for plastic and damage variables. The time-fractional stress-strain relationship and yield function are discretized using the L1 FD scheme from Lin and Xu [91].
- We develop a fully-implicit scheme for the SB Helmholtz free-energy density, and hence to the fractional damage energy release rate. We then exploit the structure of the discretized energy and apply Fast Fourier Transforms (FFTs) to obtain an efficient scheme.
- The accuracy of free-energy discretization is proved to be of order  $O(\Delta t^{2-\beta})$ , and numerical tests show a computational complexity of order  $O(N^2 \log N)$ , with N being the number of time-steps.

The developed fractional return-mapping algorithm can be easily incorporated to existing finite element (FE) frameworks as a constitutive box. Numerical tests are performed with imposed monotone and cyclic strains, and demonstrate that:

- Softening, hysteresis and low-cycle fatigue can be modeled.
- Memory-dependent damage energy release rates induce anomalous damage evolutions with competing visco-elastic/plastic effects, without changing the form of Lemaitre's damage potential.

The developed model motivates applications to failure of biological materials [21], where micro-structural evolution can be upscaled to the continuum through evolving fractional orders  $\beta_E$ ,  $\beta_K$  [40] and damage D. The memory-dependent fractional damage energy release rates motivate studies on anomalous bulk-to-surface energy loss in damage accumulation/crack propagation of, *e.g.*, bone tissue, where intrinsic/extrinsic plasticity/crack-bridging mechanisms [228] lead to a complex nature of failure.

This work is organized as follows: In Section 5.2 we present definitions of fractional operators. In Section 5.3, we present the thermodynamics and rheology of SB elements. In Section 5.4, we develop the fractional visco-elasto-plastic model with damage, followed by its discretization. A series of numerical tests are shown in Section 5.5.

# **5.2 Definitions of Fractional Calculus**

We start with some preliminary definitions of fractional calculus [31]. The left-sided Riemann-Liouville integral of order  $\beta \in (0, 1)$  is defined as

$$\binom{RL}{t_L} \mathcal{I}_t^{\beta} f(t) = \frac{1}{\Gamma(\beta)} \int_{t_L}^t \frac{f(s)}{(t-s)^{1-\beta}} \, ds, \quad t > t_L,$$
(5.1)

where  $\Gamma$  represents the Euler gamma function and  $t_L$  denotes the lower integration limit. The corresponding inverse operator, i.e., the left-sided fractional derivative of order  $\beta$ , is then defined based on (1.1) as

$$\binom{RL}{t_L}\mathcal{D}^\beta_t f)(t) = \frac{d}{dt} \binom{RL}{t_L} \mathcal{I}^{1-\beta}_t f)(t) = \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \int_{t_L}^t \frac{f(s)}{(t-s)^\beta} \, ds, \quad t > t_L.$$

Also, the left-sided Caputo derivative of order  $\beta \in (0, 1)$  is obtained as

$$\binom{C}{t_L}\mathcal{D}_t^{\beta}f(t) = \binom{RL}{t_L}I_t^{1-\beta}\frac{df}{dt}(t) = \frac{1}{\Gamma(1-\beta)}\int_{t_L}^t \frac{f'(s)}{(t-s)^{\beta}}\,ds, \quad t > t_L$$

The definitions of Riemann-Liouville and Caputo derivatives are linked by the following relationship:

$$\binom{RL}{t_L}\mathcal{D}_t^{\beta}f(t) = \frac{f(t_L)}{\Gamma(1-\beta)(t+t_L)^{\beta}} + \binom{C}{t_L}\mathcal{D}_t^{\beta}f(t),$$

which denotes that the definition of the aforementioned derivatives coincide when dealing with homogeneous Dirichlet initial/boundary conditions.

#### 5.2.1 Interpretation of Caputo derivatives in terms of nonlocal vector calculus

In this section we show that the Caputo derivative can be reinterpreted as the limit of a nonlocal truncated time derivative [229]. This fact establishes a connection between nonlocal initial value problems and their fractional counterparts, which can benefit from the nonlocal theory.

Given a nonnegative and symmetric kernel function  $\rho_{\delta}(s) = \rho_{\delta}(|s|)$ , a nonlocal, weighted, gradient operator can be defined as [230]

$$\mathcal{G}_{\delta}f(t) = \lim_{\epsilon \to 0} \int_{\epsilon}^{\delta} (f(t) - f(t-s))s\rho_{\delta}(s) \, ds, \tag{5.2}$$

when the limit exists in  $L^2(0,T)$  for a function  $f \in L^2(0,T)$ . It is common to assume that the kernel function  $\rho_{\delta}$  has compact support in  $[-\delta, \delta]$  and a normalized moment:

$$\int_0^\delta s^2 \rho_\delta(s) \, ds = 1. \tag{5.3}$$

Here, the parameter  $\delta > 0$  represents the extent of the nonlocal interactions or, in case of time dependence, the memory span. In the nonlocal theory it is usually referred to as *horizon*.

Note that at the limit of vanishing nonlocality, *i.e.* as  $\delta \to 0$ ,  $\mathcal{G}_{\delta}$  corresponds to the classical first order time derivative operator  $\frac{d}{dt}$ . In this work, we are interested in the limit of infinite interactions, *i.e.* as  $\delta \to \infty$ . Specifically, when the initial data f(t) := f(0) for all  $t \in (-\infty, 0)$  and the kernel function is defined as

$$\rho_{\infty}(s) = \frac{\beta}{\Gamma(1-\beta)} s^{-\beta-2}, \quad \text{for } \beta \in (0,1),$$
(5.4)

the nonlocal operator  $\mathcal{G}_{\delta}$  corresponds to the Caputo fractional derivative for t > 0, for a piecewise differentiable function  $f \in C(-\infty, T)$  such that  $f' \in L^1(0, T) \cap C(0, T]$ . Formally,

$$\mathcal{G}_{\infty}f(t) = \begin{pmatrix} C \mathcal{D}_t^{\beta}f(t) \\ 0 \end{pmatrix}$$
(5.5)



Figure 5.1: *(left)* Schematics of the SB element recovering standard limit cases. *(right)* The SB element seen as an infinite, hierarchical mechanical representation of canonical elements, coding an infinite number of relaxation times. The pair  $(\mathbb{E}, \beta)$  represents a dynamic process of the material.

Note that a similar property holds true for fractional derivatives in space, see [231].

## 5.2.1.1 Note on well-posedness

Paper [229] analyzes the well-posedness of nonlocal initial value problems. More specifically, it proves, under certain conditions on the parameters, that the following equation has a unique solution and depends continuously upon the data.

$$\mathcal{G}_{\delta}\gamma + H\gamma = F \qquad t \in (0, T],$$
  
$$\gamma = G \qquad t \in (-\delta, 0),$$
  
(5.6)

for H > 0 and F and G in suitable functional spaces.

# **5.3** Thermodynamics of Fractional Scott-Blair Elements

We present the thermodynamic principles used in this work, and then we introduce the Helmholtz free-energy density and constitutive law for the fractional SB element. Such fractional element is the rheological building block of our modeling approach, providing a constitutive interpolation between a Hookean ( $\beta \rightarrow 0$ ) and Newtonian ( $\beta \rightarrow 1$ ) element (*see Figure 5.1*). Furthermore, the SB element can be interpreted as an infinite self-similar arrangement of standard Maxwell elements, which naturally leads to fractional operators in the constitutive law [34].

## 5.3.1 Thermodynamic principles

Let a closed system undergo an irreversible, isothermal, strain-driven thermodynamic process. We analyze an infinitesimal material region at a position x and time t of a continuum deformable body  $\mathcal{B}$ . Let the first law of thermodynamics in rate form [232] be defined as:

$$\dot{e} = \dot{q} - \dot{w},\tag{5.7}$$

where  $\dot{e}(x,t) [J.s^{-1}.kg^{-1}]$  denotes the specific rate of internal energy,  $\dot{q}(x,t) [J.s^{-1}.kg^{-1}]$  represents the rate of specific heat exchange and the term  $\dot{w}(x,t) [J.s^{-1}.kg^{-1}]$  denotes the stress power transferred into the bulk due to external forces [233]. In this work,  $\tau(x,t)$  represents the stress state and  $\dot{\varepsilon}$  the strain rate. We also consider the second law of thermodynamics, postulating the irreversibility of entropy production, given, in specific form, by:

$$\dot{s} \ge \dot{q}/\theta,$$
 (5.8)

where  $\dot{s}(x,t) [J.s^{-1}.kg^{-1}.K^{-1}]$  denotes the rate of specific entropy production and  $\theta(x,t) = \theta_0 [K]$ represents the constant temperature. Let  $\psi(x,t) : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}^+$  be the Helmholtz free-energy density with units  $[J.m^{-3}]$ , representing the available energy to perform work, defined by  $\psi := \rho (e - \theta s)$ , with the rate form  $\dot{\psi} = \rho (\dot{e} - \theta \dot{s})$  for the isothermal case. Combining the first and second laws, respectively, (5.7) and (5.8), with  $\dot{\psi}$  and taking the stress power  $\dot{w} = -\tau \dot{\varepsilon}$ , we obtain the Clausius-Duhem inequality, which states the non-negative dissipation rates [234]:

$$-\dot{\psi} + \tau \dot{\varepsilon} \ge 0, \quad \forall x \in \mathcal{B}.$$
 (5.9)

Satisfying the dissipation inequality (5.9) is here taken as the necessary condition for the potential  $\psi$  and the stress  $\tau$  to be thermodynamically admissible.

# 5.3.2 Helmholtz free-energy density

We present the free-energy under consideration for the employed SB element, here referred to a given material coordinate of a continuum body or a lumped mechanical system. We start with the

fractional Helmholtz free-energy density developed by Lion [35], obtained through an integration of a continuum spectrum of Maxwell branches leading to the following definition for  $\psi(\varepsilon) : \mathbb{R} \to \mathbb{R}^+$ :

$$\psi(\varepsilon) = \frac{1}{2} \int_0^\infty \tilde{E}(z) \left[ \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) \, ds \right]^2 \, dz, \tag{5.10}$$

where we the strain  $\varepsilon$  is taken as the state variable. The term  $\tilde{E}(z) : \mathbb{R}^+ \to \mathbb{R}^+$  denotes the power-law relaxation spectrum, given by

$$\tilde{E}(z) = \frac{\mathbb{E}}{\Gamma(1-\beta)\Gamma(\beta)z^{\beta+1}}, \quad 0 < \beta < 1, \quad \mathbb{E} \in \mathbb{R}^+,$$

which with (5.10), codes an infinite number of relaxation times. The pseudo-constant  $\mathbb{E}$  has units  $[Pa.s^{\beta}]$ , where the unique pair ( $\mathbb{E}, \beta$ ) codes a dynamic process instead of an equilibrium state of the material [24]. Let  $\mathcal{D}_{mech}$  denote the mechanical dissipation of the SB element. We introduce the following Lemmas:

**Lemma 5.3.1.** The SB element stress-strain relationship  $\tau(t) : \mathbb{R}^+ \to \mathbb{R}$  resulting from (5.10) and the Clausius-Duhem inequality (5.9) is given by

$$\tau(t) = \int_0^\infty \tilde{E}(z) \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) \, ds \right) \, dz = \mathbb{E}_0^C \mathcal{D}_t^\beta \varepsilon(t), \tag{5.11}$$

where the Caputo definition for the fractional derivative is a consequence of the adopted free-energy. The mechanical dissipation  $\mathcal{D}_{mech}(\varepsilon) : \mathbb{R} \to \mathbb{R}^+$  for the SB element is given by the following form:

$$\mathcal{D}_{mech}(\varepsilon) = \int_0^\infty \frac{\tilde{E}(z)}{z} \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) \, ds \right)^2 dz.$$
(5.12)

Proof. See Appendix B.1.

**Remark 5.3.2.** The limit cases for the fractional free-energy (5.10) with respect to  $\beta$  are consistent with the well-known stress-strain relationship (5.11). Therefore,  $\psi(\varepsilon)$  recovers a fully conserving Hookean spring when  $\lim_{\beta\to 0} \psi = \mathbb{E}\varepsilon^2/2$ , and a fully dissipative Newtonian dashpot when  $\lim_{\beta\to 1} \psi = 0$ . We refer the readers to [35, 73] for additional details regarding memory-dependent free-energies.



Figure 5.2: Damaged fractional visco-elasto-plastic model. (A) Constitutive diagram with viscoelastic/plastic rheological elements. (B) Stress response showing the yield surface expansion (hardening) and contraction (softening).

# 5.4 Fractional Visco-Elasto-Plastic Model with Damage

We develop a damage formulation for a fractional visco-elasto-plastic model (M1) by Suzuki *et al.* [1]. The closure for the damage variable is obtained through a Lemaitre-type approach [211, 213]. We later prove the thermodynamic consistency of the damage model, and hence for the visco-elasto-plastic model (M1) as a limiting, undamaged case.

## 5.4.1 Thermodynamic formulation

The fractional visco-elasto-plastic device is illustrated in Figure 5.2. It consists of a SB element with material pair  $(\mathbb{E}, \beta_E)$  for the visco-elastic part, under a corresponding logarithmic viscoelastic strain  $\varepsilon^{ve}(t) : \mathbb{R}^+ \to \mathbb{R}$ . The visco-plastic part is given by a parallel combination of a Coulomb frictional element with yield stress  $\tau^Y [Pa] \in \mathbb{R}^+$ , a linear hardening Hooke element with constant  $H[Pa] \in \mathbb{R}^+$ , and a SB element with material pair  $(\mathbb{K}, \beta_K)$ , with  $\mathbb{K}[Pa.s^{\beta K}] \in \mathbb{R}^+$ , all subject to a logarithmic visco-plastic strain  $\varepsilon^{vp}(t) : \mathbb{R}^+ \to \mathbb{R}$  and an internal hardening variable  $\alpha(t) : \mathbb{R}^+ \to \mathbb{R}^+$ . The entire device is subject to a Kirchhoff stress  $\tau$ . The total logarithmic strain is given by:

$$\varepsilon(t) = \varepsilon^{ve}(t) + \varepsilon^{vp}(t). \tag{5.13}$$

Let  $D(t) : \mathbb{R}^+ \to \Omega_D$ , with  $\Omega_D = [0, 1)$  be a time-dependent and monotonically increasing internal damage variable representing the internal material degradation. Our model has the following

assumptions:

Assumption 1. The visco-elastic response is linear, under an isothermal strain-driven process.

**Assumption 2.** There is a state coupling between the visco-elastic strains/hardening variable  $\varepsilon^{ve}$ ,  $\alpha$ , and damage D. However, the damage evolution is solely driven by the visco-elastic free-energy potential.

**Assumption 3.** There is no state coupling between visco-elasticity and visco-plasticity.

**Assumption 4.** The damage D(t) and hardening  $\alpha(t)$  are irreversible, i.e., there is no material healing. Also, there are no crack closure effects.

Assumption 5. All state and internal variables are subject to homogeneous initial conditions, e.g.,  $\varepsilon(0) = \varepsilon^{ve}(0) = \varepsilon^{vp}(0) = \alpha(0) = D(0) = 0.$ 

Assumption (3) implies a linearity between the visco-elastic and visco-plastic free-energy components, both multiplicatively coupled with damage.

## 5.4.1.1 Free-energy densities

We write the Helmholtz free-energy density  $\psi(\varepsilon^{\nu e}, \alpha, D) : \mathbb{R} \times \mathbb{R}^+ \times \Omega_D \to \mathbb{R}^+$  for the model as:

$$\psi(\varepsilon^{ve}, \alpha, D) = (1 - D) \left( \bar{\psi}^{ve}(\varepsilon^{ve}) + \bar{\psi}^{vp}(\alpha) \right), \tag{5.14}$$

where  $\bar{\psi}^{ve}(\varepsilon^{ve}) : \mathbb{R} \to \mathbb{R}^+$  and  $\bar{\psi}^{vp}(\alpha) : \mathbb{R}^+ \to \mathbb{R}^+$  represent the undamaged visco-elastic and visco-plastic free-energy densities. Utilizing (5.10) for the SB elements and the Hookean spring, the free-energy density is given by:

$$\psi(\varepsilon^{ve}, \alpha, D) = \frac{1}{2} (1 - D) \left[ \int_0^\infty \tilde{E}(z) \left( \int_0^t \exp\left(-\frac{t - s}{z}\right) \dot{\varepsilon}^{ve}(s) \, ds \right)^2 \, dz \qquad (5.15) + \int_0^\infty \tilde{K}(z) \left( \int_0^t \exp\left(-\frac{t - s}{z}\right) \dot{\alpha}(s) \, ds \right)^2 \, dz + H\alpha^2 \right],$$

with the following relaxation spectra for visco-elasticity and visco-plasticity:

$$\tilde{E}(z) = \frac{\mathbb{E}}{\Gamma(1-\beta_E)\Gamma(\beta_E)z^{\beta_E+1}}, \quad \tilde{K}(z) = \frac{\mathbb{K}}{\Gamma(1-\beta_K)\Gamma(\beta_K)z^{\beta_K+1}},$$

where  $0 < \beta_E$ ,  $\beta_K < 1$ .

**Remark 5.4.1** (Recovery of classical free-energy potentials). Similar to the SB element case, we recover the Hookean and Newtonian limit cases for the asymptotic values of  $\beta_E$ ,  $\beta_K$ . Also, if  $D \rightarrow 0$ , we recover an undamaged case, and when  $D \rightarrow 1$ , we have  $(1 - D)\psi \rightarrow 0$  (material failure).

# 5.4.1.2 Constitutive laws

We use the Clausius-Duhem inequality (5.9) in the local form of classical thermodynamics of internal variables, which induces *near-equilibrium* states for every time *t* of the thermodynamic process. However, the fractional free-energy densities introduce memory effects and therefore *far-from-equilibrium* states in the scope of rational thermodynamics [72]. Using (5.14) and (5.13), inequality (5.9) is given by:

$$-\rho\dot{\psi}(\varepsilon^{\nu e},\alpha,D) + \tau\left(\dot{\varepsilon}^{\nu e} + \dot{\varepsilon}^{\nu p}\right) \ge 0,\tag{5.16}$$

where we evaluate  $\dot{\psi}$  as follows:

$$\dot{\psi}(\varepsilon^{ve}, \dot{\varepsilon}^{ve}, \alpha, \dot{\alpha}, D, \dot{D}) = \frac{\partial \psi}{\partial \varepsilon^{ve}} \dot{\varepsilon}^{ve} + \frac{\partial \psi}{\partial \alpha} \dot{\alpha} + \frac{\partial \psi}{\partial D} \dot{D}.$$
(5.17)

Similar to the proof of Lemma 5.3.1, the partial derivatives are obtained by chain and Leibniz rules. For the first term on the RHS of (5.17), we have:

Recalling (5.12), we rewrite the above equation as:

$$\frac{\partial \psi}{\partial \varepsilon^{ve}} \dot{\varepsilon}^{ve} = (1 - D) \left[ \int_0^\infty \tilde{E}(z) \left( \int_0^t \exp\left(-\frac{t - s}{z}\right) \dot{\varepsilon}^{ve}(s) \, ds \right) dz \, \dot{\varepsilon}^{ve} -\mathcal{D}_{mech}^{ve}(\varepsilon^{ve}) \right], \tag{5.18}$$

where  $\mathcal{D}_{mech}^{ve}(\varepsilon^{ve}): \mathbb{R} \to \mathbb{R}^+$  represents the visco-elastic mechanical energy dissipation, given by:

$$\mathcal{D}_{mech}^{ve}(\varepsilon^{ve}) = \int_0^\infty \frac{\tilde{E}(z)}{z} \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}^{ve}(s) \, ds \right)^2 \, dz.$$

Similarly, we obtain the second term on the RHS of (5.17):

$$\frac{\partial \psi}{\partial \alpha} \dot{\alpha} = R(t) \dot{\alpha} - (1 - D) \mathcal{D}_{mech}^{vp}(\alpha), \qquad (5.19)$$

where  $R(t) : \mathbb{R}^+ \to \mathbb{R}^+$  represents the accumulated stress acting on the SB and Hooke elements on the visco-plastic part due to the accumulated visco-plastic strains. Recalling Lemma 5.3.1, R(t)reads:

$$\begin{split} R(t) &= (1-D) \left[ \int_0^\infty \tilde{K}(z) \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\alpha}(s) \, ds \right) dz + H\alpha \right] \\ &= (1-D) \left[ \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha) + H\alpha \right]. \end{split}$$

On the other hand, the term  $\mathcal{D}_{mech}^{vp}(\alpha) : \mathbb{R}^+ \to \mathbb{R}^+$  denotes the visco-plastic mechanical energy dissipation in the model, which is given by:

$$\mathcal{D}_{mech}^{vp}(\alpha) = \int_0^\infty \frac{\tilde{K}(z)}{z} \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\alpha}(s) \, ds \right)^2 \, dz.$$

Finally, the direct calculation of the last term on the RHS of (5.17) yields:

$$\frac{\partial \psi}{\partial D} \dot{D} = \left[ Y^{\nu e}(\varepsilon^{\nu e}) + Y^{\nu p}(\alpha) \right] \dot{D} = Y(\varepsilon^{\nu e}, \alpha) \dot{D}, \qquad (5.20)$$

where  $Y^{ve}(\varepsilon^{ve}) : \mathbb{R} \to \mathbb{R}^-$  and  $Y^{vp}(\alpha) : \mathbb{R}^+ \to \mathbb{R}^-$  denote, respectively, the *visco-elastic/plastic* damage energy release rates. From (5.14), they are respectively given by:

$$Y^{ve}(\varepsilon^{ve}) = -\bar{\psi}^{ve}(\varepsilon^{ve}) = -\frac{1}{2} \int_0^\infty \tilde{E}(z) \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}^{ve}(s) \, ds \right)^2 dz.$$
(5.21)

$$Y^{\nu p}(\alpha) = -\bar{\psi}^{\nu p}(\alpha) = -\frac{1}{2} \int_0^\infty \tilde{K}(z) \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\alpha}(s) \, ds \right)^2 dz.$$
(5.22)

We observe from the above result that, in principle, both visco-elastic and visco-plastic parts release bulk energy with respect to damage. Inserting (5.18), (5.19) and (5.20) into (5.16), recalling Lemma 5.3.1, and dropping the function variables, we obtain:

$$\left[\tau - (1 - D) \mathbb{E}_{0}^{C} \mathcal{D}_{t}^{\beta E} \left(\varepsilon^{v e}\right)\right] \dot{\varepsilon}^{v e} + \tau \dot{\varepsilon}^{v p} - R\dot{\alpha}$$

$$- Y \dot{D} + (1 - D) \left(\mathcal{D}_{mech}^{v e} + \mathcal{D}_{mech}^{v p}\right) \ge 0.$$
(5.23)

Since the strain rate  $\dot{\varepsilon}^{ve}$  in (5.23) is arbitrary, without violating the inequality, we can set its multiplying argument to zero, and obtain the following stress-strain relationship:

$$\tau(t) = (1 - D) \mathbb{E}_0^C \mathcal{D}_t^{\beta_E} \left( \varepsilon^{ve} \right), \qquad (5.24)$$

and alternatively, using (5.13), we obtain:

$$\tau(t) = (1 - D) \mathbb{E}_{0}^{C} \mathcal{D}_{t}^{\beta_{E}} \left(\varepsilon - \varepsilon^{v_{p}}\right), \qquad (5.25)$$

and hence, the total energy dissipation (5.23) becomes:

$$\tau \dot{\varepsilon}^{vp} - R\dot{\alpha} - Y\dot{D} + (1 - D) \left( \mathcal{D}_{mech}^{ve} + \mathcal{D}_{mech}^{vp} \right) \ge 0.$$
(5.26)

Hence, we obtained the stress-strain relationships and dissipation potentials.

## 5.4.1.3 Evolution laws for visco-plasticity and damage

In order to obtain the kinematic equations for the internal variables, we define a combined hardening and damage dissipation potential  $F(\tau, \alpha, Y, D) : \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^- \times \mathbb{R}^+ \to \mathbb{R}$ , in the form [211, 213]:

$$F(\tau, \alpha, Y, D) := f(\tau, \alpha, D) + F_D(Y^{ve}, D), \qquad (5.27)$$

where  $f(\tau, \alpha, D) : \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^- \cup \{0\}$  represents a yield function, defined here as the difference between the absolute value of the applied stress in the device and the stress acting on the

visco-plastic part [1]:

$$f(\tau, \alpha, D) := |\tau| - \left[ (1 - D)\tau^Y + R \right]$$
$$= |\tau| - (1 - D) \left[ \tau^Y + \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha) + H\alpha \right], \tag{5.28}$$

which softens the visco-plastic stresses.

**Lemma 5.4.2.** The set of admissible stresses lies in a closed convex space (see Fig.5.2) with respect to the associated thermodynamic variables  $\tau$  and R [211], given by:

$$E_{\tau} = \{ \tau \in \mathbb{R} | f(\tau, \alpha, D) < 0 \}.$$

$$(5.29)$$

The boundary of  $E_{\tau}$ , denoted by  $\partial E_{\tau}$ , is the convex set given by:

$$\partial E_{\tau} = \{ \tau \in \mathbb{R} | f(\tau, \alpha, D) = 0 \},\$$

where  $f(\tau, \alpha, D) = 0$  denotes the yield condition in classical plasticity.

Proof. See Appendix B.3.

The term  $F_D(Y^{ve}, D) : \mathbb{R}^- \times \mathbb{R}^+ \to \mathbb{R}^+$  represents a damage potential driven by the plastic strains and visco-elastic free-energy (*see Assumption 2*), where we adopt Lemaitre's form for ductile materials [211]:

$$F_D(Y,D) := \frac{S}{(s+1)(1-D)} \left(-\frac{Y^{ve}}{S}\right)^{s+1},$$
(5.30)

where  $S \in \mathbb{R}^+$  [*Pa*] and  $s \in \mathbb{R}^+$  represent material parameters, identified, *e.g.*, by Cao *et al.* [235] for a Zirconium alloy, and by Bouchard *et al.* [236] for highly ductile metals. In the latter, an inverse power-law form for  $F_D$  was defined with respect to the equivalent plastic strains to avoid damage over-estimation. The sensitivity of Lemaitre's model with respect to *S* and *s* was studied by Roux and Bouchard [237].

From the defined yield function (5.28), and the principle of maximum plastic dissipation [192], the following properties hold: i) associativity of the flow rule, ii) associativity in the hardening law,

iii) Kuhn-Tucker complimentary conditions, and iv) convexity of  $E_{\tau}$ . Therefore, we obtain a set of evolution equations for  $\varepsilon^{vp}$ ,  $\alpha$  and D:

$$\dot{\varepsilon}^{vp} = \frac{\partial f}{\partial \tau} \dot{\gamma}, \quad \dot{\alpha} = -\frac{\partial f}{\partial R} \dot{\gamma}, \quad \dot{D} = -\frac{\partial F_D}{\partial Y^{ve}} \dot{\gamma},$$

where  $\dot{\gamma}(t) : \mathbb{R}^+ \to \mathbb{R}^+$  denotes the plastic slip rate. For simplicity, we consider only variations of the potential  $F_D$  with respect to the free-energy from the visco-elastic component for the damage evolution. Evaluating the above equations using (5.28) and (5.30), we obtain, respectively, the evolution for visco-plastic strains, hardening variable, and damage:

$$\dot{\varepsilon}^{vp} = \operatorname{sign}(\tau)\dot{\gamma},\tag{5.31}$$

$$\dot{\alpha} = \dot{\gamma},\tag{5.32}$$

$$\dot{D} = \frac{\dot{\gamma}}{(1-D)} \left(-\frac{Y^{ve}}{S}\right)^s,\tag{5.33}$$

where the first two evolution laws coincide with the ones defined for the model M1 by Suzuki *et al.* [1] for fractional visco-elasto-plasticity.

**Remark 5.4.3.** The obtained nonlinear damage evolution (5.33) coincides with the local Lemaitre form [211, 213]. However, due to the time-fractional form of  $Y^{ve}$ , power-law memory effects for damage are introduced in the model.

**Theorem 5.4.4** (Positive dissipation). *The mechanical dissipation for the damaged, fractional visco-elasto-plastic model is positive and given by,* 

$$(1 - D(t)) \left[ \tau^{Y} \dot{\gamma}(t) + \mathcal{D}_{mech}^{ve}(\varepsilon^{ve}) + \mathcal{D}_{mech}^{vp}(\alpha) \right] - Y(\varepsilon^{ve}, \alpha) \dot{D}(t) \ge 0,$$

where the above Clausius-Duhem inequality holds. Therefore, the defined Helmholtz free-energy density (5.15), the obtained stress-strain relationship (5.25) and evolution equations (5.31)-(5.33) of the developed model are thermodynamically admissible.

Proof. See Appendix B.2.

## 5.4.2 Time-fractional integration

We develop two new algorithms for time-fractional integration of the developed model. The first one is a semi-implicit *fractional return-mapping algorithm*, that can be implemented in zero- or one- dimensional systems as a constitutive box. The second one is an FD discretization for the fractional Helmholtz free-energy density and damage energy release rate Y (5.21). Let  $t \in (0, T]$ , and an uniform time grid given by  $t_n = n\Delta t$ , with n = 0, 1, ..., N and time-step size  $\Delta t = T/N$ .

## 5.4.2.1 Semi-implicit fractional return-mapping algorithm

We

employ a backward-Euler scheme considering all variables to be implicit, except the damage D in the stress-strain relationship and yield function. We refer the readers to [236] for a comparison between implicit/semi-implicit integer-order return-mapping algorithms. Such explicit treatment of D weakly couples the damage and plastic slip, simplifying the visco-plastic time-integration. Given known total strains  $\varepsilon_n$  at time  $t_n$ , and a strain increment  $\Delta \varepsilon_{n+1}$  we have  $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_{n+1}$ . The discrete form of the stress-strain relationship (5.25) reads:

$$\tau_{n+1} = (1 - D_n) \mathbb{E}_0^C \mathcal{D}_t^{\beta_E} \left(\varepsilon - \varepsilon^{v_p}\right)|_{t=t_{n+1}}.$$
(5.34)

The backward-Euler discretization of the flow rule (5.31) yields:

$$\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \operatorname{sign}(\tau_{n+1})\Delta\gamma, \qquad (5.35)$$

with  $\Delta \gamma = \gamma_{n+1} - \gamma_n$  representing the plastic slip increment in the interval [ $t_n$ ,  $t_{n+1}$ ]. Similarly, the discretization of the hardening law (5.32) and the damage evolution (5.33) are given, respectively, by

$$\alpha_{n+1} = \alpha_n + \Delta \gamma, \tag{5.36}$$

$$D_{n+1} = D_n + \frac{\Delta \gamma}{1 - D_{n+1}} \left(\frac{Y_{n+1}^{ve}}{S}\right)^s,$$
(5.37)

with the following discrete form for the damage energy release rate (5.21):

$$Y_{n+1}^{ve} = -\bar{\psi}_{n+1}^{ve} = -\frac{1}{2} \int_0^\infty \tilde{E}(z) \left( \int_0^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{z}\right) \dot{\varepsilon}^{ve}(s) \, ds \right)^2 dz.$$

Similarly, the yield function (5.28) evaluated at  $t_{n+1}$  is given by:

$$f_{n+1} = |\tau_{n+1}| - (1 - D_n) \left[ \tau^Y + \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha) |_{t=t_{n+1}} + H\alpha_{n+1} \right].$$
(5.38)

We utilize trial states, were we freeze the internal variables (except for damage) for the prediction step at  $t_{n+1}$ . Therefore, we have:

$$\varepsilon_{n+1}^{vp^{trial}} = \varepsilon_n^{vp}, \quad \alpha_{n+1}^{trial} = \alpha_n.$$

The trial visco-elastic stress and yield function are given, respectively, by

$$\tau_{n+1}^{trial} = (1 - D_n) \mathbb{E}_0^C \mathcal{D}_t^{\beta E} (\varepsilon - \varepsilon^{v p^{trial}})|_{t=t_{n+1}},$$

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - (1 - D_n) \left[ \tau^Y + \mathbb{K}_0^C \mathcal{D}_t^{\beta K} (\alpha^{trial})|_{t=t_{n+1}} + H \alpha^{trial} \right].$$
(5.39)

Substituting (5.35) into (5.34) and recalling (5.39), we obtain:

$$\tau_{n+1} = \tau_{n+1}^{trial} - \operatorname{sign}(\tau_{n+1})(1 - D_n) \mathbb{E}_0^C \mathcal{D}_t^{\beta E} (\Delta \gamma) \mid_{t=t_{n+1}},$$

where we observe that

$$\left[|\tau_{n+1}| + (1-D_n)\mathbb{E}_0^C \mathcal{D}_t^{\beta E}(\Delta \gamma)|_{t=t_{n+1}}\right]\operatorname{sign}(\tau_{n+1}) = |\tau_{n+1}^{trial}|\operatorname{sign}(\tau_{n+1}^{trial}).$$

Since the argument inside brackets on the LHS above is positive, we note that  $sign(\tau_{n+1}) = sign(\tau_{n+1}^{trial})$ . Hence, we have the updated stress:

$$\tau_{n+1} = \tau_{n+1}^{trial} - \operatorname{sign}(\tau_{n+1}^{trial})(1 - D_n) \mathbb{E}_0^C \mathcal{D}_t^{\beta E} (\Delta \gamma) |_{t=t_{n+1}}.$$
(5.40)

Our last step is to derive the closure to for the plastic slip  $\Delta \gamma$ . Substituting (5.40) and (5.36) into (5.38), we obtain:

$$f_{n+1} = f_{n+1}^{trial} - (1 - D_n) \left[ \mathbb{E}_0^C \mathcal{D}_t^{\beta E} \left( \Delta \gamma \right) |_{t=t_{n+1}} - \mathbb{K}_0^C \mathcal{D}_t^{\beta K} \left( \Delta \gamma \right) |_{t=t_{n+1}} - H \Delta \gamma \right].$$

Finally, setting the discrete yield condition  $f_{n+1} = 0$ , we obtain the following multi-term fractional differential equation for the plastic slip:

$$\mathbb{E}_{0}^{C}\mathcal{D}_{t}^{\beta E}\left(\Delta\gamma\right)|_{t=t_{n+1}} + \mathbb{K}_{0}^{C}\mathcal{D}_{t}^{\beta K}\left(\Delta\gamma\right)|_{t=t_{n+1}} + H\Delta\gamma = \frac{f_{n+1}^{trial}}{(1-D_{n})}.$$
(5.41)
After solving (5.41) for  $\Delta \gamma$ , we directly update the internal variables  $\alpha_{n+1}$  and  $\varepsilon_{n+1}^{\nu p}$ . The damage update is done through Newton iteration. Let  $P_{n+1}^k$  given at a sub-iteration k:

$$P_{n+1}^{k} = D_{n+1}^{k} - D_n - \frac{\Delta \gamma}{1 - D_{n+1}^{k}} \left(\frac{Y_{n+1}^{ve}}{S}\right)^{s},$$

with the following derivative, obtained analytically:

$$\frac{dP}{dD^k}\Big|_{t=t_{n+1}} = 1 + \frac{\Delta\gamma}{(1-D_{n+1}^k)^2} \left(\frac{Y_{n+1}^{ve}}{S}\right)^s.$$

Therefore, the new iterated damage is given by:

$$D_{n+1}^{k+1} = D_{n+1}^k - \frac{P_{n+1}^k}{\left(\frac{dP}{dD^k}\right)|_{t=t_{n+1}}}.$$

The developed fractional return-mapping algorithm is summarized in Algorithm 5.1.

### 5.4.2.2 Numerical discretization of fractional operators

The fractional derivatives in the fractional return-mapping Algorithm 5.1 are evaluated implicitly using the L1 FD method [91]. Let  $u(t) : \mathbb{R}^+ \to \mathbb{R}$ . The time-fractional Caputo derivative of order  $0 < \beta < 1$  is discretized as:

$${}_{0}^{C} \mathcal{D}_{t}^{\beta} u(t) \Big|_{t=t_{n+1}} = \frac{1}{\Gamma(2-\beta)} \sum_{j=0}^{n} d_{j} \frac{u_{n+1-j} - u_{n-j}}{\Delta t^{\beta}} + r_{\Delta t}^{n+1},$$
(5.42)

where  $r_{\Delta t}^{n+1} \leq C_u \Delta t^{2-\beta}$  and  $d_j := (j+1)^{1-\beta} - j^{1-\beta}$ , j = 0, 1, ..., n. The above expression can be rewritten and approximated as:

$$\left. \begin{smallmatrix} C \\ 0 \end{smallmatrix} \right|_{t=t_{n+1}} \approx \frac{1}{\Delta t^{\beta} \Gamma(2-\beta)} \left[ u_{n+1} - u_n + \mathcal{H}^{\beta} u \right],$$

where the so-called *history term*  $\mathcal{H}^{\beta}u$  is given by:

$$\mathcal{H}^{\beta} u = \sum_{j=1}^{n} d_j \left[ u_{n+1-j} - u_{n-j} \right].$$
(5.43)

Using (5.42) does not cause any loss of accuracy for the return-mapping, since the backward-Euler approach for internal variables is first-order accurate. For trial state variables  $u_{n+1}^{trial} = u_n$ , the discretized Caputo fractional derivatives are given by:

$${}_{0}^{C}\mathcal{D}_{t}^{\beta}u^{trial}(t)\Big|_{t=t_{n+1}} \approx \frac{\mathcal{H}^{\beta}u}{\Delta t^{\beta}\Gamma(2-\beta)}.$$
(5.44)

Algorithm 5.1: Fractional return-mapping algorithm.

1: Database for 
$$\varepsilon$$
,  $\varepsilon^{vp}$ ,  $\alpha$ ,  $\Delta \gamma$ ,  $D_n$  and total strain  $\varepsilon_{n+1}$ .  
2:  $\varepsilon_{n+1}^{vptrial} = \varepsilon_n^{vp}$ ,  $\alpha_{n+1}^{trial} = \alpha_n$   
3:  $\tau_{n+1}^{trial} = (1 - D_n) \mathbb{E}_0^0 \mathcal{D}_0^{\beta E} (\varepsilon - \varepsilon^{vptrial})|_{t=t_{n+1}}$   
4:  $f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - (1 - D_n) \left[ \tau^Y + \mathbb{K}_0^0 \mathcal{D}_t^{\beta K} (\alpha^{trial})|_{t=t_{n+1}} + H\alpha^{trial} \right]$   
5: if  $f_{n+1}^{trial} \le 0$  then  
6:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp}$ ,  $\alpha_{n+1} = \alpha_n$ ,  $D_{n+1} = D_n$ ,  $\tau_{n+1} = \tau_{n+1}^{trial}$ .  
7: else  
8: Solve for  $\Delta \gamma$ :  
9:  $\mathbb{E}_0^0 \mathcal{D}_t^{\beta E} (\Delta \gamma)|_{t=t_{n+1}} + \mathbb{K}_0^0 \mathcal{D}_t^{\beta K} (\Delta \gamma)|_{t=t_{n+1}} + H\Delta \gamma = f_{n+1}^{trial}/(1 - D_n)$   
10:  $\tau_{n+1} = \tau_{n+1}^{trial} - \operatorname{sign}(\tau_{n+1}^{trial})(1 - D_n) \mathbb{E}_0^0 \mathcal{D}_t^{\beta E} (\Delta \gamma)|_{t=t_{n+1}}$   
11:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \operatorname{sign}(\tau_{n+1})\Delta \gamma$   
12:  $\alpha_{n+1} = \alpha_n + \Delta \gamma$   
13:  $Y_{n+1}^{ve} = -\frac{1}{2} \int_0^\infty \tilde{E}(z) \left( \int_0^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{z}\right) \dot{\varepsilon}^{ve}(s) ds \right)^2 dz$  (Algorithm 5.2).  
14: while  $|P_{n+1}^k| > \epsilon$  do  
15:  $P_{n+1}^k = D_{n+1}^k - D_n - \frac{\Delta \gamma}{1 - D_{n+1}^k} \left( \frac{Y_{n+1}^{ve}}{s} \right)^s$   
16:  $\left( dP/dD^k \right)|_{t=t_{n+1}} = 1 + \frac{\Delta \gamma}{(1 - D_{n+1}^k)^2} \left( \frac{Y_{n+1}^{ve}}{s} \right)^s$   
17:  $D_{n+1}^{k+1} = D_{n+1}^k - \frac{P_{n+1}^k}{(dP/dD^k)|_{t=t_{n+1}}}$   
18: end while

19: end if

**Free-Energy/Damage Energy Release Rate:** We now discretize the visco-elastic damage energy release rate  $Y^{ve} = -\bar{\psi}^{ve}$ . We first rewrite (5.10) as [35]:

$$\psi(\varepsilon) = \frac{\mathbb{E}}{2\Gamma(1-\beta)} \int_0^t \int_0^t \frac{\dot{\varepsilon}(s_1)\dot{\varepsilon}(s_2)}{(2t-s_1-s_2)^{\beta}} \, ds_1 \, ds_2.$$
(5.45)

We then decompose the integral signs of (5.45) into a discrete summation of *n* integrals and approximate  $\dot{\varepsilon}(t)$  using a backward-Euler scheme to obtain,

$$\begin{split} \psi(\varepsilon_{n+1}) &= \frac{\mathbb{E}}{2\Gamma(1-\beta)} \int_{0}^{t_{n+1}} \int_{0}^{t_{n+1}} \frac{\dot{\varepsilon}(s_1)\dot{\varepsilon}(s_2)}{(2t_{n+1}-s_1-s_2)^{\beta}} \, ds_1 \, ds_2 \\ &= \frac{\mathbb{E}}{2\Gamma(1-\beta)} \sum_{i=0}^{n} \sum_{j=0}^{n} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} \frac{\Delta\varepsilon_{i+1}\Delta\varepsilon_{j+1}}{\Delta t^2 (2t_{n+1}-s_1-s_2)^{\beta}} \, ds_1 \, ds_2 + \tilde{r}_{\Delta t}^{n+1}, \end{split}$$
(5.46)

with  $\Delta \varepsilon_{k+1} = \varepsilon_{k+1} - \varepsilon_k$ 

**Theorem 5.4.5.** The local truncation error  $\tilde{r}_{\Delta t}^{n+1}$  for (5.46) satisfies

$$\tilde{r}_{\Delta t}^{n+1} \le C \Delta t^{2-\beta},\tag{5.47}$$

where C denotes a constant depending only on the strain  $\varepsilon(t)$ .

Proof. See Appendix B.4.

Let the first term of the RHS of (5.46) be the approximation  $\psi_{n+1}^{\delta} \approx \psi(\varepsilon_{n+1})$  evaluated at  $t = t_{n+1}$ . Performing a change of variables  $v_1 = t_{n+1} - s_1$  and  $v_2 = t_{n+1} - s_2$ , we obtain:

$$\psi_{n+1}^{\delta} = \mathbb{E}^* \sum_{i=0}^n \sum_{j=0}^n \frac{\Delta \varepsilon_{i+1} \Delta \varepsilon_{j+1}}{\Delta t^2} \int_{t_{n-i}}^{t_{n+1-i}} \int_{t_{n-j}}^{t_{n+1-j}} (v_1 + v_2)^{-\beta} dv_1 dv_2,$$
(5.48)

with  $\mathbb{E}^* = \mathbb{E}/(2\Gamma(1 - \beta))$ . Using the symmetry between the indices of strains and integration limits in (5.48), we obtain:

$$\psi_{n+1}^{\delta} = \mathbb{E}^* \sum_{i=0}^n \sum_{j=0}^n \frac{\Delta \varepsilon_{n-i+1} \Delta \varepsilon_{n-j+1}}{\Delta t^2} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (v_1 + v_2)^{-\beta} dv_1 dv_2.$$
(5.49)

We can analytically evaluate the double integral sign in (5.49) to obtain:

$$\int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (v_1 + v_2)^{-\beta} dv_1 dv_2 = \frac{\Delta t^{2-\beta}}{(1-\beta)(2-\beta)} \left[ (i+j)^{2-\beta} - 2(i+j+1)^{2-\beta} + (i+j+2)^{2-\beta} \right].$$
(5.50)

Substituting (5.50) into (5.49), we obtain the discrete free-energy density,

$$\psi_{n+1}^{\delta} = \frac{\mathbb{E}}{2\Delta t^{\beta} \Gamma(3-\beta)} \sum_{i=0}^{n} \sum_{j=0}^{n} b_{ij}^{(\beta)} (\varepsilon_{n+1-i} - \varepsilon_{n-i}) (\varepsilon_{n+1-j} - \varepsilon_{n-j}), \tag{5.51}$$

with the following entries for the convolution weight matrix:

$$b_{ij}^{(\beta)} = (i+j)^{2-\beta} - 2(i+j+1)^{2-\beta} + (i+j+2)^{2-\beta}, \quad i, j = 0, 1, \dots, n.$$

We can also rewrite (5.51) as the following matrix-vector product:

$$\psi_{n+1}^{\delta} = \frac{\mathbb{E}}{2\Delta t^{\beta} \Gamma(3-\beta)} \Delta \varepsilon_{n+1}^{T} \mathbf{B}_{n+1} \Delta \varepsilon_{n+1}, \qquad (5.52)$$

where we note that  $\mathbf{B}_{n+1}$  is an  $n \times n$  Hankel matrix of convolution weights with 2n - 1 unique entries  $b_{ij}^{(\beta)}$ . The  $n \times 1$  vector  $\Delta \varepsilon_{n+1}$  is given by:

$$\Delta \boldsymbol{\varepsilon}_{n+1} = [\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}_n, \ \boldsymbol{\varepsilon}_n - \boldsymbol{\varepsilon}_{n-1}, \ \dots, \ \boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1, \ \boldsymbol{\varepsilon}_1 - \boldsymbol{\varepsilon}_0]^T .$$
(5.53)

**Fast Computation of Matrix-Vector Products:** The form (5.52) requires a full matrix-vector product with complexity  $O(n^2)$  for every time-step, and consequently  $O(N^3)$  for full time-integration. Our aim is to reduce such complexity by leveraging the obtained matrix forms. Since **B** is a Hankel matrix, it relates to a Toeplitz matrix  $\mathbf{T}_{n+1}$  through  $\mathbf{B}_{n+1} = \mathbf{T}_{n+1}\mathbf{J}_{n+1}$ , where  $\mathbf{J}_{n+1}$  represents a reflection matrix with ones in the secondary diagonal and zero everywhere else. Therefore, we obtain:

$$\psi_{n+1}^{\delta} = \frac{\mathbb{E}}{2\Delta t^{\beta} \Gamma(3-\beta)} \Delta \varepsilon_{n+1}^{T} \mathbf{T}_{n+1} \mathbf{J}_{n+1} \Delta \varepsilon_{n+1}.$$
(5.54)

The Toeplitz matrix has a circulant embedding of size  $2n \times 2n$  [238], fully described by a  $2n \times 1$  vector of unique coefficients:

$$\mathbf{c}_{n+1}^{(\beta)} = \begin{bmatrix} b_{0,n}^{(\beta)}, \ b_{1,n}^{(\beta)}, \ \dots, \ b_{n,n}^{(\beta)}, \ 0, \ b_{0,0}^{(\beta)}, \ b_{0,1}^{(\beta)}, \ \dots, \ b_{0,n-1}^{(\beta)} \end{bmatrix}^T.$$
(5.55)

Let the following zero-padded vector  $\Delta \varepsilon_{n+1}^*$ , with size  $2n \times 1$ :

$$\Delta \boldsymbol{\varepsilon}_{n+1}^* = \left[ (\Delta \boldsymbol{\varepsilon}_{n+1}^f)_{n \times 1}, \ (\mathbf{0})_{n \times 1} \right]^T, \tag{5.56}$$

where  $\Delta \varepsilon_{n+1}^{f} = \mathbf{J}_{n+1} \Delta \varepsilon_{n+1}$  denotes the reflection of  $\Delta \varepsilon_{n+1}$ , given by:

$$\Delta \boldsymbol{\varepsilon}_{n+1}^{f} = \left[\varepsilon_{1} - \varepsilon_{0}, \ \varepsilon_{2} - \varepsilon_{1}, \ \dots, \ \varepsilon_{n} - \varepsilon_{n-1}, \ \varepsilon_{n+1} - \varepsilon_{n}\right]^{T}.$$
(5.57)

Finally, we obtain the fast form of (5.52) for every time-step  $t_{n+1}$ :

$$\psi_{n+1}^{\delta} = \frac{\mathbb{E}}{2\Delta t^{\beta} \Gamma(3-\beta)} \Delta \varepsilon_{n+1}^{T} \mathcal{F}^{-1} \left( \mathcal{F}(\mathbf{c}_{n+1}^{(\beta)}) \odot \mathcal{F}(\Delta \varepsilon_{n+1}^{*}) \right),$$
(5.58)

where  $\mathcal{F}(\cdot)$  and  $\mathcal{F}^{-1}(\cdot)$  denote, respectively, the forward and inverse FFTs and  $\odot$  represents the Hadamard entry-wise product. Recalling  $Y^{ve}(\varepsilon^{ve}) = -\bar{\psi}^{ve}(\varepsilon^{ve})$ , the discrete damage energy release rate is given by:

$$Y_{n+1}^{ve} = -\frac{\mathbb{E}}{2\Delta t^{\beta E} \Gamma(3-\beta_E)} \Delta \varepsilon_{n+1}^{ve^T} \mathcal{F}^{-1} \left( \mathcal{F}(\mathbf{c}_{n+1}^{(\beta_E)}) \odot \mathcal{F}(\Delta \varepsilon_{n+1}^{ve^*}) \right),$$
(5.59)

Algorithm 5.2: Fast computation of fractional damage energy release rate.

- 1: Database:  $\boldsymbol{\varepsilon}^{ve}$  and 2N 1 coefficients  $b_{0,0}^{(\beta_E)}, \ldots, b_{0,N}^{(\beta_E)}, b_{1,N}^{(\beta_E)}, \ldots, b_{N,N}^{(\beta_E)}$ .
- 2: Compute  $\Delta \varepsilon_{n+1}^{ve}$  using (5.53), and form  $\Delta \varepsilon_{n+1}^{ve^*}$  using (5.56).
- 3: Compute the FFT  $\mathcal{F}(\Delta \varepsilon_{n+1}^{ve^*})$ .
- 4: Compute  $\mathbf{c}_{n+1}^{(\beta_E)}$  using (5.55), using the known  $b^{(\beta_E)}$  coefficients.
- 5: Compute the FFT  $\mathcal{F}(\mathbf{c}_{n+1}^{(\beta_E)})$ . 6:  $Y_{n+1}^{ve} = -\frac{\mathbb{E}}{2\Delta t^{\beta_E} \Gamma(3-\beta_E)} \Delta \boldsymbol{\varepsilon}_{n+1}^{ve^T} \mathcal{F}^{-1} \left( \mathcal{F}(\mathbf{c}_{n+1}^{(\beta_E)}) \odot \mathcal{F}(\Delta \boldsymbol{\varepsilon}_{n+1}^{ve^*}) \right)$ . 7: return  $Y_{n+1}^{ve}$ .

where,

$$\Delta \boldsymbol{\varepsilon}_{n+1}^{ve} = \left[ \boldsymbol{\varepsilon}_{n+1}^{ve} - \boldsymbol{\varepsilon}_{n}^{ve}, \ \boldsymbol{\varepsilon}_{n}^{ve} - \boldsymbol{\varepsilon}_{n-1}^{ve}, \ \dots, \ \boldsymbol{\varepsilon}_{2}^{ve} - \boldsymbol{\varepsilon}_{1}^{ve}, \ \boldsymbol{\varepsilon}_{1}^{ve} - \boldsymbol{\varepsilon}_{0}^{ve} \right]^{T},$$
(5.60)

and with  $\Delta \varepsilon_{n+1}^{ve^*}$  being the reflected and zero-padded form of (5.60). Also, the vector  $\mathbf{c}_{n+1}^{(\beta_E)}$  is given by:

$$\mathbf{c}_{n+1}^{(\beta_E)} = \begin{bmatrix} b_{0,n}^{(\beta_E)}, \ b_{1,n}^{(\beta_E)}, \ \dots, \ b_{n,n}^{(\beta_E)}, \ 0, \ b_{0,0}^{(\beta_E)}, \ b_{0,1}^{(\beta_E)}, \ \dots, \ b_{0,n-1}^{(\beta_E)} \end{bmatrix}^T,$$
(5.61)

with  $b_{ij}^{(\beta E)} = (i+j)^{2-\beta E} - 2(i+j+1)^{2-\beta E} + (i+j+2)^{2-\beta E}$  and i, j = 0, 1, ..., n. Algorithm 5.2 demonstrates the numerical evaluation of the damage energy release rate for every time-step  $t = t_{n+1}$ .

**Computational Complexity of the Developed Scheme:** Employing (5.59) for full timefractional integration over  $\Omega$  yields a total computational complexity of  $O(N^2 \log N)$ , similar to the  $O(N^2)$  complexity of the employed L1 FD scheme for fractional Caputo derivatives. Furthermore, the required storage for the developed scheme is O(N).

### 5.5 Numerical Tests

We present two qualitative examples with monotone/cyclic loads for the SB free-energy density and the developed damaged, visco-elasto-plastic model, where we verify the convergence and computational complexity of the developed algorithms. For convergence analyses, let  $\mathbf{u}^*$  and  $\mathbf{u}^{\delta}$ be, respectively, the reference and approximate solutions in  $\Omega = (0, T]$ , for a specific time-step size  $\Delta t$ . The global relative error and convergence order are given, respectively, as:

$$\operatorname{err}(\Delta t) = \frac{||\mathbf{u}^* - \mathbf{u}^o||_{L^{\infty}(\Omega)}}{||\mathbf{u}^*||_{L^{\infty}(\Omega)}}, \quad \operatorname{Order} = \log_2\left[\frac{\operatorname{err}(\Delta t)}{\operatorname{err}(\Delta t/2)}\right]$$
(5.62)

We consider homogeneous initial conditions for all model variables in all cases. The presented algorithms were implemented in MATLAB R2019a and were run in a system with Intel Core i7-6700 CPU with 3.40 GHz, 16 GB RAM and Ubuntu 18.04.2 LTS operating system.

**Example 1** (Convergence for Free-Energy Density). We start with two convergence tests for the fractional Helmholtz free-energy density using fabricated solutions. The first one employs second-order increasing monotone strains, and the second uses cyclic varying strains.

•Monotone Strains. Let  $t \in (0, T]$ , with total time T = 1 [s]. We define the quadratic strain form  $\varepsilon(t) = (t/T)^2$ . Therefore, analytical solution for the Helmholtz free-energy (5.10) can be obtained directly as:

$$\psi^*(\varepsilon) = \frac{2^{2-\beta} \left[8 + 2^\beta \left(\beta - 5\right)\right]}{\Gamma(5-\beta)} T^4 \mathbb{E} \varepsilon^{2-\frac{\beta}{2}}.$$

We set  $\mathbb{E} = 100 [Pa.s^{\beta}]$ , and estimate the computational complexity of the direct (5.54) and fast (5.58) forms, with varying  $\Delta t$ . Figure 5.3 presents the approximate free-energy solution, where we recover the standard limit cases of a Hookean spring ( $\beta \rightarrow 0$ ) and a Newtonian dashpot ( $\beta \rightarrow 1$ ), as well as second-order accuracy for the developed discretization. Figure 5.4 presents the obtained  $O(N^3)$  and  $O(N^2 \log N)$  computational complexities, respectively, for the direct and FFT-based free-energy time-integration schemes. The break-even point lies at N = 200 time-steps.

•Cyclic Strains. We utilize a fabricated sinusoidal strain solution  $\varepsilon(t) = \varepsilon_0 \sin(\omega t)$ , with  $t \in (0, T]$ , with amplitude  $\epsilon_0$  and frequency  $\omega$ . The corresponding analytical solution for  $\psi^*$  is cumbersome, and therefore not shown here. We set  $\varepsilon_0 = 1$ ,  $\omega = \pi [s^{-1}]$ , T = 50 [s],  $\beta = 0.5$  and  $\mathbb{E} = 1 [Pa.s^{0.5}]$ , and start with a sufficient number of time-steps to capture the oscillation modes. Figure 5.5 illustrates the obtained results, where we capture the highly oscillatory behavior for both transient and steady-state parts with second-order accuracy.

**Example 2** (Fractional Visco-Elasto-Plastic Model with Damage). We test our developed model and fractional return-mapping algorithm subject to prescribed monotone/cyclic strains. The con-



Figure 5.3: Numerical results for the free-energy computation with a quadratic form for  $\varepsilon(t)$ . (*Left*)  $\psi^{\delta}$  vs strain with varying  $\beta$ . (*Right*) Relative error vs time-step size for varying  $\beta$ , with second-order accuracy.



Figure 5.4: CPU time *vs* number of time-steps of the developed time-integration schemes for the fractional Helmholtz free-energy density under monotone strains.

vergence analysis is done with a benchmark solution and we analyze the quality of the anomalous damage response with respect to the fractional orders  $\beta_E$ ,  $\beta_K$  from visco-elasticity/plasticity under different strain amplitudes/frequencies.

• Monotone Strains. Let  $\varepsilon(t) = \dot{\varepsilon}t$ , where  $t \in (0, T]$ , final time T = 0.03125 [s] and strain rate  $\dot{\varepsilon} = 0.64 [s^{-1}]$ , and therefore  $\varepsilon(T) = 0.02$ . We set  $\beta_E = 0.5$ ,  $\mathbb{E} = 50 [Pa.s^{0.5}]$ ,  $\mathbb{K} = 10 [Pa.s^{\beta K}]$ ,  $\tau^Y = 1 [Pa]$ ,  $S = 10^{-4} [Pa]$  and s = 1. A benchmark solution for the stress (see Fig.5.6) is computed with time-step size  $\Delta t = 2^{-20} [s]$  and varying fractional orders  $\beta_K$ , where we observe that higher



Figure 5.5: (A) Free-energy density computations for cyclic strains vs time, N = 3200 time-steps and  $\beta = 0.5$ . (B) Convergence analysis showing second-order accuracy.



Figure 5.6: Stress vs strain for the benchmark solution with time-step size  $\Delta t = 2^{-20}$ ,  $\beta_E = 0.5$  and different  $\beta_K$  values.

values for  $\beta_K$  led to increased hardening and damage for the prescribed strain rate. We observe a linear convergence rate in Figure 5.7a, due to the employed backward-Euler discretization in the fractional return-mapping algorithm. A second-order computational complexity for the fractional return-mapping algorithm is also verified in Figure 5.7b. The influence of hardening and viscoelastic damage energy release rate is shown in Figure 5.8. We observe that higher damage values are obtained for  $\beta_K = 0.7$ , despite the higher accumulated plastic strains for lower values of  $\beta_K$ . The higher damage is instead due to higher values of damage energy release rates shown in Figure



Figure 5.7: Fractional visco-elasto-plastic model with damage under monotone strains. (A) First-order convergence behavior. (B) Computational time vs number of time-steps, with second-order computational complexity.



Figure 5.8: Developed model under monotone strains: (A) Damage vs accumulated plastic strain, with higher damage but less plasticity for higher  $\beta_K$ . (B) Damage energy release rate vs visco-elastic strains, which are both larger for higher values of fractional order  $\beta_K$ .

5.8b for  $\beta_K = 0.7$ . We note that similar to the stress-strain response, the visco-elastic fractional free-energy is power-law memory-dependent on the strain rates, therefore leading to the observed anomalous behavior.

• *Cyclic Strains.* To investigate the interplay between the damage/hardening/viscosity and hysteresis effects, we perform a constant rate loading/unloading cyclic strain test, mathematically

expressed as:

$$\varepsilon(t) = \frac{2\varepsilon_A}{\pi} \arcsin\left(\sin\left(2\pi\omega t\right)\right),$$

where  $\varepsilon_A$  and  $\omega$  represent, respectively, the amplitude and frequency of total strains. Here, we focus on low-cycle fatigue behavior, and therefore we set  $\varepsilon = 0.1$ , and three strain frequencies  $\omega = \{2\pi, 4\pi, 8\pi\} [s^{-1}]$ , which correspond, respectively, to approximate absolute strain rates of  $|\dot{\varepsilon}| \approx \{2.51, 5.02, 10.05\}$ . We set a total time T = 10 [s], and for each frequency, we use  $N = \{8\ 000, 16\ 000, 32\ 000\}$  time-steps, corresponding to  $\Delta t = \{1.25 \times 10^{-3}, 6.25 \times 10^{-4}, 3.125 \times 10^{-4}\} [s]$ . The material parameters are set to  $\mathbb{E} = 25 [Pa.s^{\beta}E]$ ,  $\mathbb{K} = 10 [Pa.s^{\beta}K]$ ,  $\tau^Y = 1 [Pa]$ , S = 1 [Pa] and s = 1, where we set the fractional order values  $\beta_E = \beta_K = \{0.3, 0.5, 0.7\}$ .

The stress-strain hysteresis results are presented in Figure 5.9. We observe that higher frequencies led to more softening in the model, while higher values of fractional orders  $\beta_E$ ,  $\beta_K$  led to increased hardening, followed by softening. Such damage increase is illustrated in Fig. 5.10, where we observe that higher  $\beta_E$  and  $\beta_K$  values led to increased plasticity for all cases, with a significant increase of damage rates for  $\beta_E = \beta_K = 0.5, 0.7$  when  $\omega = 8\pi$ . We also observe from Fig. 5.11 that due to the anomalous nature of the fractional visco-elastic free-energy potential, the damage energy release rates substantially increase with higher fractional orders and loading rates, which contribute to the observed higher values of damage. Therefore, for this model, higher material viscosity in both visco-elastic and visco-plastic parts might be sufficient to yield lower values of damage at low frequencies due to internal dissipation mechanisms, but at higher frequencies and therefore more loading cycles, they lead to earlier material failure.



Figure 5.9: Stress hysteresis response for cyclic strains with frequencies (A)-(C)  $\omega = 2\pi$ , (D)-(F)  $\omega = 4\pi$ , (G)-(I)  $\omega = 8\pi$ .



Figure 5.10: Damage vs accumulated plastic strains with varying strain frequencies.



Figure 5.11: Damage energy release rate vs time for the total strain with varying frequency.

#### **CHAPTER 6**

### A GENERAL RETURN-MAPPING FRAMEWORK FOR FRACTIONAL VISCO-ELASTO-PLASTICITY

# 6.1 Background

Experimental evidence suggests that complex material behavior may possess more than a single power-law scaling in the viscoelastic regime, particularly in multi-fractal structures, which are characteristic of cells [25] and biological tissues [173], due to their complex, hierarchical and heterogeneous microstructure. For such cases, a single fractional rheological element is not sufficient to capture the observed behavior, even if data suggests a linear viscoelastic behavior. Stamenović [25] measured the complex shear modulus of cultured human airway smooth muscle and observed two distinct power-law regimes separated by an intermediate *plateau*. In [23] Kapnistos *et al.* found an unexpected tempered power-law relaxation response of entangled polystyrene ring polymers, compared to the usual relaxation plateau of linear chain polymers. Such behavior was interpreted through self-similar conformations of double-folded loops the in ring polymers, instead of the reptation observed in linear chains.

In addition to multiple viscoelastic power-law behaviors, there also exists evidence of bioplasticity in soft media [20, 21]. The creep behavior of human embrionic stem cells (ESCs) under differentiation was studied by Pajerowski *et al.* in [20] through micro-aspiration experiments at different pressures. The cell nucleous demonstrated distinguished visco-elasto-plastic power-law scalings, with  $\alpha = 0.2$  for the plastic regime, independent of the applied pressure. It is discussed that such low power-law exponent arises due to the fractal arrangement of chromatin inside the cell nucleus. Studies on force-induced mechanical plasticity of mouse embrionic fibroblasts were performed by Bonadkar *et al.* in [21]. It was found that the viscoelastic relaxation and the permanent deformations followed a stochastic, normally-distributed, power-law scaling  $\beta(\omega)$ , with values ranging from  $\beta \approx 0$  to  $\beta \approx 0.6$ . The microstructural mechanism of plastic deformation in the cytoskeleton is due to the combination of permanent stretching and buckling of actin fibers.

Regarding existing modeling approaches of anomalous plasticity, several works employed fractional calculus to account for the visco-plastic regimes of several classes of materials, and we outline three of them: Time-fractional, space-fractional and stress-fractional. Time-fractional approaches focus on introducing memory effects into non-equilibrium viscous variables [1, 46], and consequently modeling power-laws in both visco-elastic and visco-plastic regimes, which is of interest for polymers, cells, and tissues. Suzuki et al. [1] developed a fractional visco-elasto-plastic model that provides a constitutive interpolation between rate-independent plasticity and Perzyna's visco-plasticity by introducing a SB model acting the plastic regime, and utilizes a rate-dependent yield function, which was later proved to be thermodynamically consistent in a further extension of the model to account for continuum damage mechanics [75]. A three-dimensional space-fractional approach to elastoplasticity was also developed by Sumelka [47] in order to account for spatial nonlocalities. The model is based on rate-independent elastoplasticity, and nonlocal effects are accounted through a fractional continuum mechanics approach, where the strains are defined through a space-fractional Riesz-Caputo derivative of the displacements. Finally, stress-fractional models for plasticity have found to be interesting for soil mechanics and geomaterials that follow nonassociated plastic flow [48, 49], *i.e.*, the yield surface expansion in the stress space does not follow the usual normality rule, and may be non-convex. Sumelka [48] proposed a three-dimensional fractional visco-plastic model, where a fractional flow-rule with order  $0 < \alpha < 1$  in the stress domain naturally models non-associative plasticity. Interestingly, this model recovers the classical Perzyna visco-plasticity as  $\alpha \to 1$ , and the effect of the fractional flow rule can be a compact descriptor of micro-structure anisotropy. Later on, Sun and Sumelka [49] developed a similar stress-fractional model, which was successfully applied for soils under compression. We refer the reader to the interesting review work by Sun et al. [50] a review of fractional calculus applications in plasticity.

In this work we develop a generalized fractional visco-elasto-plastic models, where the viscoplastic device can be coupled several existing fractional linear/nonlinear viscoelastic representations. More specifically, we utilize a fractional viscoplastic device developed in [1, 75], which is then couple with a series of linear fractional models, such as Scott-Blair (SB), Kelvin-Voigt (FKV), Maxwell (FM), Kelvin-Zener (FKZ), Poynting-Thomson (FPT); and also a quasi-linear model for large strains. Then, a generalized fractional return-mapping algorithm is proposed, which overcomes existing difficulties in previous developments by first fully-discretizing all fractional operators, and then performing the predictor-corrector procedure. More specifically, existing approaches are built on the notion of employing the predictor-corrector approach before the full discretization of fractional operators, while treating trial states for stress and internal variables to be continuous functions of time. This prevents models with serial combinations of SB elements to be incorporated in associated yield functions in a straightforward fashion. The main features of the proposed framework are:

- We perform a full discretization of fractional viscoelastic models prior to the definition of trials states, which allows a linear decomposition between final and trial stresses regardless of the employed models.
- The fractional return-mapping algorithm is fully-implicit for linear viscoelastic rheology, and semi-implicit for quasi-linear viscoelasticity.
- Due to the full-discretization before the return-mapping procedure, the operations involving the plastic-slip are memoryless, which resembles return-mapping steps from classical elastoplasticity.
- The correction (return-mapping) step has the same structure regardless of the employed viscoelastic models.

We carry out a number of numerical experiments involving fabricated and reference solutions under monotone and general loading conditions, and observe a global accuracy ranging from  $O(\Delta t)$ to  $O(\Delta t^{2-\beta})$ , according to the regularity induced by the associated FDEs and loading conditions. This work is organized as follows. In Section 6.2 we present the mathematical definitions employed in this work. In Section 6.3 we describe the considered linear/quasi-linear fractional visco-elastic models, that are coupled with fractional visco-elasto-plasticity in Section 6.4. All corresponding models are discretized and posed in a unified fractional return-mapping form in Section 6.5. Convergence analyses and computational performance of presented models and return-mapping algorithm are performed in Section 6.6.

# 6.2 Definitions of Fractional Calculus

We start with some preliminary definitions of fractional calculus [33]. The left-sided Riemann-Liouville integral of order  $\beta \in (0, 1)$  is defined as

$$\binom{RL}{t_L} \mathcal{I}_t^{\beta} f(t) = \frac{1}{\Gamma(\beta)} \int_{t_L}^t \frac{f(s)}{(t-s)^{1-\beta}} \, ds, \quad t > t_L,$$

where  $\Gamma$  represents the Euler gamma function and  $t_L$  denotes the lower integration limit. The corresponding inverse operator, i.e., the left-sided fractional derivative of order  $\beta$ , is then defined based on (1.1) as

$$\binom{RL}{t_L}\mathcal{D}_t^{\beta}f(t) = \frac{d}{dt}\binom{RL}{t_L}\mathcal{I}_t^{1-\beta}f(t) = \frac{1}{\Gamma(1-\beta)}\frac{d}{dt}\int_{t_L}^t \frac{f(s)}{(t-s)^{\beta}}\,ds, \quad t > t_L.$$
(6.1)

Also, the left-sided Caputo derivative of order  $\beta \in (0, 1)$  is obtained as

$$\binom{C}{t_L}\mathcal{D}_t^{\beta}f(t) = \binom{RL}{t_L}I_t^{1-\beta}\frac{df}{dt}(t) = \frac{1}{\Gamma(1-\beta)}\int_{t_L}^t \frac{f'(s)}{(t-s)^{\beta}}\,ds, \quad t > t_L.$$
(6.2)

The definitions of Riemann-Liouville and Caputo derivatives are linked by the following relationship:

$$\binom{RL}{t_L}\mathcal{D}_t^{\beta}f(t) = \frac{f(t_L)}{\Gamma(1-\beta)(t+t_L)^{\beta}} + \binom{C}{t_L}\mathcal{D}_t^{\beta}f(t),$$
(6.3)

which can be obtained through integration by parts followed by the application of Leibniz rule on (6.1). We note that the aforementioned derivatives coincide when dealing with homogeneous Dirichlet initial/boundary conditions. Finally, we define the two-parameter Mittag-Leffler function  $E_{a,b}(z)$  as [32]:

$$E_{a,b}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(ak+b)}, \quad Re(a) > 0, \quad b \in \mathbb{C}, \quad z \in \mathbb{C}.$$
(6.4)

# 6.3 Fractional Visco-Elasticity

We present the linear and quasi-linear fractional visco-elastic models that we couple with the visco-plastic return-mapping procedure.

### 6.3.1 Linear visco-elasticity



Figure 6.1: Fractional linear viscoelastic models employed in this work, constructed from serial/parallel combinations of SB elements. The SB building blocks naturally account for an infinite fractal arrangement of Hookean/Newtonian elements. The fractional quasi-linear model employed is not represented by a mechanical analogue, although the time-dependent component of the relaxation function has a SB-like representation.

**Scott-Blair (SB) Model:** The rheological *building block* for our framework is the fractional *Scott-Blair* (SB) visco-elastic element, which compactly represents an anomalous visco-elastic constitutive law connecting the stresses and strains:

$$\sigma(t) = \mathbb{E} {}_{0}^{C} \mathcal{D}_{t}^{\beta} \varepsilon(t), \quad t > 0, \quad \varepsilon(0) = 0,$$
(6.5)

with pseudo-constant  $\mathbb{E}_1[Pa.s^\beta] \ge 0$  and constant fractional order in the range  $0 < \beta < 1$ , which provides a material interpolation between Hookean ( $\beta \rightarrow 0$ ) and Newtonian ( $\beta \rightarrow 1$ ) elements. The pair ( $\beta$ ,  $\mathbb{E}$ ) uniquely represent the SB constants, where the *pseudo-constant*  $\mathbb{E}[Pa.s^\beta]$  compactly describes textural properties, such as the firmness of the material [24, 172]. In this sense  $\mathbb{E}$  is interpreted as describing a snapshot of a non-equilibrium dynamic process instead of an equilibrium state. The corresponding rheological symbol for the SB model represents a fractal-like arrangement of springs and dashpots [6, 34], which we interpret as a compact, upscaled representation of a fractallike microstructure. Regarding the thermodynamic admissibility, we refer the reader to Lion[35] for the SB model, and Suzuki *et al.*[75] for the combination of the SB element with more complex mechanisms of visco-plasticity and damage. The relaxation function G(t) [*Pa*] for the SB model is given by the following inverse power-law form:

$$G^{SB}(t) := \frac{\mathbb{E}}{\Gamma(1-\alpha)} t^{-\beta}, \tag{6.6}$$

which is the convolution kernel of the differ-integral form in (6.5).

**Fractional Kelvin-Voigt (FKV) Model:** Through a parallel combination of SB elements, we obtain the following stress-strain relationship [34]:

$$\sigma(t) = \mathbb{E}_1 \ {}_0^C \mathcal{D}_t^{\beta_1} \varepsilon(t) + \mathbb{E}_2 \ {}_0^C \mathcal{D}_t^{\beta_2} \varepsilon(t), \quad t > 0, \quad \varepsilon(0) = 0, \tag{6.7}$$

with fractional orders  $0 < \beta_1, \beta_2 < 1$  and associated pseudo-constants  $\mathbb{E}_1[Pa.s^{\beta_1}] \ge 0$  and  $\mathbb{E}_2[Pa.s^{\beta_2}] \ge 0$ . The corresponding relaxation modulus G(t)[Pa], is also an additive form of two SB elements:

$$G^{FKV}(t) := \frac{\mathbb{E}_1}{\Gamma(1 - \beta_1)} t^{-\beta_1} + \frac{\mathbb{E}_2}{\Gamma(1 - \beta_2)} t^{-\beta_2}.$$
 (6.8)

Which has a response characterized by two power-law regimes, with a transition from faster to slower relaxation. Assuming  $\beta_2 > \beta_1$ , the asymptotic responses for small and large time-scales are given by  $G^{FKV} \sim t^{-\beta_2}$  as  $t \to 0$  and  $G^{FKV} \sim t^{-\beta_1}$  as  $t \to \infty$ .

**Fractional Maxwell (FM) Model:** Through a serial combination of SB elements, we obtain the fractional Maxwell (FM) model[24], given by:

$$\sigma(t) + \frac{\mathbb{E}_2}{\mathbb{E}_1} {}^C_0 \mathcal{D}_t^{\beta_2 - \beta_1} \sigma(t) = \mathbb{E}_2 {}^C_0 \mathcal{D}_t^{\beta_2} \varepsilon(t), \quad t > 0,$$
(6.9)

with pseudo-constants  $\mathbb{E}_1[Pa.s^{\beta_1}] > 0$ ,  $\mathbb{E}_2[Pa.s^{\beta_1}] \ge 0$ , fractional orders  $0 < \beta_1 < \beta_2 < 1$ , with  $0 < \beta_2 - \beta_1 < 1$  and two sets of initial conditions for strains  $\varepsilon(0) = 0$ , and stresses  $\sigma(0) = 0$ . We note that in the case of non-homogeneous ICs, there needs to be a compatibility conditions[32]

between stresses and strains at t = 0. The corresponding relaxation function for this building block model assumes a more complex, Miller-Ross form[24]:

$$G^{FM}(t) := \mathbb{E}_1 t^{-\beta_1} E_{\beta_2 - \beta_1, 1 - \beta_1} \left( -\frac{\mathbb{E}_1}{\mathbb{E}_2} t^{\beta_2 - \beta_1} \right).$$
(6.10)

Interestingly, the presence of a Mittag-Leffler function in (6.10) leads to a stretched exponential relaxation for smaller times and a power-law behavior for longer times. We also observe that the limit cases are given by  $G^{FM} \sim t^{-\beta_1}$  as  $t \to 0$  and  $G^{FM} \sim t^{-\beta_2}$  as  $t \to \infty$ , indicating that the FM model provides a behavior transitioning from slower-to-faster relaxation. We refer the reader to the works [24, 174] for a number of applications of the aforementioned models. We notice that both FKV and FM models are able to recover the SB element with a convenient set of pseudo-constants and  $\beta_1 = \beta_2$ .

**Fractional Kelvin-Zener (FKZ) model:** The fractional generalization of the standard linear solid (SLS) model is given by a FM branch in parallel with a third SB element, given by the following FDE:

$$\left[1 + \frac{\mathbb{E}_2}{\mathbb{E}_1} {}^C_0 \mathcal{D}_t^{\beta_2 - \beta_1}\right] \sigma(t) = \left[\mathbb{E}_2 {}^C_0 \mathcal{D}_t^{\beta_2} + \mathbb{E}_3 {}^C_0 \mathcal{D}_t^{\beta_3} + \frac{\mathbb{E}_2 \mathbb{E}_3}{\mathbb{E}_1} {}^C_0 \mathcal{D}_t^{\beta_2 + \beta_3 - \beta_1}\right] \varepsilon(t), \tag{6.11}$$

with fractional orders  $0 < \beta_1 < \beta_2 < 1$  and conditions  $0 < \beta_2 - \beta_1 < 1$  and  $0 < \beta_2 + \beta_3 - \beta_1 < 1$ , pseudo-constants  $\mathbb{E}_1 [Pa.s^{\beta_1}] > 0$ ,  $\mathbb{E}_3 [Pa.s^{\beta_3}] \ge 0$ ,  $\mathbb{E}_2 [Pa.s^{\beta_2}] \ge 0$  and same initial conditions as the FM model. We note that the FM model is recovered when  $\mathbb{E}_3 = 0$  and the FKV model is recovered when setting  $\mathbb{E}_1 = 0$ . The relaxation function is obtained in a straightforward fashion as the summation of relaxation functions from the SB and FM models:

$$G^{FKZ}(t) := \mathbb{E}_1 t^{-\beta_1} E_{\beta_2 - \beta_1, 1 - \beta_1} \left( -\frac{\mathbb{E}_1}{\mathbb{E}_2} t^{\beta_2 - \beta_1} \right) + \frac{\mathbb{E}_3}{\Gamma(1 - \beta_3)} t^{-\beta_3}, \tag{6.12}$$

which leads to three inverse power-law regimes for short, intermediate and long times, according to particular relationships between  $\beta_1$ ,  $\beta_2$ ,  $\beta_3$  [36].

**Fractional Poynting-Thomson (FPT) Model:** Finally, we introduce our last fractional linear visco-elastic model given by the serial combination between a FKV model and a SB element:

$$\left[1 + \frac{\mathbb{E}_1}{\mathbb{E}_3} {}^C_0 \mathcal{D}_t^{\beta_1 - \beta_3} + \frac{\mathbb{E}_2}{\mathbb{E}_3} {}^C_0 \mathcal{D}_t^{\beta_2 - \beta_3}\right] \sigma(t) = \left[\mathbb{E}_1 {}^C_0 \mathcal{D}_t^{\beta_1} + \mathbb{E}_2 {}^C_0 \mathcal{D}_t^{\beta_2}\right] \varepsilon(t), \tag{6.13}$$

with  $0 < \beta_3 < \beta_1 < 1$  and  $0 < \beta_3 < \beta_2 < 1$ , additional conditions  $0 < \beta_1 - \beta_3 < 1$  and  $0 < \beta_2 - \beta_3 < 1$ , and pseudo-constants  $\mathbb{E}_1 [Pa.s^{\beta_1}] \ge 0$ ,  $\mathbb{E}_2 [Pa.s^{\beta_2}] \ge 0$ ,  $\mathbb{E}_3 [Pa.s^{\beta_3}] > 0$  and homogeneous initial conditions  $\sigma(0) = 0$  and  $\varepsilon(0) = 0$ . Similar to the FKZ model, we recover the FM one when setting either  $\mathbb{E}_1$  or  $\mathbb{E}_2$  to zero; although the FKV model cannot be recovered except for the trivial case when  $\sigma(t) = 0$ .

### 6.3.2 Quasi-Linear Fractional Visco-Elasticity

Although fractional linear visco-elastic models provide suitable relaxation functions that describe the anomalous visco-elastic dynamics of a number of soft materials, at times, complex microstructural deformation mechanisms and large strains induce material nonlinearities, and hence the relaxation function itself depends on the applied strain levels. To incorporate this additional effect, we also consider the following quasi-linear, fractional visco-elastic model (FQLV) [10, 168]:

$$\sigma(t,\varepsilon) = \int_0^t G(t-s) \frac{\partial \sigma^e(\varepsilon)}{\partial \varepsilon} \dot{\varepsilon} \, ds, \qquad (6.14)$$

where the convolution kernel is given by a multiplicative decomposition of a reduced relaxation function G(t) and an instantaneous, nonlinear elastic tangent response with stress  $\sigma^e$ . In the work by Craiem *et al.*[10], the reduced relaxation function has a fractional Kelvin-Voigt-like form with one of the SB replaced with a Hookean element. Here, we assume a simpler rheology and adopt a Scott-Blair-like reduced relaxation in the form:

$$G(t) = Et^{-\alpha} / \Gamma(1 - \alpha), \qquad (6.15)$$

with the pseudo-constant *E* with units  $[s^{\alpha}]$ . We adopt the same, two-parameter, exponential nonlinear elastic part as in[10]:

$$\sigma^{e}(\varepsilon) = A\left(e^{B\varepsilon} - 1\right),\tag{6.16}$$

with A having units of [Pa]. Substituting Equations 6.15 and 6.16 into Eq.6.14, we obtain:

$$\sigma(t,\varepsilon) = \frac{EAB}{\Gamma(1-\alpha)} \int_0^t \frac{e^{B\varepsilon(s)}\dot{\varepsilon}(s)}{(t-s)^{\alpha}} \, ds, \tag{6.17}$$

which differs slightly from the linear SB model (6.5) in the sense that an additional exponential factor multiplies the function being convoluted.

# 6.4 Fractional Visco-Elasto-Plasticity

With all fractional viscoelastic models defined in Section 6.3, we couple any of them, subject to a viscoelastic strain  $\varepsilon^{ve}(t)$ , to the fractional viscoplastic device illustrated in Fig.6.2. The viscoplastic device is composed of a parallel combination of a Coulomb element with initial yield stress  $\sigma^{Y}[Pa]$ , a SB element with pseudo-constant  $\mathbb{K}[Pa.s^{\beta K}]$  and fractional order  $\beta_{K}$ , and a Hookean spring with constant H[Pa]. The entire visco-plastic part is subject to a visco-plastic strain  $\varepsilon^{vp}(t) : \mathbb{R}^+ \to \mathbb{R}$ . In order to obtain the kinematic equations for the internal variables, we start with an additive decomposition of the total logarithmic strain  $\varepsilon(t) : \mathbb{R}^+ \to \mathbb{R}$  acting on the visco-elasto-plastic device:

$$\varepsilon(t) = \varepsilon^{ve}(t) + \varepsilon^{vp}(t)$$



Figure 6.2: Fractional visco-elasto-plastic model diagram. Here, any of the linear and quasi-linear fractional viscoelastic models can be separately coupled with a fractional viscoplastic rheological device.

The visco-plastic effects are accounted for through the definition of a memory- and ratedependent yield function  $f(\sigma, \alpha) : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}^- \cup \{0\}$  in the following form [1]:

$$f(\sigma, \alpha) := |\sigma| - \left[\sigma^{Y} + \mathbb{K}_{0}^{C} \mathcal{D}_{t}^{\beta_{K}}(\alpha) + H\alpha\right].$$
(6.18)

Here,  $\alpha \in \mathbb{R}^+$  represents the internal hardening variable, and the above form accounts for isotropic hardening. The set of admissible stresses lie in a closed convex space, where the associated boundary respects the yield condition of classical plasticity (see [75], Lemma 4.1, setting the

*damage as* D = 0). From the defined yield function (6.18), and the principle of maximum plastic dissipation [192], the following properties hold: **i**) associativity of the flow rule, **ii**) associativity in the hardening law, **iii**) Kuhn-Tucker complimentary conditions, and **iv**) convexity. The set of evolution equations for the internal variables  $\varepsilon^{vp}$  and  $\alpha$  is obtained by:

$$\dot{\varepsilon}^{vp} = \frac{\partial f}{\partial \sigma} \dot{\gamma}, \quad \dot{\alpha} = -\frac{\partial f}{\partial R} \dot{\gamma},$$

where  $\dot{\gamma}(t) : \mathbb{R}^+ \to \mathbb{R}^+$  denotes the plastic slip rate. Evaluating the above equations using (6.18), we obtain the evolution for viscoplastic strains and hardening [1]:

$$\dot{\varepsilon}^{\nu p} = \operatorname{sign}(\tau) \dot{\gamma}, \tag{6.19}$$

$$\dot{\alpha} = \dot{\gamma}. \tag{6.20}$$

**Proposition 1.** The closure for the plastic slip rate  $\dot{\gamma}(t) \in \mathbb{R}^+$  with a SB visco-elastic part of constants ( $\mathbb{E}$ ,  $\beta_E$ ), ( $\mathbb{K}$ ,  $\beta_K$ ) and H (model M1 [1]) with homogeneous initial conditions for the internal variables and their respective rates, i.e.,  $\varepsilon^{vp}(0) = \alpha(0) = \gamma(0) = 0$  and  $\dot{\gamma}(0) = 0$  and  $\dot{\varepsilon}^{vp}(0) = \dot{\alpha}(0) = \dot{\gamma}(0) = 0$  is given by the following fractional Cauchy problem:

$$\mathbb{E} {}_{0}^{C} \mathcal{D}_{t}^{\beta_{E}} \dot{\gamma}(t) + \mathbb{K} {}_{0}^{C} \mathcal{D}_{t}^{\beta_{K}} \dot{\gamma}(t) + H \dot{\gamma}(t) = sign(\sigma) \mathbb{E} \left[ \frac{\dot{\varepsilon}(0)t^{-\beta_{E}}}{\Gamma(1-\beta_{E})} + {}_{0}^{C} \mathcal{D}_{t}^{\beta_{E}} \dot{\varepsilon}(t) \right]$$
(6.21)

Proof. See Appendix C.1.

# 6.5 A Class of Return-Mapping Algorithms for Fractional Visco-Elasto-Plasticity

Given the presented viscoelastic and viscoplastic models, respectively, in Sections 6.3 and 6.4, we now demonstrate now to solve each resulting system of nonlinear equations, according to the choice of viscoelastic models. The considered fractional return-mapping approach in this work is fully discrete, *i.e.*, we first discretize all fractional derivatives using a finite-difference approach, and then employ trial states for the internal variable in a predictor-corrector scheme.

We discretize the fractional Caputo derivatives in Equations 6.5-6.9 through an implicit L1 finite-difference scheme[176] and also through a fast time-stepping approach[106]. For simplicity,

we present here only the discretization using the L1 approach. Let  $\Omega = (0, T]$  decomposed as a uniform time-grid with *N* time-steps of size  $\Delta t$ , such that  $t_n = n\Delta t$ , with n = 0, 1, ..., N. The time-fractional Caputo derivative of a real-valued function  $u(t) \in C^2(\Omega)$  at time  $t = t_{n+1}$  is therefore discretized as [176]:

$${}_{0}^{C}\mathcal{D}_{t}^{\beta}u(t)|_{t=t_{n+1}} = \frac{1}{\Delta t^{\beta}\Gamma(2-\beta)} \left[u_{n+1} - u_{n} + \mathcal{H}^{\alpha}u\right] + O(\Delta t^{2-\beta}), \tag{6.22}$$

with history term  $\mathcal{H}^{\nu}u$  given by the following form:

$$\mathcal{H}^{\beta}u = \sum_{j=1}^{n} b_{j}^{\beta} \left[ u_{n+1-j} - u_{n-j} \right],$$

with weights  $b_j^{\beta} := (j+1)^{1-\beta} - j^{1-\beta}$ .

### 6.5.1 Time-Fractional Integration of Visco-Elastic Models

In the following, we present the discretized forms for each considered fractional viscoelastic model from Section 6.3, which are taken in a fully-implicit fashion.

**Scott-Blair Model**: Evaluating both sides of (6.5) at  $t = t_{n+1}$ , we obtain:

$$\sigma_{n+1} = \mathbb{E}_1 {}_0^C \mathcal{D}_t^{\beta_1} \varepsilon(t) |_{t=t_{n+1}},$$

which, applying (6.22), we directly obtain:

$$\sigma_{n+1} = C_1^{SB} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_1} \varepsilon \right], \tag{6.23}$$

with strain history  $\mathcal{H}^{\beta_1}\varepsilon$  and constant  $C_1^{SB}$  shown in Appendix C.2 for the SB and next model discretizations.

**Fractional Kelvin-Voigt Model**: Evaluating both sides of (6.7) at  $t = t_{n+1}$ , we obtain:

$$\sigma_{n+1} = \mathbb{E}_{10}^{\ C} \mathcal{D}_t^{\beta_1} \varepsilon(t) |_{t=t_{n+1}} + \mathbb{E}_{20}^{\ C} \mathcal{D}_t^{\beta_2} \varepsilon(t) |_{t=t_{n+1}},$$

which, applying (6.22), for the fractional derivatives of order  $\beta_1$  and  $\beta_2$ , leads to:

$$\sigma_{n+1} = C_1^{KV} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_1} \varepsilon \right] + C_2^{KV} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_2} \varepsilon \right].$$
(6.24)

**Fractional Maxwell Model**: Evaluating both sides of (6.9) at  $t = t_{n+1}$ , we obtain:

$$\sigma_{n+1} + \frac{\mathbb{E}_2}{\mathbb{E}_1} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2 - \beta_1} \sigma(t) \big|_{t=t_{n+1}} = \mathbb{E}_2 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2} \varepsilon(t) \big|_{t=t_{n+1}},$$

which, applying (6.22), for the fractional derivatives of strains and stresses, leads to:

$$\sigma_{n+1} = \frac{C_1^M \left[\varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_2}\varepsilon\right] + C_2^M \left[\sigma_n - \mathcal{H}^{\beta_2 - \beta_1}\sigma\right]}{1 + C_2^M},\tag{6.25}$$

with the emergence of a stress history term  $\mathcal{H}^{\beta_2-\beta_1}\sigma$ .

**Fractional Kelvin-Zener Model**: Evaluating both sides of (6.11) at  $t = t_{n+1}$ , we obtain:

$$\begin{split} \sigma_{n+1} + \frac{\mathbb{E}_2}{\mathbb{E}_1} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2 - \beta_1} \sigma(t) |_{t = t_{n+1}} &= \mathbb{E}_2 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2} \varepsilon(t) |_{t = t_{n+1}} + \mathbb{E}_3 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_3} \varepsilon(t) |_{t = t_{n+1}} \\ &+ \frac{\mathbb{E}_2 \mathbb{E}_3}{\mathbb{E}_1} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2 + \beta_3 - \beta_1} \varepsilon(t) |_{t = t_{n+1}}, \end{split}$$

which, applying (6.22), for the fractional derivatives of strains and stresses, leads to:

$$\sigma_{n+1} = (1 + C_4^{KZ})^{-1} \left[ C_1^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2} \varepsilon \right) + C_2^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_3} \varepsilon \right) + C_3^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2 + \beta_3 - \beta_1} \varepsilon \right) + C_4^{KZ} \left( \sigma_n - \mathcal{H}^{\beta_2 - \beta_1} \sigma \right) \right],$$
(6.26)

with  $\Delta \varepsilon_{n+1} = \varepsilon_{n+1} - \varepsilon_n$ .

Fractional Poynting-Thomson Model: Finally, we evaluate both sides of (6.13) and obtain:

$$\begin{split} \sigma_{n+1} &+ \frac{\mathbb{E}_1}{\mathbb{E}_3} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_1 - \beta_3} \sigma(t) \big|_{t = t_{n+1}} + \frac{\mathbb{E}_2}{\mathbb{E}_3} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2 - \beta_3} \sigma(t) \big|_{t = t_{n+1}} \\ &= \mathbb{E}_1 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_1} \varepsilon(t) \big|_{t = t_{n+1}} + \mathbb{E}_2 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2} \varepsilon(t) \big|_{t = t_{n+1}}, \end{split}$$

which, applying (6.22), for the fractional derivatives of strains and stresses, leads to:

$$\sigma_{n+1} = (1 + C_3^{PT} + C_4^{PT})^{-1} \left[ C_1 \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_1} \varepsilon \right) + C_2^{PT} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2} \varepsilon \right) + C_3^{PT} \left( \sigma_{n+1} + \mathcal{H}^{\beta_1 - \beta_3} \sigma \right) + C_4^{PT} \left( \sigma_n - \mathcal{H}^{\beta_2 - \beta_3} \sigma \right) \right].$$
(6.27)

**Fractional Quasi-Linear Visco-Elastic Model:** The discretization for the FQLV model (6.17) has a slightly different development than the preceding models. Nevertheless, it only involves a

slight modification of the fully-implicit L1 difference approach by with a trapezoidal rule taken on the exponential factor. More specifically, we evaluate the quasi-linear viscoelastic operator as:

$$\sigma_{n+1} = \frac{EAB}{\Gamma(1-\beta)} \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} (t_{n+1}-s)^{-\beta} \exp(B\varepsilon_{k+\frac{1}{2}}) \left(\frac{\varepsilon_{k+1}-\varepsilon_k}{\Delta t}\right) ds,$$

with  $\varepsilon_{i+\frac{1}{2}} = (\varepsilon_i + \varepsilon_{i+1})/2$ . Following similar steps as in [176], we obtain the following discretized stresses at  $t = t_{n+1}$  for the FQLV model:

$$\sigma_{n+1} = C_1^{QLV} \left[ \exp(B\varepsilon_{n+\frac{1}{2}}) \left(\varepsilon_{n+1} - \varepsilon_n\right) + \mathcal{H}^{\alpha} \left(\varepsilon, \frac{\partial \sigma^e}{\partial \varepsilon}\right) \right], \tag{6.28}$$

with constant  $C_1^{QLV} = EAB/(\Delta t^{\alpha}\Gamma(2-\alpha))$ . The discretized history load in this case is given by:

$$\mathcal{H}^{\alpha}\left(\varepsilon, \frac{\partial \sigma^{e}}{\partial \varepsilon}\right) = \sum_{k=1}^{n} \exp(B\varepsilon_{n-k+\frac{1}{2}}) \left(\varepsilon_{n-k+1} - \varepsilon_{n-k}\right) b_{k}, \tag{6.29}$$

with weights  $b_k = (k + 1)^{1-\alpha} - k^{1-\alpha}$ . Since the trapezoid approximation of the strains in the exponential term are second-order accurate, the overall accuracy of the visco-elastic models is still bounded by the native L1-difference approach, and therefore should be of  $O(\Delta t^{2-\alpha})$ .

**Remark 6.5.1.** We note that except for the quasi-linear viscoelastic model, any of the aforementioned discretizations for linear models can recover existing classical counterparts by properly setting  $\beta_i \rightarrow 0$  or  $\beta_i \rightarrow 1$ . In these cases, to achieve comparable performance to integer-order models, history terms can be selectively disregarded and the corresponding discretization constants can be adjusted to their integer-order counterparts.

### 6.5.2 Time-Fractional Integration of Visco-Plasticity

We start with the discretization of internal variables. Following [1], we assume a strain-driven process with known total strains  $\varepsilon_{n+1}$  at time  $t_{n+1}$ . The strain decomposition becomes:

$$\varepsilon_{n+1} = \varepsilon_{n+1}^{ve} + \varepsilon_{n+1}^{vp}. \tag{6.30}$$

The flow rule (6.19) is discretized through a first-order backward-Euler approach, which yields:

$$\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \operatorname{sign}(\tau_{n+1}) \Delta \gamma_{n+1}, \tag{6.31}$$

with  $\Delta \gamma_{n+1} = \gamma_{n+1} - \gamma_n$  representing the plastic slip increment in the interval  $[t_n, t_{n+1}]$ . Similarly, the discretization of the hardening law (6.20) is given by

$$\alpha_{n+1} = \alpha_n + \Delta \gamma_{n+1}, \tag{6.32}$$

Evaluating the yield function (6.18) at  $t_{n+1}$  and employing discretization (6.22) for the hardening variable, we obtain: is given by:

$$f_{n+1} = |\sigma_{n+1}| - \left[\sigma^Y + \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha)|_{t=t_{n+1}} + H\alpha_{n+1}\right]$$
$$= |\sigma_{n+1}| - \left[\sigma^Y + \mathbb{K}^*\left(\alpha_{n+1} - \alpha_n + \mathcal{H}^{\beta K}\alpha\right) + H\alpha_{n+1}\right], \tag{6.33}$$

with  $\mathbb{K}^* = \mathbb{K}/(\Delta t^{\beta_K} \Gamma(2 - \beta_K)).$ 

The next step is to define trial states for the stress and yield functions, which is the core idea to define the viscoelastic prediction phase, and the correction step after solving the internal viscoplastic variables. Therefore, we freeze the internal variables for the prediction step at  $t_{n+1}$ . Therefore the trial visco-plastic strains and hardening are given by:

$$\varepsilon_{n+1}^{vp^{trial}} = \varepsilon_n^{vp}, \quad \alpha_{n+1}^{trial} = \alpha_n.$$
(6.34)

In this token, the trial yield function is given by setting the above relationship for the hardening variable into (6.33) to obtain:

$$f_{n+1}^{trial} = |\sigma_{n+1}^{trial}| - \left[\sigma^Y + \mathbb{K}^*\left(\mathcal{H}^{\beta K}\alpha\right) + H\alpha_n\right].$$
(6.35)

In order to complete the return-mapping procedure, we need an explicit relationship between the stresses  $\sigma_{n+1}$  in terms of the known total strains  $\varepsilon_{n+1}$ . In order to achieve this, we solve for the plastic slip  $\Delta \gamma$  using a discrete consistency condition  $f_{n+1} = 0$ . We start with the trial stresses for each presented fractional visco-elastic model by substituting the visco-plastic trial strain (6.34) and (6.30) into (6.23)-(6.28), where we obtain, for each discretized model:

#### Scott-Blair:

$$\sigma_{n+1}^{trial} = C_1^{SB} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_1} (\varepsilon - \varepsilon^{vp}) \right], \tag{6.36}$$

Fractional Kelvin-Voigt:

$$\sigma_{n+1}^{trial} = C_1^{KV} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_1} (\varepsilon - \varepsilon^{\nu p}) \right] + C_2^{KV} \left[ \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_2} (\varepsilon - \varepsilon^{\nu p}) \right].$$
(6.37)

Fractional Maxwell:

$$\sigma_{n+1}^{trial} = \frac{C_1^M \left[\varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta_2}(\varepsilon - \varepsilon^{vp})\right] + C_2^M \left[\sigma_n - \mathcal{H}^{\beta_2 - \beta_1}\sigma\right]}{1 + C_2^M},\tag{6.38}$$

Fractional Kelvin-Zener:

$$\sigma_{n+1}^{trial} = (1 + C_4^{KZ})^{-1} \left[ C_1^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2} (\varepsilon - \varepsilon^{vp}) \right) + C_2^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_3} (\varepsilon - \varepsilon^{vp}) \right) + C_3^{KZ} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2 + \beta_3 - \beta_1} (\varepsilon - \varepsilon^{vp}) \right) + C_4^{KZ} \left( \sigma_n - \mathcal{H}^{\beta_2 - \beta_1} \sigma \right) \right].$$
(6.39)

Fractional Poynting-Thomson:

$$\sigma_{n+1}^{trial} = (1 + C_3^{PT} + C_4^{PT})^{-1} \left[ C_1^{PT} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_1} (\varepsilon - \varepsilon^{vp}) \right) + C_2^{PT} \left( \Delta \varepsilon_{n+1} + \mathcal{H}^{\beta_2} (\varepsilon - \varepsilon^{vp}) \right) + C_3^{PT} \left( \sigma_{n+1} + \mathcal{H}^{\beta_1 - \beta_3} \sigma \right) + C_4^{PT} \left( \sigma_n - \mathcal{H}^{\beta_2 - \beta_3} \sigma \right) \right].$$
(6.40)

Fractional Quasi-Linear Viscoelastic Model:

For this model, we follow a similar procedure of substituting the viscoelastic strains into (6.28), however we evaluate the exponential term explicitly in time for all stages of the return-mapping algorithm. Therefore, the corresponding trial state becomes:

$$\sigma_{n+1}^{trial} = C_1^{QLV} \left[ \exp(B(\varepsilon_n - \varepsilon_n^{vp})) \left(\varepsilon_{n+1} - \varepsilon_n\right) + \mathcal{H}^{\alpha} \left(\varepsilon - \varepsilon^{vp}, \frac{\partial \sigma^e}{\partial \varepsilon}\right) \right], \quad (6.41)$$

### 6.5.3 Generalized fractional return-mapping algorithm

From the aforementioned trial states, each discretized visco-elastic constitutive laws (6.23)-(6.28) and recalling (6.31), one can show the following stress correction onto the yield surface:

$$\sigma_{n+1} = \sigma_{n+1}^{trial} - \operatorname{sign}(\sigma_{n+1}^{trial}) C_{RM}^{ve}(\mathbb{E}, \Delta t, \varepsilon) \Delta \gamma_{n+1},$$
(6.42)

where interestingly, all discretized, aforementioned visco-elastic models change the return-mapping procedure by a scaling factor  $C_{RM}^{ve}(C, \varepsilon_n, \varepsilon_n^{vp}) \in \mathbb{R}^+$  acting on the Lagrange multiplier  $\Delta \gamma$ , which is given by, for each model:

$$C_{RM}^{ve} = \begin{cases} C_1^{SB} & (Scott - Blair) \\ C_1^{KV} + C_2^{KV} & (FractionalKelvin - Voigt) \\ C_1^M / (1 + C_2^M) & (FractionalMaxwell) \\ (C_1^{KZ} + C_2^{KZ} + C_3^{KZ}) / (1 + C_4^{KZ}) & (FractionalKelvin - Zener) \\ (C_1^{PT} + C_2^{PT}) / (1 + C_3^{PT} + C_4^{PT}) & (FractionalPoynting - Thomson) \\ (C_1^{QLV} \exp(B(\varepsilon_n - \varepsilon_n^{vp}))) & (FractionalQuasi - Linear - Viscoelastic). \end{cases}$$

$$(6.43)$$

Most of the above cases can be obtained through the derivation of the fractional Kelvin-Zener model, from which the Scott-Blair, fractional Maxwell and fractional Kelvin-Voigt models can be directly recovered, and note that the derivation for the fractional Poynting-Thomson and quasi-linear viscoelasticity follow similarly in a straightforward fashion. Substituting the updated stresses (6.42) into the discrete yield function (6.33) and recalling (6.35), we obtain:

$$f_{n+1} = f_{n+1}^{trial} - \left(C_{RM}^{ve} + \mathbb{K}^* + H\right) \Delta \gamma.$$

Enforcing the discrete yield condition  $f_{n+1} = 0$ , we obtain the solution for the discrete plastic slip:

$$\Delta \gamma_{n+1} = \frac{f_{n+1}^{trial}}{C_{RM}^{ve} + \mathbb{K}^* + H}.$$
(6.44)

### 6.5.3.1 Comparison of the return-mapping algorithm to existing approaches

In [1], trial states were defined prior to the discretization of fractional operators, and the corresponding trial variables were taken as continuous functions of time, therefore making the return-mapping Algorithm 6.1: Fractional return-mapping algorithm.

1: Database for  $\varepsilon$ ,  $\varepsilon^{vp}$ ,  $\sigma$ ,  $\alpha$ , and total strain  $\varepsilon_{n+1}$ . 2:  $\varepsilon_{n+1}^{vp^{trial}} = \varepsilon_n^{vp}$ ,  $\alpha_{n+1}^{trial} = \alpha_n$ 3: Compute  $\sigma_{n+1}^{trial}$  from (6.23)-(6.28) according to the selected fractional visco-elastic model. 4:  $f_{n+1}^{trial} = |\sigma_{n+1}^{trial}| - [\sigma^Y + \mathbb{K}^* (\mathcal{H}^{\beta} K \alpha) + H \alpha_n]$ 5: **if**  $f_{n+1}^{trial} \le 0$  **then** 6:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp}$ ,  $\alpha_{n+1} = \alpha_n$ ,  $\sigma_{n+1} = \sigma_{n+1}^{trial}$ . 7: **else** 8: Return-Mapping: 9: Compute  $C_{RM}^{ve}$  from (6.43) according to the selected fractional visco-elastic model. 10:  $\Delta \gamma_{n+1} = f_{n+1}^{trial} / (C_{RM}^{ve} + K^* + H)$ 11:  $\sigma_{n+1} = \sigma_{n+1}^{trial} - \operatorname{sign}(\sigma_{n+1}^{trial}) C_{RM}^{ve} \Delta \gamma$ 12:  $\varepsilon_{n+1}^{vp} = \varepsilon_n^{vp} + \operatorname{sign}(\tau_{n+1}) \Delta \gamma$ 13:  $\alpha_{n+1} = \alpha_n + \Delta \gamma$ 

procedure "semi-discrete". Let the quantities ( $\overline{\cdot}$ ) be the corresponding solutions for the procedure developed in [1]. For the SB viscoelastic case, one has the following trial stresses at  $t = t_{n+1}$ :

$$\bar{\sigma}_{n+1}^{\text{trial}} = \mathbb{E}_{0}^{C} \mathcal{D}_{t}^{\beta E} (\varepsilon - \bar{\varepsilon}^{v p^{trial}})|_{t=t_{n+1}},$$

where, after employing the discretized plastic flow rule, the following relationship between the corrected and trial stresses is obtained:

$$\bar{\sigma}_{n+1} = \bar{\sigma}_{n+1}^{\text{trial}} - \mathbb{E}\text{sign}(\bar{\sigma}_{n+1}) {}_{0}^{C} \mathcal{D}_{t}^{\beta E}(\Delta \gamma)|_{t=t_{n+1}},$$

which can be explicitly be inserted in the discrete yield function to solve for the plastic slip rate. While such procedure is straightforward for SB and FKV viscoelastic elements, it is non-trivial for serial combinations such as the FM, FKZ and FPT models. For instance, if we follow the same procedure for the FM model, we obtain:

$$\bar{\sigma}_{n+1}^{trial} + \frac{\mathbb{E}_2}{\mathbb{E}_1} {}_0^C \mathcal{D}_t^{\beta_2 - \beta_1} (\bar{\sigma}^{trial}) |_{t=t_{n+1}} = \mathbb{E}_2 {}_0^C \mathcal{D}_t^{\beta_2} (\varepsilon - \bar{\varepsilon}^{vp^{trial}}) |_{t=t_{n+1}},$$

which yields the following relationship between  $\bar{\sigma}$  and  $\bar{\sigma}^{trial}$ :

$$\left(\bar{\sigma}_{n+1} - \bar{\sigma}_{n+1}^{trial}\right) + \frac{\mathbb{E}_2}{\mathbb{E}_1} \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2 - \beta_1} (\bar{\sigma} - \bar{\sigma}^{trial})|_{t=t_{n+1}} = -\mathbb{E}_2 \mathop{}_{0}^{C} \mathcal{D}_t^{\beta_2} (\varepsilon - \bar{\varepsilon}^{vp^{trial}})|_{t=t_{n+1}}.$$

We note that, different from the SB case, when a fractional viscoelastic model involving a serial combination of SB elements cannot be incorporated to the yield function in differential form, unless a full discretization is performed at this stage. This happens since the discretized yield function (6.33) requires a closed description of  $\sigma_{n+1}$ , which would require an equivalent Boltzmann representation for such models, which is impractical due to complex forms of relaxation kernels. Therefore, our approach in this work carry trial states in already fully-discretized fractional operators, which closely completely resembles classical elastoplastic approaches.

Regarding the obtained discretizations in this work, we note that the plastic slip (6.44) assumes a simple form similar to rate-independent elasto-plasticity. As discussed above, in the returnmapping procedure developed in [1], the trial states and plastic slip were assumed to have memory in the discretization procedure, and therefore a fractional relaxation equation in the following form was obtained:

$$\Delta \bar{\gamma}_{n+1} = \frac{\mathbb{E}^* \left( \Delta \bar{\gamma}_n - \mathcal{H}^{\beta E} \Delta \bar{\gamma} \right) + \mathbb{K}^* \left( \Delta \bar{\gamma}_n - \mathcal{H}^{\beta K} \Delta \bar{\gamma} \right) + \bar{f}_{n+1}^{trial}}{\mathbb{E}^* + \mathbb{K}^* + H}, \tag{6.45}$$

Furthermore, we observe that the obtained plastic slip discretization in this work has two less history terms to be evaluated. Although this does not influence the computational complexity of the original scheme, we show in the numerical examples that this fact still leads to about 50 % less CPU time. Regarding the difference in stress solutions, let  $t = t_p$  be the time-step of onset of plasticity for the first time. Therefore, we have the following estimate:

$$|\sigma_{p+1} - \bar{\sigma}_{p+1}| = \frac{\mathbb{E}^*}{\mathbb{E}^* + \mathbb{K}^* + H} \left[ \mathbb{K}^* \left( \mathcal{H}^{\beta E} \Delta \bar{\gamma} - \mathcal{H}^{\beta K} \Delta \bar{\gamma} \right) - H \left( \Delta \bar{\gamma}_p - \mathcal{H}^{\beta E} \Delta \bar{\gamma} \right) \right], \quad (6.46)$$

which shows that at such stage, both discretizations coincide when  $\beta_E = \beta_K$  and H = 0. In the following Section, we verify such estimate by obtaining an analytical solution with the aid of Proposition 1.

### 6.6 Numerical Tests

We present three convergence examples with different loading conditions to verify the employed fractional visco-elastic models, the validity of the new fractional visco-plastic return-mapping

algorithm, and the full visco-elasto-plastic response of the models. For the convergence analyses, let  $\mathbf{u}^*$  and  $\mathbf{u}^{\delta}$  be, respectively, the reference and approximate solutions in  $\Omega = (0, T]$ , for a specific time-step size  $\Delta t$ . We define the following relative error measures:

$$\operatorname{err}_{N}(\Delta t) = \frac{|u_{N}^{*} - u_{N}^{\delta}|}{|u_{N}^{*}|}, \ \operatorname{err}(\Delta t) = \frac{||\mathbf{u}^{*} - \mathbf{u}^{\delta}||_{L^{2}(\Omega)}}{||\mathbf{u}^{*}||_{L^{2}(\Omega)}}, \ \operatorname{Order} = \log_{2}\left[\frac{\operatorname{err}(\Delta t)}{\operatorname{err}(\Delta t/2)}\right]$$
(6.47)

We consider homogeneous initial conditions for all model variables in all cases. The presented algorithms were implemented in MATLAB R2020b and were run in a system with Intel Core i7-8850H CPU with 2.60 GHz, 32 GB RAM and MacOS 11.5 operating system.

**Example 3** (Convergence of fractional visco-elastic algorithms). We perform a convergence study of the fractional visco-elastic component of our framework, under stress relaxation and monotone loading experiments. For the experiments in this example, we set  $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (1, 1, 1)$  and  $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$  for fractional linear visco-elastoc models, ensuring all fractional derivatives are taken with an equivalent order  $\beta \in (0, 1)$ . For the fractional quasi-linear viscoelastic model we set E = 1,  $\beta = 0.3$ , A = 1 and B = 1.

For the stress relaxation test, we impose a step strain  $\varepsilon(t) = H(t)\varepsilon_0$ , with  $\varepsilon_0 = 1$  for T = 1000 [s], where H(t) denotes the Heaviside step function. We compare the obtained solutions at t = T for the SB, FKV, FM, and FKZ models to their corresponding relaxation functions (6.6), (6.8), (6.10), and (6.12). The FPT and QLV models are not analyzed in this step, since their time-dependent stress relaxation functions are not readily available, and they are instead analyzed under monotone strains. The obtained results are illustrated in Fig.6.3a, where an expected linear convergence behavior is obtained for all models, given the non-smooth nature of the stress relaxation solution.

For the monotone strain case, we set T = 1 and fabricate a solution for strains in the form  $\varepsilon(t) = \varepsilon_T(t/T)$ , with total applied strain fixed at  $\varepsilon_f = 1$ . Since analytical solutions for all fractional visco-elastic models are difficult to obtain, we compute a reference solution for each model, taken with  $\Delta t = 2^{-17}$  [s]. Particularly for the fractional QLV model, we utilize the the fabricated strain function  $\varepsilon(t)$ , to obtain the following analytical stress solution:

$$\sigma^{QLV^*}(t) = EAB^{\beta} \exp(Bt) \left[ 1 - \frac{\Gamma(1-\beta, Bt)}{\Gamma(1-\beta)} \right],$$



Figure 6.3: Convergence analysis for the fractional visco-elastic models with known analytical solutions. (a) A stress relaxation test with non-smooth step-strains, and material parameters  $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (1, 1, 1)$  and  $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$ , yielding first-order convergence. (b) Convergence for the fractional QLV model with a fabricated solution of linearly increasing strains and material properties  $(E, \beta, A, B) = (1, 0.3, 1, 1)$ . The slopes of the error curves are  $q \approx 2 - \beta$ .

where  $\Gamma(\cdot, \cdot)$  denotes the upper incomplete gamma function. The convergence results for all fractional visco-elastic models with respect to the reference numerical solution are presented in Fig.6.4, while the results for the QLV model with analytical solution are illustrated in Fig.6.3b. We observe for all both cases that the accuracy of the implemented and developed schemes is of order  $O(\Delta t^{2-\beta})$ . The difference in error slopes among models in Fig.6.4 is due to the highest fractional order assigned to each model. For the SB and QLV models, the fractional order is set as  $\beta = 0.3$ , and therefore the observed slope is  $q \approx 1.7$ . For all remaining models and choice of fractional orders, the error slopes are determined by the fractional derivative of highest order, which is  $\beta_2 = 0.7$  in this example, yielding  $q \approx 1.3$ .

**Example 4** (Convergence of fractional visco-plastic algorithms). *The purpose of this example is to demonstrate the conditions where the presented plastic slip discretization* (6.44), *the form* (6.45) *from* [1] *and their associated return-mapping algorithms are equivalent, and also provide a numerical estimate for their difference when such conditions are not satisfied. For this purpose, we test a monotone load where an analytical solution is available, and a case with a cyclic load* 



Figure 6.4: Convergence analysis for all fractional visco-elastic models with  $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (1, 1, 1)$ and  $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$ . A cubic strain function was employed and a reference solution with time-step size  $\Delta t = 2^{-17}$  Monotone loading test with convergence rates  $q \approx 1.3$  for all models.

under high strain rates. For both cases, we set a SB visco-elastic part with  $\mathbb{E} = 50 [Pa.s^{\beta E}]$ ,  $\mathbb{K} = 5 [Pa.s^{\beta K}]$ .

For the monotone strain case, we start with a fabricated solution for strains in the form  $\varepsilon(t) = At^3$ , with  $A = \varepsilon_T/T^3 [s^{-3}]$ . Here,  $\varepsilon_f$  denotes the total applied stress and T represents the final simulation time. Utilizing the result of Lemma 1 and setting  $\beta_E = \beta_K = 0$  and  $\sigma^Y = H = 0$ , we obtain the following analytical solution for stresses:

$$\sigma^*(t) = \frac{6A\mathbb{E}\mathbb{K}}{\mathbb{E}+\mathbb{K}} \frac{t^{3-\beta_E}}{\Gamma(4-\beta_E)}.$$
(6.48)

We note that the proposed fabricated solution ensures that no internal variable is a linear function, and therefore not computed exactly by the L1 discretization. We set  $\varepsilon_T = 1$ , T = 1 [s], and therefore A = 1 [s<sup>-3</sup>]. Table 6.1 presents the obtained convergence results for the fabricated solution (6.48) for both return-mapping algorithms and under the same fractional-orders  $\beta_E$  and  $\beta_K$ . We observe that the errors coincide for this particular case, while the accuracy of order  $O(\Delta t^{2-\beta})$  of the L1 approach is also achieved. The computational times are illustrated in Fig.6.5, where the developed fractional return-mapping approach, when using a SB visco-elastic element, is about 50% faster than the original return-mapping approach from [1], since about half the amount of history terms need to be computed.

	$\beta_E = \beta_K = 0.1$		$\beta_E = \beta_K = 0.5$		$\beta_E = \beta_K = 0.9$	
$\Delta t$	$\operatorname{err}(\Delta t)$	Order	$\operatorname{err}(\Delta t)$	Order	$\operatorname{err}(\Delta t)$	Order
2 <sup>-9</sup>	3.2426e-06	_	9.2971e-05	_	1.3246e-03	_
$2^{-10}$	9.1853e-07	1.8197	3.3109e-05	1.4895	6.1875e–04	1.0981
$2^{-11}$	2.5845e-07	1.8294	1.1763e-05	1.4929	2.8884e-04	1.0991
$2^{-12}$	7.2323e-08	1.8374	4.1731e-06	1.4951	1.3479e-04	1.0995
$2^{-13}$	2.0145e-08	1.8440	1.4788e-06	1.4966	6.2895e-05	1.0998
$2^{-14}$	5.5891e-09	1.8497	5.2369e-07	1.4977	2.9344e-05	1.0999

Table 6.1: Convergence behavior for the return-mapping Algorithm 6.1 obtained in this work and the original approach from [1] for an FVEP device with a SB element.



Figure 6.5: CPU times for the developed fractional return-mapping algorithm and the original one [1] for a SB visco-elastic part. The black line has slope q = 2.

Despite the identical results obtained for the monotone case and equal visco-elastic/plastic fractional orders, this is not the case under general loading conditions. To demonstrate the difference between the visco-elasto-plastic discretization  $\sigma_{n+1}$  developed in this work, and  $\bar{\sigma}_{n+1}$ from [1], we take the latter as a reference solution with  $\Delta t = 2^{-19}$  [s] and T = 1 [s]. We also consider  $\sigma^Y = 10$  [Pa],  $\beta_E = 0.3$  and  $\beta_K = 0.7$  with same pseudo-constants as the previous test case. A constant rate loading/unloading cyclic strain test of the following form is employed:

$$\varepsilon(t) = \frac{2\varepsilon_A}{\pi} \arcsin\left(\sin\left(2\pi\omega t\right)\right),\tag{6.49}$$

where we consider a strain amplitude  $\varepsilon_A = 0.25$ , and two strain frequencies of  $\omega = 1 [Hz]$  and  $\omega = 60 [Hz]$ . The difference between both approaches is illustrated in Fig.6.6. Here, higher

frequencies result in higher strain rates, and consequently a significant plastic strain history, even after a number of hysteresis cycles. The obtained results confirm the estimates from (6.46), which is already valid at the onset of plasticity. Furthermore, we observe that a tenfold increase in strain rates approximately leads to a tenfold increase in the difference between both algorithms.



Figure 6.6: Comparison between the presented return-mapping algorithm and the reference approach from [1], under low and high frequency loading.

**Example 5** (Convergence of fractional visco-elasto-plasticity). Finally, we perform a verification on the entire fractional visco-elasto-plastic framework under cyclic strain. Since no fabricated solutions are available, we employ reference solutions with time-step size  $\Delta t = 2^{-18} [s]$ . Let T = 1 [s] with the same applied strains (6.49) as the previous example. The visco-elastic material parameters are taken as  $(\mathbb{E}_1, \mathbb{E}_2, \mathbb{E}_3) = (50, 50, 50)$  and  $(\beta_1, \beta_2, \beta_3) = (0.3, 0.7, 0.1)$ , and viscoplastic parameters taken as  $\mathbb{K} = 5$ ,  $\beta_K = 0.7$ , H = 0 and  $\sigma^Y = 1$ . Figure 6.7 illustrates the obtained convergence results, where all models except the FKV one showed a convergence rate of order  $q \approx 1.3$ , which is compatible with the employed L1 discretization scheme, and given that  $\beta_2 = \beta_K = 0.7$ . The FKV model achieved linear asymptotic convergence for the considered example, which is the expected worst case scenario from the backward-Euler discretization of internal variables. We believe the difference in convergence behavior between the FKV model and the others could be due to the sharper response of the FKV model, due to a stiffer rheology combined with the nonlinear loading/unloading response. This combination of effects could result in a lower solution regularity and therefore a lower convergence rate.



Figure 6.7: Convergence analysis for the fractional visco-elasto-plastic models under cyclic loads. Due to the particular choice of fractional orders (with  $\beta_2 = \beta_K = 0.7$  being dominant), we observed convergence rates  $q \approx 1.3$  for all models, except for the FKV. In the latter case, we observe a linear convergence to the reference solution.



Figure 6.8: Visco-elasto-plastic reference solutions for the employed models for the first 30 loading cycles. We notice a similar behavior for most models under the choice of material parameters, except for the FPT and FKV models. The FKV particularly yielded a very stiff response due to the combination of high fractional order values and high strain rates.
#### **CHAPTER 7**

# ANOMALOUS NONLINEAR DYNAMICS BEHAVIOR OF FRACTIONAL VISCOELASTIC STRUCTURES

# 7.1 Background

Nonlinearities are intrinsic in real physical systems, arising from multiple sources, such as changes in geometry, material response (*e.g.*, ageing), and boundary effects (*e.g.*, emergence of boundary-layers/shock). We focus on the analysis of nonlinear systems where anomalous dynamics arise from nonlocal/history effects. Despite the existing "nearly-pure" systems, where standard features evolve to anomalous qualities, *e.g.*, laminar-to-turbulent flows [239, 240] and dislocation pile-up in plasticity [116], in our study, the anomaly source is from the employment of extraordinary materials.

Power-law rheology is a characteristic of a wide range of anomalous materials. This complex response exhibits macroscopic *memory-effects* through single-to-multiple power-law relaxation/creep [23] and dynamic storage/dissipation in visco-elasticity [6]. Such power-laws are multi-scale fingerprints of spatio-temporal sub-diffusive processes in fractal-like micro-structures, where the mean squared displacement of constituents/defects scales nonlinearly in time as  $\langle \Delta r \rangle^2 \propto t^{\alpha}$  [22]. When subject to mechanical loads, such materials undergo micro-structural changes, *e.g.* rearrangement/unfolding of polymer networks/chains [23], plastic stretching/buckling of micro-fibers [21], formation, arresting, relaxation of dislocations [26], which propagate the evolving micro-rheology to the larger scales. Classical (integer-order) viscoelastic models accurately fit exponential data with a limited number of relaxation times [241]. However, a large number of relaxation time is usually required to estimate complex hereditary behaviors observed for a broad class of anomalous (non-exponential) materials. This yields high-dimensional parameter spaces, worsening the conditioning of already ill-posed parameter estimations [242]. In addition, multi-exponential approximations are mere truncations of power-law relaxation [243], only providing accurate results for short times, thus lacking predictability and requiring recalibration for multiple time-scales [24].

Fractional differential equations (FDEs) are predictive tools for anomalous materials across multiple time-scales. Nutting and Gemant [244, 245] showed that power law kernels are more descriptive of creep/relaxation. Bagley and Torvik [246] proposed a link between fractional viscoelasticity and polymer dynamics through dynamic moduli. The building block of fractional viscoelasticity is the so-called *Scott-Blair* (SB) element with fractional order  $0 < \alpha < 1$ , that interpolates between Hookean ( $\alpha \rightarrow 0$ ) and Newtonian ( $\alpha \rightarrow 1$ ) elements. Distinct arrangements of SB elements model multiple experimentally observed power-laws through multi-term FDEs. Such flexible and compact mathematical tool led to multi-disciplinary developments *e.g.*, in bio-engineering[187, 247], visco-elasto-plasticity [1, 75], among others [248–250]. The most general forms of viscoelasticity are described by distributed order differential equations (DODEs) [251, 252], where fractional-order distributions (distributions of SB elements) code evolving, heterogeneous multi-scale material properties. DODEs were employed for anomalous diffusion in [253–255] with applications also in control theory and signal processing [256, 257], vibration [258], frequency domain analysis [259], and uncertainty quantification [260, 261]. We refer the reader to [262] for a thorough review on applications of DODEs.

Regarding the dynamics of anomalous beams, Łabędzki *et al.* [76] investigated the resonance of Euler-Bernoulli piezoelectric beams by introducing fractional derivatives in the equation of motion, and solved the strong form of the system using a Rayleigh-Ritz method. Ansari *et al.* [77] studied the free vibration of a nonlocal, fractional Kelvin-Voigt (KV) Euler-Bernoulli nanobeam. A direct Ritz method in space and a fractional Adams-Moulton scheme in time were employed, observing increased damping for larger fractional orders. Under the same model, Faraji Oskouie *et al.* [78] incorporated surface stress effects through the Gurtin-Murdoch theory. Recently, Eyebe *et al.* [79] studied the nonlinear vibration of a nanobeam over a fractional Winkler-Pasternak foundation, utilizing D'Alembert principle to obtain a nonlinear system of equations, solved by a method of multiple scales. Lewandowski *et al.* [80] analyzed the nonlinear, steady-state vibration of a fractional Zener beam, obtaining amplitude equations with explicit finite-element tangent

matrices. The authors also studied the stability and parametric influence of their model.

An important application of interest is the dynamics of human's outer *hair cells* inside the fluid-filled cochlea of the inner ear. The corresponding structures are indeed '*beam-shaped*' whose dysfunction leads to sensorineural hearing loss. Direct measurements from the cochlea is not possible, which makes computational modeling a valuable (noninvasive) tool to study the health and function of the hair cells. The outer hair cells sit on the basilar membrane (i.e., the beam base) and are embedded into the tectorial membrane at the other end. The sound transmission in the cochlea leads to a pressure difference across the basilar membrane leading to the vibration of hair cells [263]. The cochlea has been modelled previously based on a fractional-modeling approach [187, 247]. The proposed distributed-order fractional modeling in the current work can be readily employed in studying the fluid-induced vibrations of the hair cells, leading to new experiment setups and sensor developments.

The sophistication of numerical methods allowed numerous applications of fractional models in the last two decades, such as spectral methods for spatio-temporal discretization of FDEs [264, 265] and DODEs [266]. Among many schemes for time-fractional integration [177, 267– 269], for simplicity, we outline the L1 finite-difference (FD) scheme by Lin and Xu [176] and refer to [224] for a brief review of numerical methods for time-fractional ODEs. Despite the existing works on nonlinear vibration of fractional viscoelastic beams, they employed direct Ritz discretizations in the strong forms of the equations of motion, requiring more smoothness on basis functions. Spectral methods for nonlinear fractional beam models with proper finite dimensional function spaces suitable for fractional operators are still lacking. Furthermore, from the rheology standpoint, studying the emergence of anomalous dynamics from evolving extraordinary material properties and their sensitivity is fundamental for physics- and mathematically-informed learning of constitutive laws from data, and also requires more attention.

In this work, we study how the evolving power-law rheology, in the language of fractional constitutive laws lead to (counter-intuitive) anomalous dynamics in mechanical systems. Our representation of choice is a geometrically nonlinear, fractional KV Euler-Bernoulli cantilever

beam under free and forced vibration, where:

- The fractional KV model with order  $\alpha$  is obtained from both the Boltzmann superposition principle and general distributed-order viscoelasticity.
- Motivated by the effect of evolving fractal microstructures on macroscopic material dynamics, we study the effects of fractional orders on the continuum response.
- We employ Hamilton's principle to avoid a non-trivial decomposition of conservative (elastic) and non-conservative (viscous) parts of SB elements.
- The weak form of the governing equation is obtained, followed by a single-mode approximation in space.
- We solve the resulting nonlinear system through a method of multiple scales, followed by a sensitivity analysis of amplitude decay rates with respect to  $\alpha$ .

Our numerical and semi-analytical experiments demonstrate several anomalous responses linked to far-from-equilibrium dynamics, such as  $\alpha$ -dependent hardening-like drifts in linear amplitudefrequency behavior and long-term power law response. An interesting new result indicating a super sensitivity of amplitude response with respect to  $\alpha$  was obtained, which could be potentially related to the identification of early damage precursors, before the onset of macroscopic plasticity and cracks [116]. Specifically, a softening-like behavior is observed until a critical  $\alpha$ - value, followed by a hardening-like response, both justified from the constitutive standpoint. This motivates the notion of evolving anomalies, where the changing fractal material microstructure drives the fractional operator form through  $\alpha$  [40]. Finally, we observe the usual bifurcation behavior under steady-state amplitude at primary resonance in the presence of geometrical nonlinearity, which is also driven by material nonlinearity through the fractional order.

This work is organized as follows. In Section 7.2, we introduce the model assumptions, fractional viscoelasticity definitions, the extended Hamilton's principle, and obtain the strong/weak forms of equation of motion under base excitation. We employ assumed modes in space to reduce

the problem to a system of fractional ODEs. In Section 7.3, we obtain the linearized equation of motion. Perturbation analysis in carried out Section 7.4 to solve the resulting nonlinear fractional ODE.

# 7.2 Mathematical Formulation

We formulate our anomalous physical system and discuss the main assumptions utilized to derive the corresponding equation of motion.

## 7.2.1 Nonlinear In-Plane Vibration of a Viscoelastic Cantilever Beam

Let the nonlinear response of a slender viscoelastic cantilever beam with symmetric cross-section, subject to harmonic vertical base excitation denoted by  $v_b$  (see Figures 7.1a and 7.1b). We employ the nonlinear Euler-Bernoulli beam theory, where the geometric nonlinearities are taken into account in the equations of motion. We consider the following kinematic and geometric assumptions:

- The beam is inextensional, i.e., the strech along the neutral axis is negligible. The effects of warping and shear deformation are ignored. Therefore, the strain states in the cross section are only due to bending.
- The beam is slender with symmetric cross section, and undergoes purely planar flexural vibration.
- The length L, cross section area A, mass per unit length ρ, mass M and rotatory inertia J of the lumped mass at the tip of beam are constant.
- The axial displacement along length of beam and the lateral displacement are respectively denoted by *u*(*s*, *t*) and *v*(*s*, *t*).
- We consider the in-plane vertical vibration of the beam and reduce the problem to 1dimension.



Figure 7.1: (a) In-plane kinematics of the cantilever beam subject to a base displacement  $v_b(t)$  with respect to an inertial coordinate system (x, y, z). The terms u(s, t) and v(s, t) denote, respectively, the axial and vertical displacements with respect to a (x', y', z') coordinate system attached to the base, and  $\psi(s, t)$  is the rotation angle about the z'-axis. (b) The total deformation of an arbitrary (red) point, composed of an axial displacement u and vertical displacement v, as well as the displacement due to rotation  $\psi$ .

Figures 7.1a and 7.1b illustrates the kinematics of the cantilever beam under consideration. Let (x, y, z) be an inertial coordinate system and (x', y', z') be a moving coordinate system attached to the base of the beam, such that  $(x'_0, y'_0, z'_0) = (0, v_b, 0)$ . We note that both systems coincide when the base displacement is zero, *i.e.*,  $v_b(t) = 0$ . Furthermore, a differential element of the beam rotates about the z'-axis with an angle  $\psi(s, t)$  to the coordinate system  $(\xi, \eta, \zeta)$ , where

$$\begin{bmatrix} \mathbf{e}_{\xi} \\ \mathbf{e}_{\eta} \\ \mathbf{e}_{\zeta} \end{bmatrix} = \begin{pmatrix} \cos(\psi) & \sin(\psi) & 0 \\ -\sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{bmatrix} \mathbf{e}_{x'} \\ \mathbf{e}_{y'} \\ \mathbf{e}_{z'} \end{bmatrix},$$

and  $\mathbf{e}_i$  is the unit vector along the *i*<sup>th</sup> coordinate. The angular velocity and curvature at any point *s* along the length of the beam at time *t* can be written, respectively, as

$$\boldsymbol{\omega}(s,t) = \frac{\partial \psi}{\partial t} \, \mathbf{e}_{z'}, \quad \boldsymbol{\rho}(s,t) = \frac{\partial \psi}{\partial s} \, \mathbf{e}_{z'} \tag{7.1}$$

Therefore, the total displacement and velocity of an arbitrary point of the beam with respect to the inertial coordinate system takes the form:

$$\mathbf{r} = (u - \eta \sin(\psi)) \mathbf{e}_x + (v + v_b + \eta \cos(\psi)) \mathbf{e}_y, \tag{7.2}$$

$$\frac{\partial \mathbf{r}}{\partial t} = \left(\frac{\partial u}{\partial t} - \eta \,\frac{\partial \psi}{\partial t} \,\cos(\psi)\right) \,\mathbf{e}_x + \left(\frac{\partial v}{\partial t} + \frac{\partial v_b}{\partial t} - \eta \,\frac{\partial \psi}{\partial t} \,\sin(\psi)\right) \,\mathbf{e}_y. \tag{7.3}$$



Figure 7.2: Deformation of an arbitrary element of the beam. The initial configuration CD translates, rotates and elongates to an updated configuration  $C^*D^*$ .

We also let an arbitrary element CD with initial length ds on the neutral axis, located at a distance s from the origin O of the moving system (x', y', z'), to deformation to an updated configuration  $C^*D^*$  (see Fig. 7.2). The displacement components of points C and D are denoted by the pairs (u, v) and (u + du, v + dv), respectively. The axial strain e(s, t) at point C is given by

$$e = \frac{ds^* - ds}{ds} = \frac{\sqrt{(ds + du)^2 + dv^2} - ds}{ds} = \sqrt{(1 + \frac{\partial u}{\partial s})^2 + (\frac{\partial v}{\partial s})^2} - 1.$$
(7.4)

Applying the inextensionality assumption, i.e. e = 0, (7.4) becomes

$$1 + \frac{\partial u}{\partial s} = \left(1 - \left(\frac{\partial v}{\partial s}\right)^2\right)^{1/2}.$$
(7.5)

Moreover, based on the assumption of negligible vertical shear strains, and using (7.5), we have the following expression for the rotation:

$$\psi = \tan^{-1} \frac{\frac{\partial v}{\partial s}}{1 + \frac{\partial u}{\partial s}} = \tan^{-1} \frac{\frac{\partial v}{\partial s}}{\left(1 - \left(\frac{\partial v}{\partial s}\right)^2\right)^{1/2}}.$$
(7.6)

Using the expansion  $\tan^{-1}(x) = x - \frac{1}{3}x^3 + \cdots$ , the curvature can be approximated up to third-order terms as

$$\psi = \frac{\partial v}{\partial s} (1 - (\frac{\partial v}{\partial s})^2)^{-1/2} - \frac{1}{3} (\frac{\partial v}{\partial s})^3 (1 - (\frac{\partial v}{\partial s})^2)^{-3/2} + \cdots$$
$$\approx \frac{\partial v}{\partial s} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) - \frac{1}{3} (\frac{\partial v}{\partial s})^3 \approx \frac{\partial v}{\partial s} + \frac{1}{6} (\frac{\partial v}{\partial s})^3$$
(7.7)

Therefore, the angular velocity and curvature of the beam, i.e.  $\frac{\partial \psi}{\partial t}$  and  $\frac{\partial \psi}{\partial s}$ , respectively, can be

approximated as:

$$\frac{\partial \psi}{\partial t} \simeq \frac{\partial^2 v}{\partial t \partial s} + \frac{1}{2} \frac{\partial^2 v}{\partial t \partial s} \left(\frac{\partial v}{\partial s}\right)^2 \simeq \frac{\partial^2 v}{\partial t \partial s} \left(1 + \frac{1}{2} \left(\frac{\partial v}{\partial s}\right)^2\right),\tag{7.8}$$

$$\frac{\partial \psi}{\partial s} \simeq \frac{\partial^2 v}{\partial s^2} + \frac{1}{2} \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 \simeq \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2). \tag{7.9}$$

By the Euler-Bernoulli beam assumptions a slender beam without vertical shear strains, the strain-curvature relationship takes the form

$$\varepsilon(s,t) = -\eta \, \frac{\partial \psi(s,t)}{\partial s} \tag{7.10}$$

## 7.2.2 Linear Viscoelasticity: Boltzmann Superposition Principle

In this section, we start with a *bottom-up* derivation of our rheological building block, *i.e.*, the Scott-Blair model through the Boltzmann superposition principle. Then, in a *top-bottom* fashion, we demonstrate how the fractional Kelvin-Voigt model is obtained from a general distributed-order form. Assuming linear viscoelasticity, and applying a small step strain increase, denoted by  $\delta \varepsilon(t)$ , at a given time  $t = \tau_1$ , the resulting stress in the material is given by:

$$\sigma(t) = G(t - \tau_1)\delta\varepsilon(\tau_1), \quad t > \tau_1, \tag{7.11}$$

where G(t) denotes the relaxation function. The Boltzmann superposition principle states that resulting stresses from distinct applied small strains are additive. Therefore, the total tensile stress of the specimen at time t is obtained from the superposition of infinitesimal changes in strain at some prior time  $\tau_i$ , given as  $G(t - \tau_i)\delta\varepsilon(\tau_i)$ . Therefore,

$$\sigma(t) = \sum_{\tau_j < t} G(t - \tau_j) \frac{\delta \varepsilon(\tau_j)}{\delta \tau_j} \delta \tau_j, \qquad (7.12)$$

where the limiting case  $\delta \tau_i \rightarrow 0$  yields the following integral form:

$$\sigma(t) = \int_{-\infty}^{t} G(t-\tau) \dot{\varepsilon}(\tau) d\tau, \qquad (7.13)$$

where  $\dot{\varepsilon}$  denotes the strain rate.



Figure 7.3: Classical viscoelastic models as a combination of spring (purely elastic) and dash-pot (purely viscous) elements. Kelvin-Voigt (top) and Maxwell (bottom) rheological models.

# 7.2.2.1 Exponential Relaxation (Classical Models) vs. Power-Law Relaxation (Fractional Models)

The relaxation function G(t) is traditionally expressed as the summation of exponential functions with different exponents and constants, which yields the *so-called* generalized Maxwell form as:

$$G(t) = \sum C_i e^{-t/\tau_i}.$$
(7.14)

For the simple case of a single exponential term (a single Maxwell branch), we have  $G(t) = Ee^{-t/\tau}$ . Therefore, in the case of zero initial strain ( $\varepsilon(0) = 0$ ), we have:

$$\sigma(t) = E \int_0^t e^{-(t-\tilde{t})/\tau} \dot{\varepsilon}(\tilde{t}) d\tilde{t}, \qquad (7.15)$$

which solves the integer-order differential equation  $\frac{\partial \varepsilon}{\partial t} = \frac{1}{E} \frac{\partial \sigma}{\partial t} + \frac{1}{\eta} \sigma$ , where the relaxation time constant  $\tau = \eta/E$  is obtained from experimental observations. The Maxwell model is in fact a combination of purely elastic and purely viscous elements in series, as illustrated in Fig. 7.3.

By letting the relaxation function (kernel) in (7.13) have a modulated power-law form  $G(t) = E_{\alpha} g(\alpha)(t - \tau)^{-\alpha}$ , equation (7.13) for the stress takes the following form,

$$\sigma(t) = E_{\alpha} g(\alpha) \int_{-\infty}^{t} \frac{\dot{\varepsilon}(\tau)}{(t-\tau)^{\alpha}} d\tau.$$
(7.16)

where  $E_{\alpha}$  denotes a *pseudo-constant* with units  $[Pa.s^{\alpha}]$ . If we choose the modulation  $g(\alpha) = \frac{1}{\Gamma(1-\alpha)}$ , then the integro-differential operator (7.16) gives the Liouville-Weyl fractional derivative [270]. Although the lower integration limit of (7.16) is taken as  $-\infty$ , under hypothesis of causal histories, which states that the viscoelastic body is quiescent for all time prior to some starting point

t = 0, (7.16) can be re-written as

$$\sigma(t) = \varepsilon(0^{+}) \frac{E_{\alpha} g(\alpha)}{t^{\alpha}} + E_{\alpha} g(\alpha) \int_{0}^{t} \frac{\dot{\varepsilon}}{(t-\tau)^{\alpha}} d\tau,$$
  
$$= \varepsilon(0^{+}) \frac{E_{\alpha} g(\alpha)}{t^{\alpha}} + E_{\alpha} {}_{0}^{C} \mathcal{D}_{t}^{\alpha} \varepsilon,$$
  
$$= E_{\alpha} {}^{RL}_{0} \mathcal{D}_{t}^{\alpha} \varepsilon, \qquad (7.17)$$

where  ${}_{0}^{C}\mathcal{D}_{t}^{\alpha}$  and  ${}_{0}^{RL}\mathcal{D}_{t}^{\alpha}$  denote, respectively, the Caputo and Riemann-Liouville fractional derivatives [270]. Both definitions are equivalent here due to homogeneous initial conditions for the strain.

**Remark 7.2.1.** The constitutive equation (7.17) can be thought of as an interpolation between a pure elastic (spring) and a pure viscous (dash-pot) elements, i.e., the Scott Blair element [1, 271–273]. It should be noted that in the limiting cases of  $\alpha \rightarrow 0$  and  $\alpha \rightarrow 1$ , the relation (7.17) recovers the corresponding equations for spring and dash-pot, respectively.

#### 7.2.2.2 Multi-Scale Power-Laws, Distributed-Order Models

In the most general sense, materials intrinsically possess a spectrum of power-law relaxations, and therefore we need a distributed-order representation for the stress-strain relationship. Consequently, the relaxation function G(t) in (7.13) does not only contain a single power-law as in (7.16), but rather a distribution over a range of values. Considering nonlinear viscoelasticity with material heterogeneities, the distributed order constitutive equations over t > 0 with orders  $\alpha \in [\alpha_{min}, \alpha_{max}]$ and  $\beta \in [\beta_{min}, \beta_{max}]$  can be expressed in the general form as

$$\int_{\beta_{min}}^{\beta_{max}} \Phi(\beta; x, t, \sigma) {}_{0}^{*} \mathcal{D}_{t}^{\beta} \sigma(t) d\beta = \int_{\alpha_{min}}^{\alpha_{max}} \Psi(\alpha; x, t, \varepsilon) {}_{0}^{*} \mathcal{D}_{t}^{\alpha} \varepsilon(t) d\alpha,$$
(7.18)

in which the prescript \* stands for any type of fractional derivative, and initial conditions also depending on such definitions. The functions  $\Phi(\beta; x, t, \sigma)$  and  $\Psi(\alpha; x, t, \varepsilon)$  can be thought of as distribution functions, where  $\alpha \mapsto \Psi(\alpha; x, t, \varepsilon)$  and  $\beta \mapsto \Phi(\beta; x, t, \sigma)$  are continuous mappings in  $[\alpha_{min}, \alpha_{max}]$  and  $[\beta_{min}, \beta_{max}]$ . Furthermore, the dependence of the distributions on the (thermodynamically) conjugate pair ( $\sigma, \varepsilon$ ) introduces the notion of nonlinear viscoelasticity, and the dependence on a material coordinate *x* induces material heterogeneties in space.

**Remark 7.2.2.** The pairs  $(\alpha_{min}, \alpha_{max})$  and  $(\beta_{min}, \beta_{max})$  are only the theoretical lower and upper terminals in the definition of distributed order models. In general, the distribution function  $\Phi(\beta; x, t, \sigma)$  and  $\Psi(\alpha; x, t, \varepsilon)$  can arbitrarily confine the domain of integration in each realization of practical rheological problems and material design. If we let the distribution be summation of some delta functions, then, the distributed order model becomes the following multi-term model:

$$\left(1 + \sum_{k=1}^{p_{\sigma}} a_{k} {}_{0}\mathcal{D}_{t}^{\beta_{k}}\right) \sigma(t) = \left(c + \sum_{k=1}^{p_{\varepsilon}} b_{k} {}_{0}\mathcal{D}_{t}^{\alpha_{k}}\right) \varepsilon(t)$$

In order to obtain the fractional Kelvin-Voigt model, we let  $\Phi(\beta) = \delta(\beta)$  and  $\Psi(\alpha) = E_{\infty}\delta(\alpha) + E_{\alpha}\delta(\alpha - \alpha_0)$  in (7.18), and therefore,

$$\sigma(t) = E_{\infty} \varepsilon(t) + E_{\alpha} \, {}^{RL}_{0} \mathcal{D}^{\alpha}_{t} \, \varepsilon(t), \quad \alpha \in (0, 1).$$
(7.19)

## 7.2.3 Extended Hamilton's Principle

We derive the equations of motion by employing the extended Hamilton's principle

$$\int_{t_1}^{t_2} \left(\delta T - \delta W\right) \, dt = 0,$$

where  $\delta T$  and  $\delta W$  denote the variations of kinetic energy and total work [274]. The only source of external input to our system of interest is the base excitation, which is linearly superposed to the beam's vertical displacement v(t), and therefore contributes to the kinetic energy taken in the inertial (Lagrangian) coordinate system. Hence, the total work only contains the internal work done by the stress state, with the variation expressed as [275]

$$\delta W = \int_{\mathbb{V}} \sigma \, \delta \varepsilon \, d\nu, \tag{7.20}$$

where the integral is taken over the whole system volume  $\mathbb{V}$ .

**Remark 7.2.3.** It is remarked in (7.2.1) that the fractional Scott-Blair elements exhibit both elasticity and viscosity behaviors. There have been attempts in the literature to separate the conservative

(elastic) and non-conservative (viscous) parts of fractional constitutive equations at the free-energy level [276]. However, we note this separation in the time domain is not trivial for sophisticated fractional constitutive equations, and therefore we choose to formulate our problem in terms of the total work in order to avoid such additional complexities.

The full derivation of the governing equation using the extended Hamilton's principle is given in D.1. We recall that M and J are the mass and rotatory inertia of the lumped mass at the tip of beam,  $\rho$  is the mass per unit length of the beam,  $I = \int_A \eta^2 dA$ , and let  $m = \frac{\rho}{E_{\infty} I}$  and  $E_r = \frac{E_{\alpha}}{E_{\infty}}$ . We approximate the nonlinear terms up to third order and use the following dimensionless variables

$$s^* = \frac{s}{L}, \ v^* = \frac{v}{L}, \ t^* = t \left(\frac{1}{mL^4}\right)^{1/2}, \ E_r^* = E_r \left(\frac{1}{mL^4}\right)^{\alpha/2}, \ J^* = \frac{J}{\rho L^3}, \ M^* = \frac{M}{\rho L}, \ v_b^* = \frac{v_b}{L},$$

and derive the strong form of the equation of motion. Therefore, by choosing a proper function space *V*, the problem reads as: find  $v \in V$  such that

$$\frac{\partial^2 v}{\partial t^2} + \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) - \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) = -\ddot{v_b},$$
(7.21)

which is subject to the following boundary conditions:

$$\begin{aligned} v \Big|_{s=0} &= \frac{\partial v}{\partial s} \Big|_{s=0} = 0, \\ J \left( \frac{\partial^3 v}{\partial t^2 \partial s} (1 + (\frac{\partial v}{\partial s})^2) + \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s \partial t})^2 \right) \\ &+ \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \Big|_{s=1} = 0, \\ M (\frac{\partial^2 v}{\partial t^2} + v_b^i) - \frac{\partial v}{\partial s} \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \\ &+ \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \Big|_{s=1} = 0. \end{aligned}$$
(7.22)

## 7.2.4 Weak Formulation

The common practice in analysis of numerical methods for PDEs are mostly concerned with linear equations. Analyses for linear PDEs are well-developed and well-defined, however they are still scarce for nonlinear PDEs. The linear theories are usually applicable to nonlinear problems if the solution is sufficiently smooth [277]. We do not intend to investigate/develop analysis for our proposed nonlinear model. Instead, by assuming smooth solution, we employ linear theories in our analysis. Let  $v : \mathbb{R}^{1+1} \to \mathbb{R}$  for  $\alpha \in (0, 1)$  and  $\Omega = [0, T] \times [0, L]$ . Here, we construct the solution space,  $\mathcal{B}^{\alpha}(\Omega)$ , endowed with proper norms [265], in which the corresponding weak form of (7.21) can be formulated. If we recall the equation (7.21) as E, then:

$$\mathcal{B}^{\alpha}(\Omega) := \left\{ v \in {}_{0}^{l} H^{\alpha}(\Omega) \left| \int_{\Omega} E \, d\Omega < \infty \right\}$$
(7.23)

where

$${}_{0}^{l}H^{\alpha}(\Omega) = {}_{0}^{l}H^{\alpha}\left(I;L^{2}(\Omega)\right) \cap L^{2}(I;{}_{0}H^{2}(\Omega)),$$
$${}_{0}H^{2}(\Omega) = \left\{v \in H^{2}(\Omega) \mid v \mid_{s=0} = \frac{\partial v}{\partial s} \mid_{s=0} = 0\right\}$$

We obtain the weak form of the problem by multiplying the strong form (7.21) with proper test functions  $\tilde{v}(s) \in \mathcal{B}^{\alpha}(\Omega)$  and integrating over the dimensionless spatial computational domain  $\Omega_s = [0, 1]$ . The test functions satisfy the boundary conditions, i.e.  $\tilde{v}(0) = \frac{\partial \tilde{v}}{\partial s}(0) = 0$ . Therefore, we obtain:

$$\int_{0}^{1} \frac{\partial^{2} v}{\partial t^{2}} \tilde{v} ds + \int_{0}^{1} \frac{\partial^{2}}{\partial s^{2}} \left( \frac{\partial^{2} v}{\partial s^{2}} + \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \tilde{v} ds$$

$$- \int_{0}^{1} \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial s^{2}})^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2} v}{\partial s^{2}} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \tilde{v} ds = -\int_{0}^{1} \dot{v_{b}} \tilde{v} ds.$$

$$(7.24)$$

Integrating the above equation by parts, we obtain:

$$\begin{aligned} \frac{\partial^2}{\partial t^2} \int_0^1 v \tilde{v} ds \\ + \int_0^1 \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \frac{\partial^2 \tilde{v}}{\partial s^2} ds \\ + \int_0^1 \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \frac{\partial \tilde{v}}{\partial s} ds + M (\frac{\partial^2 v}{\partial t^2} + \ddot{v}_b) \tilde{v} \Big|_{s=1} \\ + J \left( \frac{\partial^3 v}{\partial t^2 \partial s} (1 + (\frac{\partial v}{\partial s})^2) + \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial t \partial s})^2 \right) \frac{\partial \tilde{v}}{\partial s} \Big|_{s=1} = -\ddot{v}_b \int_0^1 \tilde{v} \, ds. \end{aligned}$$
(7.25)

By rearranging the terms, we get

$$\frac{\partial^{2}}{\partial t^{2}} \left( \int_{0}^{1} v \,\tilde{v} \,ds + M \,v \,\tilde{v} \,\Big|_{s=1} + J \,\frac{\partial v}{\partial s} \,\frac{\partial \tilde{v}}{\partial s} \,\Big|_{s=1} \right) + J \left( \frac{\partial^{3} v}{\partial t^{2} \partial s} (\frac{\partial v}{\partial s})^{2} + \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial t \partial s})^{2} \right) \frac{\partial \tilde{v}}{\partial s} \,\Big|_{s=1} \\ + \int_{0}^{1} \frac{\partial^{2} v}{\partial s^{2}} \,\frac{\partial^{2} \tilde{v}}{\partial s^{2}} \,ds + E_{r} \int_{0}^{1} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \,ds \\ + \int_{0}^{1} \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} \,\frac{\partial^{2} \tilde{v}}{\partial s^{2}} \,ds + \int_{0}^{1} \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial s^{2}})^{2} \,\frac{\partial \tilde{v}}{\partial s} \,ds \\ + \frac{E_{r}}{2} \int_{0}^{1} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} \right] \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \,ds + \frac{E_{r}}{2} \int_{0}^{1} (\frac{\partial v}{\partial s})^{2} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \frac{\partial^{2} \tilde{v}}{\partial s} \,ds \\ + E_{r} \int_{0}^{1} \frac{\partial v}{\partial s} \frac{\partial^{2} v}{\partial s^{2}} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \frac{\partial \tilde{v}}{\partial s} \,ds = -v_{b}^{r} \left( \int_{0}^{1} \tilde{v} \,ds + M \tilde{v} \right|_{s=1} \right).$$
(7.26)

# 7.2.5 Assumed Mode: A Spectral Approximation in Space

We employ the following modal discretization to obtain a reduced-order model of the beam. Therefore,

$$v(s,t) \simeq v_N(s,t) = \sum_{n=1}^{N} q_n(t) \phi_n(s),$$
 (7.27)

where the spatial functions  $\phi_n(s)$ ,  $n = 1, 2, \dots, N$  are assumed *a priori* and the temporal functions  $q_n(t)$ ,  $n = 1, 2, \dots, N$  are the unknown modal coordinates. The assumed modes  $\phi_n(s)$  in (7.27) are obtained in D.4, by solving the corresponding linear eigenvalue problem of our nonlinear model.

Subsequently, we construct the proper finite dimensional spaces of basis/test functions as:

$$V_N = \tilde{V}_N = span \left\{ \phi_n(x) : n = 1, 2, \cdots, N \right\}.$$
 (7.28)

Since  $V_N = \tilde{V}_N \subset V = \tilde{V}$ , problem (7.26) read as: find  $v_N \in V_N$  such that

$$\frac{\partial^{2}}{\partial t^{2}} \left( \int_{0}^{1} v_{N} \tilde{v}_{N} ds + M v_{N} \tilde{v}_{N} \Big|_{s=1} + J \frac{\partial v_{N}}{\partial s} \frac{\partial \tilde{v}_{N}}{\partial s} \Big|_{s=1} \right) + J \left( \frac{\partial^{3} v_{N}}{\partial t^{2} \partial s} (\frac{\partial v_{N}}{\partial s})^{2} + \frac{\partial v_{N}}{\partial s} (\frac{\partial^{2} v_{N}}{\partial t \partial s})^{2} \right) \frac{\partial \tilde{v}_{N}}{\partial s} \Big|_{s=1} \\ + \int_{0}^{1} \frac{\partial^{2} v_{N}}{\partial s^{2}} \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} ds + E_{r} \int_{0}^{1} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v_{N}}{\partial s^{2}} \right] \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} ds \\ + \int_{0}^{1} \frac{\partial^{2} v_{N}}{\partial s^{2}} (\frac{\partial v_{N}}{\partial s})^{2} \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} ds + \int_{0}^{1} \frac{\partial v_{N}}{\partial s} (\frac{\partial^{2} v_{N}}{\partial s})^{2} \frac{\partial \tilde{v}_{N}}{\partial s} ds \\ + \frac{E_{r}}{2} \int_{0}^{1} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v_{N}}{\partial s^{2}} (\frac{\partial v_{N}}{\partial s})^{2} \right] \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} ds + \frac{E_{r}}{2} \int_{0}^{1} (\frac{\partial v_{N}}{\partial s})^{2} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} ds \\ + E_{r} \int_{0}^{1} \frac{\partial v_{N}}{\partial s} \frac{\partial^{2} v_{N}}{\partial s^{2}} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v_{N}}{\partial s^{2}} \right] \frac{\partial \tilde{v}_{N}}{\partial s} ds = -\tilde{v}_{b} \left( \int_{0}^{1} \tilde{v}_{N} ds + M \tilde{v}_{N} \Big|_{s=1} \right),$$
(7.29)

for all  $\tilde{v}_N \in \tilde{V}_N$ .

## 7.2.6 Single Mode Approximation

In general, the modal discretization (7.27) in (7.29) leads to a coupled nonlinear system of fractional ordinary differential equations. We note that while the fractional operators already impose numerical challenges, these are increased by the presence of nonlinearities, leading to failure of existing numerical schemes. However, without loss of generality, we can assume that only one mode (primary mode) of motion is involved in the dynamics of system of interest.

## 7.2.6.1 Why is single-mode approximation useful?

Although single-mode approximations are simplistic in nature, they encapsulate the most fundamental dynamics and the highest energy mode in the motion of nonlinear systems. Furthermore, as shown by numerous studies below, such approximation also proved capable of capturing the complex behavior of structures. Azrar et al. [278] demonstrated sufficient approximations of single- and multi-modal representation for the nonlinear forced vibration of a simply supported beam under a uniform harmonic distributed force. Tseng and Dugundji [279] showed similar results between single and two mode approximations for nonlinear vibrations of clamped-clamped beams far from the crossover region. Loutridis et al. [280] implemented a crack detection method for beams using a single-degree-offreedom system with time varying stiffness. In [281], the effects of base stiffness and attached mass on the nonlinear, planar flexural free vibrations of beams were studied. Lestari and Hanagud [282] studied the nonlinear free vibrations of buckled beams with elastic end constraints, where the single-mode assumption led to a closed-form solution in terms of elliptic functions.

Of particular interest, Habtour *et al.* [116] detected and validated the response of a nonlinear cantilever beam subject to softening due to local stress-induced, early fatigue damage precursors *prior* to crack formation. Their findings demonstrate that the pragmatism of a single-mode approximation provides sufficient sensitivity of the amplitude response with respect to the nonlinear stiffness, making their framework an effective practical tool for early fatigue detection. We also refer the reader to [283–286] for additional applications.

Therefore, we let the anomalous dynamics of our system be driven by the fractional-order  $\alpha$ , and following the aforementioned studies, we replace (7.27) with the one-mode discretization  $v_N = q(t) \phi(s)$  (where we let N = 1 and drop the subscript 1 for simplicity). Upon substituting in (7.29), we obtain the unimodal governing equation of motion as (see D.2),

$$\mathcal{M}\ddot{q} + \mathcal{J}(\ddot{q}q^2 + q\dot{q}^2) + \mathcal{K}_l q + E_r C_l \frac{R_L}{0} \mathcal{D}_t^{\alpha} q + 2\mathcal{K}_{nl} q^3 + \frac{E_r C_{nl}}{2} \left( {}^{R_L}_0 \mathcal{D}_t^{\alpha} q^3 + 3q^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} q \right) = -\mathcal{M}_b \ddot{v_b},$$
(7.30)

in which

$$\mathcal{M} = \int_{0}^{1} \phi^{2} ds + M \phi^{2}(1) + J {\phi'}^{2}(1), \quad \mathcal{J} = J {\phi'}^{4}(1),$$
  
$$\mathcal{K}_{l} = C_{l} = \int_{0}^{1} {\phi''}^{2} ds, \quad \mathcal{K}_{nl} = C_{nl} = \int_{0}^{1} {\phi'}^{2} {\phi''}^{2} ds, \quad \mathcal{M}_{b} = \int_{0}^{1} {\phi} ds + M \phi(1).$$
(7.31)

**Remark 7.2.4.** We note that one can isolate any mode of vibration  $\phi_n(s)$ ,  $n = 1, 2, \dots, N$  (and not necessarily the primary mode) by assuming that  $\phi_n(s)$  is the only active one, and thus, end up with

similar equation of motion as (7.30), where the coefficients in (7.31) are obtained based on the active mode  $\phi_n(s)$ . Therefore, we can also make sense of (7.30) as a decoupled equation of motion associated with mode  $\phi_n(s)$ , in which the interaction with other inactive modes is absent.

# 7.3 Linearized Equation: Direct Numerical Time Integration

We linearize our equation of motion for the cantilever beam by assuming small motions (*see D.3*), and obtain the following form:

$$\ddot{q} + E_r c_l \frac{RL}{0} \mathcal{D}_t^{\alpha} q + k_l q = -m_b \ddot{v}_b, \quad q(0) = \frac{v(L,0)}{\phi(L)}, \quad \dot{q}(0) = \frac{\dot{v}(L,0)}{\phi(L)}$$
(7.32)

with the coefficients

$$c_l = \frac{C_l}{\mathcal{M}}, \qquad k_l = \frac{\mathcal{K}_l}{\mathcal{M}}, \qquad m_b = \frac{\mathcal{M}_b}{\mathcal{M}}.$$
 (7.33)

The linearized, unimodal form (7.32) is equivalent to the vibration of a lumped fractional Kelvin-Voigt rheological element, and can be thought of as a fractional oscillator, shown schematically in Fig.7.4. Let a uniform time-grid with *N* time-steps of size  $\Delta t$ , such that  $t_n = n\Delta t$ , n = 0, 1, ..., N.



Figure 7.4: Lumped representation of the system as a fractional damper, with constants  $E_r c_l$  and fractional order  $\alpha$ .

We employ the following equivalence relationship between the Riemann-Liouville and Caputo definitions:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}q(t) = {}^{C}_{0}\mathcal{D}^{\alpha}_{t}q(t) + \frac{q(0)}{\Gamma(1-\alpha)t^{\alpha}}.$$
(7.34)

Substituting (7.34) into (7.32), evaluating both sides implicitly at  $t = t_{n+1}$ , and approximating the time-fractional Caputo derivative through an L1-difference scheme [176], we obtain:

$$\ddot{q}_{n+1} + E_r c_l \left[ \frac{1}{\Delta t^{\alpha} \Gamma(2-\alpha)} \left( q_{n+1} - q_n + \mathcal{H}^{\alpha} q_{n+1} \right) + \frac{q_0}{\Gamma(1-\alpha) t_{n+1}^{\alpha}} \right] + k_l q_{n+1} = -m_b \ddot{v}_{b,n+1}, \quad (7.35)$$

where  $\mathcal{H}_{k+1}^{\alpha} = \sum_{j=0}^{n-1} b_j (q_{n-j+1} - q_{n-j})$  represents the discretized history term, with  $\alpha$ -dependent convolution coefficients  $b_j = (j+1)^{\alpha} - j^{\alpha}$ . We approximate the acceleration  $\ddot{q}_{n+1}$  and velocity  $\dot{q}_{n+1}$  through a Newmark- $\beta$  method as follows:

$$\ddot{q}_{n+1} = a_1 \left( q_{n+1} - q_n \right) - a_2 \dot{q}_n - a_3 \ddot{q}_n, \tag{7.36}$$

$$\dot{q}_{n+1} = a_4 \left( q_{n+1} - q_n \right) + a_5 \dot{q}_n + a_6 \ddot{q}_n, \tag{7.37}$$

with approximation coefficients given by

$$a_1 = \frac{1}{\beta \Delta t^2}, \quad a_2 = \frac{1}{\beta \Delta t}, \quad a_3 = \frac{1 - 2\beta}{2\beta}, \quad a_4 = \frac{\gamma}{\beta \Delta t^2}, \quad a_5 = \left(1 - \frac{\gamma}{\beta}\right), \quad a_6 = \left(1 - \frac{\gamma}{2\beta}\right) \Delta t,$$

where we choose  $\beta = 0.5$ ,  $\gamma = 0.25$  for unconditional stability. Inserting (7.36) into (7.35), we obtain the following closed form for  $q_{n+1}$ :

$$q_{n+1} = \frac{(a_1 + E^*) q_n + a_2 \dot{q}_n + a_3 \ddot{q}_n - m_b \ddot{v}_{b,n+1} - E^* \left[ \mathcal{H}^{\alpha}_{n+1} + q_0 \frac{(1-\alpha)}{(n+1)^{\alpha}} \right]}{a_1 + E^* + k_l}$$
(7.38)

with  $E^* = (E_r c_l)/(\Delta t^{\alpha} \Gamma(2 - \alpha))$ . We observe that since the Newmark method is second-order accurate with respect to  $\Delta t$ , the overall accuracy is dominated by the accuracy of the L1 scheme, which is of  $O(\Delta t^{2-\alpha})$ . We also observe that a discretization of a Caputo-variant of the FDE (7.32) is recovered if we remove the term  $q_0(1 - \alpha)/(n + 1)^{\alpha}$  from (7.38).

We consider two numerical tests. In the first one, we solve the above system under harmonic base excitation, and in the second one, we consider a free-vibration response. For both tests, we set  $E_r = 1$  and consider the lumped mass at the tip, with M = J = 1, that is, we utilize (D.56) for  $\phi(s)$ , which yields the coefficients  $c_l = k_l = 1.24$ .

## 7.3.1 Harmonic Base Excitation

We solve (7.32) in the presence of base excitation in the harmonic form  $v_b = a_b sin(\omega_b t)$ , where  $\omega_b \in [0.5, 3.5]$  and  $a_b = 0.01$  denote, respectively, the base frequency and displacement amplitude. The coefficient  $m_b = -0.042$  is calculated through (7.33) and (7.31). We employ homogeneous initial conditions, *i.e.*, q(0) = 0,  $\dot{q}(0) = 0$ , and set the time  $t \in (0, 100]$ , with step size  $\Delta t = 10^{-3}$ . The maximum displacement amplitude after reaching the steady state response of the system is evaluated. Figure 7.5 illustrates the amplitude vs base frequency response with respect to varying fractional orders  $\alpha$ . We observe the existence of a critical point at  $\omega_b = 1$  that changes the dissipation nature of the fractional order parameter. Regarding the maximum observed amplitudes, increasing the fractional order in the range  $\alpha \in [0.1, 0.4]$ , decreases and slightly shifts the amplitude peaks to higher (right) frequencies (an anomalous quality). On the other hand, as the fractional order is increased in the range  $\alpha \in [0.5, 0.6]$ , the peak amplitudes slightly shift towards the lower (left) frequencies, which is also observed in standard systems with the increase of modal damping values.



Figure 7.5: Anomalous change of the maximum amplitude vs frequency at the tip of the beam in presence of harmonic base excitation for different fractional order  $\alpha$ . The solid black line represents the standard, undamped natural frequency of the system.

## 7.3.2 Free Vibration

Following the observed anomalous amplitude *vs*. base frequency behaviors and presence of a critical point nearby the standard natural frequency of the system illustrated in Figure 7.5, we solve (7.32) in a free-vibration setting employing Riemann-Liouville and Caputo definitions, where we set  $\ddot{v}_b = 0$ , and q(0) = 0.01,  $\dot{q}(0) = 0$ . Figure 7.6 (left) illustrates the obtained results for q(t)

for varying fractional orders using a Riemann-Liouville definition. We observe an  $\alpha$ -dependent amplitude decay, which converges to a classical integer-oder oscillator as  $\alpha \rightarrow 1$ . Furthermore, an anomalous transient region is observed at the short time-scale  $t \in [0.1, 1]$ . On the other hand, in Figure 7.6 (right), anomalies are present at large time-scales through a (far-from-equilibrium) power-law relaxation, while the short-time behavior is "standard-like". Such contrast between the obtained results provides interesting insights towards modeling desired anomalous ranges in such power-law materials. By replacing the fractional damper with a classical integer-order one (*see Fig.7.7*), we notice that neither anomalous dynamics are present. The obtained results are in agreement with the power-law and exponential relaxation kernels described in Sec.7.2.2. We note that since the fractional element provides a constitutive interpolation between spring and dash-pot elements (see Sec.7.2.2 for more discussion and references), it contributes to both effective stiffness and damping ratio of the system, and therefore increasing values of  $\alpha$  (decreasing stiffness), yield a reduction in the frequency response.

Fractional linear oscillators are also considered in [287] for systems with memory, where their interaction with a fluctuating environment causes the time evolution of the system to be intermittent. The authors in [287] apply the Koopman operator theory to the corresponding integer order system and then make a Lèvy transformation in time to recover long-term memory effects; they observe a power-law behavior in the amplitude decay of the system's response. Such an anomalous decay rate has also been investigated in [288] for an extended theory of decay of classical vibrational models brought into nonlinear resonances. The authors report a "non-exponential" decay in variables describing the dynamics of the system in the presence of dissipation and also a sharp change in the decay rate close to resonance.

# 7.4 Perturbation Analysis of Nonlinear Equation

We use perturbation analysis to investigate the behavior of a nonlinear system, where we reduce a nonlinear fractional differential equation to an algebraic equation to solve for the steady state amplitude and phase of vibration.



Figure 7.6: Anomalous linear free vibration modal displacement vs. time. (*Left*) Riemman-Liouville definition with short-time anomalies. (*Right*) Caputo definition with long-time anomalies.



Figure 7.7: Classical linear free vibration modal displacement vs. time under varying values of  $E_r$ .

## 7.4.1 Method of Multiple Scales

To investigate the dynamics of the system described by (7.30), we use the method of multiple scales [289, 290]. The new independent time scales and the integer-order derivative with respect to them are defined as

$$T_m = \epsilon^m t, \qquad D_m = \frac{\partial}{\partial T_m}, \qquad m = 0, 1, 2, \cdots.$$
 (7.39)

It is also convenient to utilize another representation of the fractional derivative (*see* [291], Equation 5.82), which according to the Rieman-Liouville fractional derivative, is equivalent to the fractional power of the operator of conventional time-derivative, i.e.  ${}^{RL}_{0}\mathcal{D}^{\alpha}_{t} = (\frac{d}{dt})^{\alpha}$ . Therefore,

$$\frac{d}{dt} = D_0 + \epsilon D_1 + \cdots, \quad \frac{d^2}{dt^2} = D_0^2 + 2\epsilon D_0 D_1 + \cdots, \quad {}^{RL}_0 \mathcal{D}_t^{\alpha} = (\frac{d}{dt})^{\alpha} = D_0^{\alpha} + \epsilon \alpha D_0^{\alpha-1} D_1 + \cdots$$
(7.40)

The solution q(t) can then be represented in terms of series expansion:

$$q(T_0, T_1, \dots) = q_0(T_0, T_1, \dots) + \epsilon q_1(T_0, T_1, \dots) + \epsilon^2 q_2(T_0, T_1, \dots) + \dots$$
(7.41)

We assume that the coefficients in the equation of motion have the following scaling

$$\frac{\mathcal{J}}{\mathcal{M}} = \epsilon m_{nl}, \quad \frac{\mathcal{K}_l}{\mathcal{M}} = k_l = \omega_0^2, \quad \frac{C_l}{\mathcal{M}} = \epsilon c_l, \quad \frac{\mathcal{K}_{nl}}{\mathcal{M}} = \epsilon k_{nl}, \quad \frac{C_{nl}}{\mathcal{M}} = \epsilon c_{nl}, \quad (7.42)$$

and the base excitation  $-\frac{M_b}{M} \ddot{v_b}$  is a harmonic function in the form  $\epsilon F \cos(\Omega t)$ . Thus, (7.30) can be expanded as

$$\begin{aligned} &(D_0^2 + 2\epsilon D_0 D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots) + \epsilon \, m_{nl} (D_0^2 + 2\epsilon D_0 D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots) \\ &\times (q_0 + \epsilon q_1 + \cdots)^2 + \epsilon \, m_{nl} (q_0 + \epsilon q_1 + \cdots) \\ &\times ((D_0 + \epsilon D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots))^2 + \omega_0^2 (q_0 + \epsilon q_1 + \cdots) \\ &+ \epsilon \, E_r \, c_l \, (D_0^\alpha + \epsilon \alpha D_0^{\alpha - 1} D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots) + 2\epsilon \, k_{nl} \, (q_0 + \epsilon q_1 + \cdots)^3 \\ &+ \frac{1}{2} \epsilon \, E_r \, c_{nl} \, (D_0^\alpha + \epsilon \alpha D_0^{\alpha - 1} D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots)^3 + \frac{3}{2} \epsilon \, E_r \, c_{nl} (q_0 + \epsilon q_1 + \cdots)^2 \\ &+ \epsilon q_1 + \cdots)^2 \left[ (D_0^\alpha + \epsilon \alpha D_0^{\alpha - 1} D_1 + \cdots)(q_0 + \epsilon q_1 + \cdots) \right] = \epsilon \, F \cos(\Omega \, T_0). \end{aligned}$$

By collecting similar coefficients of zero-th and first orders of  $\epsilon$ , we obtain the following equations

$$O(\epsilon^0): D_0^2 q_0 + \omega_0^2 q_0 = 0, (7.44)$$

$$O(\epsilon^{1}): D_{0}^{2}q_{1} + \omega_{0}^{2}q_{1} = -2D_{0}D_{1}q_{0} - m_{nl} \left(q_{0}^{2}D_{0}^{2}q_{0} + q_{0}(D_{0}q_{0})^{2}\right) - E_{r}c_{l}D_{0}^{\alpha}q_{0} - 2k_{nl}q_{0}^{3} - \frac{1}{2}E_{r}c_{nl}D_{0}^{\alpha}q_{0}^{3} - \frac{3}{2}E_{r}c_{nl}q_{0}^{2}D_{0}^{\alpha}q_{0} + F\cos(\Omega T_{0}).$$

$$(7.45)$$

The solution to (7.44) is of the form

$$q_0(T_0, T_1) = A(T_1) e^{i \omega_0 T_0} + c.c$$
(7.46)

where "c.c" denotes the complex conjugate. By substituting (7.46) into the right-hand-side of (7.45), we observe that different resonance cases are possible. In each case, we obtain the corresponding solvability conditions by removing the secular terms, i.e. the terms that grow in time unbounded. Then, we utilize the polar form  $A = \frac{1}{2}a e^{i\varphi}$ , where the real valued functions a and  $\varphi$  are the amplitude and phase lag of time response, respectively. Thus, the solution q(t) becomes

$$q(t) = a(\epsilon t)\cos(\omega_0 t + \varphi(\epsilon t)) + O(\epsilon), \qquad (7.47)$$

where the governing equations of a and  $\varphi$  are obtained by separating the real and imaginary parts.

#### 7.4.1.1 Case 1: No Lumped Mass At The Tip

In this case, M = J = 0, and thus, given the form (D.57) for the eigenfunctions  $\phi(s)$  in D.4, the coefficients are computed as  $\mathcal{M} = 1$ ,  $\mathcal{K}_l = C_l = 12.3624$ ,  $\mathcal{M}_b = 0.782992$ , and  $\mathcal{K}_{nl} = C_{nl} = 20.2203$ . We consider the following cases:

• Free Vibration, F = 0: Super Sensitivity to  $\alpha$ 

In this case, the beam is not externally excited and thus, F = 0. By removing the secular terms that are the coefficients of  $e^{i\omega_0 T_0}$  in the solvability condition, we find the governing equations of solution amplitude and phase as

$$\frac{da}{dT_1} = -E_r \,\omega_0^{\alpha - 1} \sin(\alpha \frac{\pi}{2}) \left( \frac{1}{2} \,c_l \,a + \frac{3}{8} \,c_{nl} \,a^3 \right),\tag{7.48}$$

$$\frac{d\varphi}{dT_1} = \frac{1}{2}c_l E_r \,\omega_0^{\alpha-1} \cos\left(\frac{\pi\alpha}{2}\right) + \frac{3}{4}c_{nl} E_r \,\omega_0^{\alpha-1} \cos\left(\frac{\pi\alpha}{2}\right) \,a^2 + \frac{3}{4}\,\omega_0^{-1} \,k_{nl} \,a^2. \tag{7.49}$$

We can see from the first equation (7.48) that the amplitude of free vibration decays out, where the decay rate  $\tau_d = c_l E_r \omega_0^{\alpha-1} \sin(\alpha \frac{\pi}{2})$  directly depends on values of the fractional derivative  $\alpha$  and the coefficients  $E_r$  (see Fig. 7.8). We introduce the sensitivity index  $S_{\tau_d,\alpha}$  as the partial derivative



Figure 7.8: Nonlinear anomalous free vibration of a viscoelastic cantilever beam with no lumped mass at the tip and  $E_r = 0.1$ . The rate of amplitude decay strongly depends on the fractional order  $\alpha$ , where a rapid decay is observed as  $\alpha$  is increased (*left*). On the other hand, for increasing  $\alpha$ , the phase lag  $\varphi(\epsilon t)$ , increases in the lower range of  $\alpha$ , and decreases in the higher range of  $\alpha$ 

of decay rate with respect to  $\alpha$ , i.e.

$$S_{\tau_d,\alpha} = \frac{d\tau_d}{d\alpha} = \frac{\pi}{2} c_l E_r \,\omega_0^{\alpha-1} \,\cos(\alpha \frac{\pi}{2}) + c_l E_r \,\omega_0^{\alpha-1} \sin(\alpha \frac{\pi}{2}) \log(\omega_0). \tag{7.50}$$



Figure 7.9: Anomalous super-sensitivity of the decay rate  $\tau_d$  with respect to  $\alpha$  under free vibration. Increasing  $\alpha$  when  $\alpha < \alpha_{cr}$  leads to higher dissipation and decay rate. The reverse effect is observed when  $\alpha > \alpha_{cr}$ . Here, the notions of softening/hardening are associated to high/lower decay rates as  $\alpha$  is increased (introducing extra viscosity).

The sensitivity index is computed and plotted in Fig. 7.9 for the same set of parameters as in Fig. 7.8. There exists a critical value

$$\alpha_{cr} = -\frac{2}{\pi} \tan^{-1} \left( \frac{\pi}{2 \log(\omega_0)} \right), \tag{7.51}$$

where  $(dS_{\tau_d,\alpha}/d\alpha) = 0$ . We observe in Fig.7.9 that by increasing  $\alpha$  when  $\alpha < \alpha_{cr}$ , i.e. introducing more viscosity to the system, the dissipation rate, and thus decay rate, increases; this can be interpreted as a softening (stiffness-decreasing) region. Further increasing  $\alpha$  when  $\alpha > \alpha_{cr}$ , will reversely results in decrease of decay rate; this can be interpreted as a hardening (more stiffening) region. We also note that  $\alpha_{cr}$  solely depends on value of  $\omega_0$ , given in (7.42), and even though the value of  $E_r$  affects decay rate, it does not change the value of  $\alpha_{cr}$ . Therefore, the region of super-sensitivity, where the anomalous transition between softening/hardening regimes takes place only depends on the *standard* natural frequency of the system.

Although the observed hardening response after a critical value of  $\alpha$  in Fig.7.9 might seem counter-intuitive at first, we remark that here the notions of softening and hardening have a mixed nature regarding energy dissipation and time-scale dependent material stress response, which have anomalous nature for fractional viscoelasticity. Similar anomalous dynamics were also observed in ballistic, strain-driven yield stress responses of fractional visco-elasto-plastic truss structures [1, 292]. In the following, we demonstrate two numerical tests by purely utilizing the constitutive

response of the fractional Kelvin-Voigt model (7.19) to justify the observed behavior in Fig.7.9 by employing the *tangent loss* and the stress-strain response under monotone loads/relaxation.

**Dissipation** *via* **tangent loss**: By taking the Fourier transform of (7.19), we obtain the so-called complex modulus  $G^*$  [270], which is given by:

$$G^*(\omega) = E_{\infty} + E_{\alpha}\omega^{\alpha} \left( \cos\left(\alpha \frac{\pi}{2}\right) + i\sin\left(\alpha \frac{\pi}{2}\right) \right), \tag{7.52}$$

from which the real and imaginary parts yield, respectively, the storage and loss moduli, as follows:

$$G'(\omega) = E_{\infty} + E_{\alpha}\omega^{\alpha}\cos\left(\alpha\frac{\pi}{2}\right), \qquad G''(\omega) = E_{\alpha}\omega^{\alpha}\sin\left(\alpha\frac{\pi}{2}\right),$$

which represent, respectively, the stored and dissipated energies per cycle. Finally, we define the tangent loss, which represents the ratio between the dissipated/stored energies, and therefore related to the mechanical damping of the anomalous medium:

$$\tan \delta^{loss} = \frac{G''(\omega)}{G'(\omega)} = \frac{E_r \omega^\alpha \sin\left(\alpha \frac{\pi}{2}\right)}{1 + E_r \omega^\alpha \cos\left(\alpha \frac{\pi}{2}\right)}$$
(7.53)

We set  $\omega = \omega_0$  and  $E_r = 1$  and demonstrate the results for (7.53) with varying fractional orders  $\alpha$ . We present the obtained results in Fig.7.10 (*left*), where we observe that increasing fractional orders lead to increased dissipation per loading cycle with the increase of the tangent loss, and the hardening part ( $\alpha > \alpha_c$ ) is not associated with higher storage in the material. Instead, the increasing dissipation with  $\alpha$  suggests an increasing damping of the mechanical structure.

Stress-time response for monotone loads/relaxation: In this test, we demonstrate how increasing fractional orders for the fractional model leads to increased hardening for sufficiently high strain rates. Therefore, we directly discretize (7.19) utilizing an L1-scheme [176] in a uniform time-grid and set  $E_{\infty} = 1$ ,  $E_{\alpha} = 1$ . We also assume the following piecewise strain function:  $\varepsilon(t) = (1/24)t$ , for  $0 \le t < 2.5$  (monotone stress/strain), and  $\varepsilon(t) = 1/10$  for  $2.5 \le t \le 6$  (stress relaxation). The obtained results are illustrated in Fig.7.10 (*right*), where we observe that even for relatively low strain rates, there is a ballistic region nearby the initial time where higher fractional orders present higher values of stress, characterizing a rate-dependent stress-hardening response. However, due to

the dissipative nature of fractional rheological elements, the initially higher-stress material softens after passing a critical point, due to its faster relaxation nature.



Figure 7.10: (*Left*) Storage and loss moduli, and tangent loss for the fractional Kelvin-Voigt model at  $\omega_0$  with varying fractional-orders and  $E_r = 1$ . (*Right*) Stress-time response under a monotone load with constant strain rate undergoing ballistic hardening response for short-time and higher  $\alpha$ , followed by a stress relaxation.

• Primary Resonance Case,  $\Omega \approx \omega_0$ 

In the case of primary resonance, the excitation frequency is close to the natural frequency of the system. We let  $\Omega = \omega_0 + \epsilon \Delta$ , where  $\Delta$  is called the detuning parameter and thus, write the force function as  $\frac{1}{2}F e^{i\Delta T_1} e^{i\omega_0 T_0} + c.c$ . In this case, the force function also contributes to the secular terms. Therefore, we find the governing equations of solution amplitude and phase as

$$\frac{da}{dT_1} = -E_r \,\omega_0^{\alpha - 1} \sin(\alpha \frac{\pi}{2}) \left(\frac{1}{2} \,c_l \,a + \frac{3}{8} \,c_{nl} \,a^3\right) + \frac{1}{2} f \,\omega_0^{-1} \,\sin(\Delta T_1 - \varphi), \tag{7.54}$$

$$a \frac{d\varphi}{dT_1} = \frac{1}{2} c_l E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2}) \,a + \frac{3}{4} c_{nl} E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2}) \,a^3 + \frac{3}{4} \,\omega_0^{-1} \,k_{nl} \,a^3 \tag{7.55}$$
$$- \frac{1}{2} f \,\omega_0^{-1} \,\cos(\Delta T_1 - \varphi),$$

in which the four parameters  $\{\alpha, E_r, f, \Delta\}$  mainly change the frequency response of the system. The equations (7.54) and (7.55) can be transformed into an autonomous system, where the  $T_1$  does not appear explicitly, by letting

$$\gamma = \Delta T_1 - \varphi.$$

The steady state solution occur when  $\frac{da}{dT_1} = \frac{d\varphi}{dT_1} = 0$ , that gives

$$E_r \,\omega_0^{\alpha - 1} \sin(\frac{\pi \alpha}{2}) \left(\frac{c_l}{2}a + \frac{3c_{nl}}{8}a^3\right) = \frac{f}{2\,\omega_0} \sin(\gamma),\tag{7.56}$$

$$\left(\Delta - \frac{c_l}{2} E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2})\right) a - \frac{3}{4} \left(c_{nl} \,E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2}) + \omega_0^{-1} \,k_{nl}\right) a^3 = \frac{f}{2\,\omega_0} \cos(\gamma), \quad (7.57)$$

and thus, by squaring and adding these two equations, we get

$$\left[\frac{c_l}{2}E_r\,\omega_0^{\alpha-1}\sin(\frac{\pi\alpha}{2})\,a + \frac{3c_{nl}}{8}E_r\,\omega_0^{\alpha-1}\sin(\frac{\pi\alpha}{2})\,a^3\right]^2 + \left[\left(\Delta - \frac{c_l}{2}E_r\,\omega_0^{\alpha-1}\cos(\frac{\pi\alpha}{2})\right)a^3 - \frac{3}{4}\left(c_{nl}\,E_r\,\omega_0^{\alpha-1}\cos(\frac{\pi\alpha}{2}) + \omega_0^{-1}\,k_{nl}\right)a^3\right]^2 = \frac{f^2}{4\,\omega_0^2}.$$
(7.58)

This can be written in a simpler way as

$$\left[A_1 a + A_2 a^3\right]^2 + \left[B_1 a + B_2 a^3\right]^2 = C,$$
(7.59)

where

$$\begin{aligned} A_1 &= \frac{c_l}{2} E_r \,\omega_0^{\alpha - 1} \sin(\frac{\pi \alpha}{2}), \quad A_2 &= \frac{3c_{nl}}{8} E_r \,\omega_0^{\alpha - 1} \sin(\frac{\pi \alpha}{2}), \\ B_1 &= \Delta - \frac{c_l}{2} E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi \alpha}{2}), \quad B_2 &= -\frac{3}{4} \left( c_{nl} \, E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi \alpha}{2}) + \omega_0^{-1} \,k_{nl} \right), \quad C = \frac{f^2}{4 \,\omega_0^2}. \end{aligned}$$

Hence, the steady state response amplitude is the admissible root of

$$(A_2^2 + B_2^2)a^6 + (2A_1A_2 + 2B_1B_2)a^4 + (A_1^2 + B_1^2)a^2 - C = 0, (7.60)$$

which is a cubic equation in  $a^2$ . The discriminant of a cubic equation of the form  $ax^3+bx^2+cx+d = 0$ is given as  $\vartheta = 18abcd - 4b^3d + b^2c^2 - 4ac^3 - 27a^2d^2$ . The cubic equation (7.60) has one real root when  $\vartheta < 0$  and three distinct real roots when  $\vartheta > 0$ . The main four parameters { $\alpha, E_r, f, \Delta$ } dictate the value of coefficients { $A_1, A_2, B_1, B_2, C$ }, the value of discriminant  $\vartheta$ , and thus the number of admissible steady state amplitudes. We see that for fixed values of { $\alpha, E_r, f$ }, by sweeping the detuning parameter  $\Delta$  from lower to higher excitation frequency, the stable steady state amplitude bifurcates into two stable branches and one unstable branch, where they converge back to a stable amplitude by further increasing  $\Delta$ . Fig. 7.11 (left) shows the bifurcation diagram by sweeping the detuning parameter  $\Delta$  and for different values of  $\alpha$  when  $E_r = 0.3$  and f = 1. The solid and dashed black lines are the stable and unstable amplitudes, respectively. The blue lines connect the bifurcation points (red dots) for each value of  $\alpha$ . We see that the bifurcation points are strongly related to the value of  $\alpha$ , meaning that by introducing extra viscosity to the system, i.e. increasing the value of  $\alpha$ , the amplitudes bifurcate and then converge back faster. Figure 7.11 (right) shows the frequency response of the system, i.e. the magnitude of steady state amplitudes versus excitation frequency. As the excitation frequency is swept to the right, the steady state amplitude increases, reaches a peak value, and then jumps down (see e.g. red dashed line for  $\alpha = 0.4$ ). The peak amplitude and the jump magnitude decreases as  $\alpha$  is increased.



Figure 7.11: Primary resonance of the viscoelastic cantilever beam with no lumped mass at the tip. Steady state amplitude (*right*) and its bifurcation diagram (*left*) by changing the detuning parameter  $\Delta$  for different values of  $\alpha$  and  $E_r = 0.3$ , f = 1.

The coefficient  $E_r = \frac{E_{\infty}}{E_{\alpha}}$  is the proportional contribution of fractional and pure elastic element. At a certain value while increasing this parameter, we see that the bifurcation disappears and the frequency response of system slightly changes. Fig. 7.12 shows the frequency response of the system for different values of  $\{\alpha, E_r\}$  when f = 0.5. In each sub-figure, we let  $\alpha$  be fixed and then plot the frequency response for  $E_r = \{0.1, 0.2, \dots, 1\}$ ; the amplitude peak moves down as  $E_r$  is increased. For higher values of  $E_r$ , we see that as  $\alpha$  is increased, the amplitude peaks drift back to the left, showing a softening behavior in the system response.



Figure 7.12: Frequency-Response curve for the case of primary resonance in the viscoelastic cantilever beam with no lumped mass at the tip. Each sub-figure corresponds to a fixed value of  $\alpha$  and f when  $E_r = \{0.1, 0.2, \dots, 1\}$ . As effect of fractional element becomes more pronounced, i.e.  $\alpha$  and  $E_r$  increase, the corresponding amplitude peaks decrease and shift towards the lower frequency range.

## 7.4.1.2 Case 2: Lumped Mass At The Tip

In this case, M = J = 1, and thus, given the functions  $\phi_1(x)$  in Appendix D.4, the coefficients are computed as  $\mathcal{M} = 1 + 70.769J + 7.2734M$ ,  $\mathcal{J} = 5008.25$ ,  $\mathcal{K}_l = C_l = 98.1058$ ,  $\mathcal{M}_b = -0.648623 - 2.69692M$ , and  $\mathcal{K}_{nl} = C_{nl} = 2979.66$ . Similar to Case 1, we consider the following cases:

• Free Vibration, F = 0

Following the same steps as in Case 1, we see that the equation governing amplitude preserve its structure, but the governing equation of phase contains an extra term accommodating the  $m_{nl}$ .

$$\frac{da}{dT_1} = -E_r \,\omega_0^{\alpha - 1} \sin(\alpha \frac{\pi}{2}) \left( \frac{1}{2} c_l \,a + \frac{3}{8} c_{nl} \,a^3 \right), \tag{7.61}$$

$$\frac{d\varphi}{dT_1} = \frac{1}{2} c_l \,E_r \,\omega_0^{\alpha - 1} \,\cos\left(\frac{\pi \alpha}{2}\right) + \frac{3}{4} c_{nl} \,E_r \,\omega_0^{\alpha - 1} \,\cos\left(\frac{\pi \alpha}{2}\right) \,a^2 + \frac{3}{4} \,\omega_0^{-1} \,k_{nl} \,a^2 - \frac{1}{4} \,m_{nl} \,\omega_0 \,a^2. \tag{7.62}$$

This extra term does not significantly alter the behavior of phase and the whole system.

# • Primary Resonance Case, $\Omega \approx \omega_0$

Similar to the free vibration, we see that the equation governing amplitude preserves its structure while the governing equation of phase contains an extra term accommodating the  $m_{nl}$ 

$$\frac{da}{dT_1} = -E_r \,\omega_0^{\alpha - 1} \sin(\alpha \frac{\pi}{2}) \left(\frac{1}{2} \,c_l \,a + \frac{3}{8} \,c_{nl} \,a^3\right) + \frac{1}{2} f \,\omega_0^{-1} \,\sin(\Delta T_1 - \varphi), \tag{7.63}$$

$$a \frac{d\varphi}{dT_1} = \frac{1}{2} c_l E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2}) \,a + \frac{3}{4} c_{nl} E_r \,\omega_0^{\alpha - 1} \,\cos(\frac{\pi\alpha}{2}) \,a^3 + \frac{3}{4} \,\omega_0^{-1} \,k_{nl} \,a^3 - \frac{1}{2} f \,\omega_0^{-1} \,\cos(\Delta T_1 - \varphi) - \frac{1}{4} \,m_{nl} \,\omega_0 \,a^3.$$
(7.64)

Transforming the equations into an autonomous system by letting  $\gamma = \Delta T_1 - \varphi$ , we obtain the governing equation of steady state solution as

$$\left[\frac{c_l}{2}E_r\,\omega_0^{\alpha-1}\sin(\frac{\pi\alpha}{2})\,a + \frac{3c_{nl}}{8}E_r\,\omega_0^{\alpha-1}\sin(\frac{\pi\alpha}{2})\,a^3\right]^2 \left[\left(\Delta - \frac{c_l}{2}E_r\,\omega_0^{\alpha-1}\cos(\frac{\pi\alpha}{2})\right)a - \frac{3}{4}\left(c_{nl}\,E_r\,\omega_0^{\alpha-1}\cos(\frac{\pi\alpha}{2}) + \omega_0^{-1}\,k_{nl} + \frac{1}{3}\,m_{nl}\,\omega_0\right)a^3\right]^2 = \frac{f^2}{4\,\omega_0^2},\tag{7.65}$$

which, similar to Case 1, can be written as

$$(A_2^2 + B_2^2)a^6 + (2A_1A_2 + 2B_1B_2)a^4 + (A_1^2 + B_1^2)a^2 - C = 0,$$

where all the  $A_1$ ,  $A_2$ ,  $B_1$ , and C are the same as in Case 1, but

$$B_2 = -\frac{3}{4} \left( c_{nl} E_r \, \omega_0^{\alpha - 1} \, \cos(\frac{\pi \alpha}{2}) + \omega_0^{-1} \, k_{nl} + \frac{1}{3} \, m_{nl} \, \omega_0 \right).$$

The corresponding cubic equation can be solved to obtain the bifurcation diagram and also the frequency response of the system. However, in addition to Case 1, we have an extra parameter  $m_{nl}$  which affects the response of the system.

#### **CHAPTER 8**

# A SELF-SINGULARITY-CAPTURING APPROACH FOR FRACTIONAL DIFFERENTIAL EQUATIONS

# 8.1 Background

Fractional differential equations (FDEs) have been successfully applied in diverse problems that present the fingerprint of power-laws/heavy-tailed statistics, such as visco-elastic modeling of bio-tissues [8, 10, 43, 187, 293], cell rheology behavior [12], food preservatives [24], complex fluids [128], visco-elasto-plastic modeling for power-law-dependent stresses/strains [1, 223, 294], earth sciences [295], anomalous diffusion in Sephadex<sup>™</sup>gels [296], among others.

The increasing number of works involving fractional modeling in the past two decades is largely due to the development of efficient numerical schemes for fractional-order/partial differential equations (FDEs/FPDEs). Starting with Lubich's early works [86, 88] on finite-difference schemes, and followed by several developments, e.g., on discretizing Burger's equation [196], fractional Adams methods for nonlinear problems [94, 108, 112, 113], and fractional diffusion processes [30, 91, 197, 199]. Also, other classes of global methods were developed, such as spectral methods for FDEs/FPDEs [95–101, 297–299], distributed-order differential equations (DODEs) [260, 261, 266], and also mesh-free schemes, such as the improved singular boundary method (SBM) developed by Chen and Gu [300]. Of particular interest, we highlight a family of fast convolution schemes for time-fractional integrals/derivatives, initially developed by Lubich [103]. In such schemes, instead of a direct discretization by splitting the fractional operator in N uniform time-integration intervals, it is split in exponentially increasing intervals, reducing the overall computational complexity from  $O(N^2)$  to  $\approx O(N \log N)$ . Furthermore, the power-law kernels are computed through a convolution quadrature using complex integration contours [103–105, 301, 302]. The storage requirements are also reduced from O(N) to  $\approx O(\log N)$ . Recently, Zeng *.et.al* [5] developed an improved version of the scheme using a Gauss-Laguerre convolution quadrature, which utilizes real-valued integration

contours. In the same work, the authors also addressed the short memory principle and applied Lubich's correction terms [86], leading to a more accurate and stable fast time-stepping scheme. We also refer readers to other classes of fast schemes for time-fractional operators that make use of the resulting matrix structures [303], kernel compression [304], and divide-and-conquer fast finite-difference schemes [305].

There have also been works on 'tunable accuracy', spectral collocation methods for FDEs/FPDEs that utilize singular basis functions [96, 102, 306]. Zayernouri and Karniadakis [96] developed an exponentially accurate spectral collocation method utilizing fractional Lagrange basis functions, given by the product of a singular term with real power  $\mu$  and a smooth part given by Lagrange interpolands. Zeng *.et.al* [306] later generalized the scheme for variable-order FDEs/FPDEs with endpoint singularities and demonstrated that a proper tuning of the power  $\mu$  enhanced the accuracy of the numerical solutions. Lischke *.et.al* [102] developed a Laguerre Petrov-Galerkin method for multi-term FDEs with tunable accuracy and linear computational complexity. Despite the high precision obtained by fine-tuning the bases in the developed works, such numerical accuracy is extremely sensitive to the 'single'-singularity basis parameter  $\mu$  and no self-capturing scheme was developed to find its correct, application-specific value.

In order to deal with weak singularities nearby the initial time, Brunner and Tang [81] developed graded mesh approaches with spline collocation methods to a first-order Volterra integro-differential equation arising in fluid dynamics. Later on, graded meshes were incorporated in usual finite-difference discretizations for FDEs [82–85]. In such schemes, a nonuniform time-grid with  $t_n = (n\Delta t)^r$  is utilized instead the uniform counterpart, where *r* denotes a grading parameter which optimal value is crucial to obtain the theoretical accuracy and convergence rates of the corresponding original schemes. Recently, stability issues of graded meshes were addressed by Stynes *.et.al* [85] in a reaction-diffusion problem, where they obtained an optimal grading parameter of  $r = (2-\alpha)/\alpha$ . Zeng *.et.al* [5] compared the performance of the optimally graded meshes developed by Stynes *.et.al* [85] against their developed fast time-stepping scheme with Lubich's correction scheme [86]. They demonstrated that, for a nonsmooth solution, Lubich's correction scheme using M = 3 terms

yielded competitive results with similar convergence rates and smaller errors than the optimally graded mesh approach. Zeng *.et.al* [5] further observed that when  $\alpha$  is close to zero, utilizing Lubich's correction scheme is even more efficient than the graded mesh approach with optimal r in [85].

The accuracy and efficiency of the aforementioned numerical schemes strongly depend on the regularity of the solution. To address such problem, a correction method was introduced by Lubich [86], which utilizes M correction terms with singular powers  $\sigma_k$ , with k = 1, ..., M, given regularity assumptions for u(t). The corresponding correction weights are obtained through the solution of a Vandermonde-type linear system of size M. Given a convenient choice of singular powers, some developed schemes were able to attain their theoretical accuracy with non-smooth solutions [5, 87], where the evaluation of correction weights can have the same computational complexity of the original methods, e.g., by employing Fast Fourier Transforms. However, such works utilize *ad-hoc* choices of  $\sigma_k$ , even without prior knowledge of the regularity of the solution. According to Zeng .et.al [5], for such cases, a reasonable choice would be  $\sigma_k = 0.1k$ , which could improve the numerical accuracy when strong singularities are present, and without loss of accuracy when there is enough regularity for u(t). However, such procedure could still lead to arbitrary choices of  $\sigma_k$  far from the true singularities of the solution. There are higher chances of approximating the singularities by increasing the number of correction terms, but using M > 9 terms induces a large condition number on the Vandermonde system (see Figure 8.2a), and consequently large residuals, leading to large errors when computing the correction weights, which are propagated to the discretized fractional operator [307].

Regarding the numerical solution of FDEs with correction terms, let N be the total number of time-steps with size  $\Delta t$ . For the first M time-steps, prior information of the numerical solution for u(t), see (8.19), is required. The procedure proposed in [5] involves the solution of a sub-problem with time domain  $t \in (0, M\Delta t]$  using a time-step size  $\tau = \Delta t^2$  and one correction term to obtain the numerical solution  $u_n^N$  for n = 1, ..., M. However, the choice of smaller step size  $\tau$  even for a short time might be too expensive, and the numerical solution for the M initial time-steps

might experience total loss of accuracy in the presence of strong singularities, not captured by the single guessed correction term. Such deficiencies outline the need for I) Capturing the multisingularities of u(t) and II) Efficient and accurate schemes that incorporate all captured singularities for time-integration of the (most crucial) initial M time-steps.

The main contribution of the present work is to develop a two-stage data-infused computational framework for accurate time-integration of FDEs. In Stage-I, we formulate a self-singularity-capturing framework where:

- The scheme utilizes available data for initial diminutive time (application-oriented), and selfcaptures/determines multi-singular solution behaviors through the knowledge introduced by the FDE and its corresponding fractional operators. *No knowledge of the analytical solution is required a-priori*, and some of the numerical tests throughout this work sample from analytical solution points only for verification purposes.
- We develop a new (finite-difference based) algorithm for automatic determination of the underlying power-law singularities nearby the initial data, employing gradient descent op-timization. Despite the several aforementioned schemes to address the singularities of the FDE solutions, our choice here is to introduce such singularities through Lubich's correction method [86].
- We introduce the capturing scheme for M correction terms and construct a hierarchical, self-capturing framework. We test the framework for the particular case of up to S = 3 singularities and M = 3 correction terms.
- The self-capturing procedure makes use of two stopping criteria for the error minimization, namely ε (for solution error) and ε<sub>1</sub> (for gradient norm error), where the numerical convergence with respect to ε defines if the singularities are captured. Numerical convergence towards the tolerance ε<sub>1</sub> defines if additional correction terms are needed to capture the true solution singularities.

In Stage-II we utilize the captured multi-singularities for the full time-integration of the FDE in question, where a variety of the aforementioned numerical methods could be, in general, employed. At this stage, no knowledge of the solution data is required, but only the usual forcing terms. Our approach is explained as the following:

- To handle the numerical solution of the FDE using multiple correction terms, we develop an implicit finite-difference method, where we solve a linear system of size *M* for the first *M* time-steps. Therefore, we incorporate the captured singular behavior up to the desired precision *ε*, without the need of using a fine time-grid;
- We numerically show that the developed methodology has order  $O(\Delta t^{3-\alpha})$ .

We perform a set of numerical tests, where we demonstrate that the developed scheme is able to capture multiple singularities using a few number of time-steps, which can later be utilized for efficient time-integration of FDEs with relatively large time-step size  $\Delta t$ , being much more accurate than *ad-hoc* choices of singularities when the regularity of the solution is unknown. The successful capturing of singularities motivates the development of kernel- and knowledge-based refinement of time-grids nearby the initial time [85], especially with values of  $\alpha$  close to zero, as well as self-construction of basis function spaces using Müntz polynomials [308, 309] for spectral element methods for FDEs/FPDEs [101].

This paper is organized as follows: Section 8.2 introduces the definitions for fractional operators and the FDE in consideration. In section 8.3 we develop the two-stage framework for efficient time-integration of FDEs, where we start with the self-singularity-capturing scheme (Stage-I) in Section 8.3.1, followed by the finite-difference scheme for solution of FDEs (Stage-II) in Section 8.3.2 using the captured singularities. The numerical results with discussions for self-capturing up to three singularities are shown in Section 8.4.

# 8.2 **Definitions**

We start with some preliminary definitions of fractional calculus [31]. The left-sided Riemann-Liouville (RL) integrals of order  $\alpha \in \mathbb{R}$ , with  $0 < \alpha < 1$  and  $t \in \mathbb{R}$ , is defined, as

$$\binom{RL}{a}\mathcal{I}_{t}^{\alpha}v(t) = \frac{1}{\Gamma(\alpha)}\int_{a}^{t}\frac{v(s)}{(t-s)^{1-\alpha}}\,ds, \quad t > a,$$
(8.1)

where  $\Gamma$  represents the Euler gamma function and *a* denotes the lower integration limit. The corresponding inverse operator, i.e., the left-sided RL fractional derivatives of order  $\alpha$ , is then defined based on (8.1) as

$$\binom{RL}{a}\mathcal{D}_t^{\alpha}v(t) = \frac{d}{dt}\binom{RL}{a}\mathcal{I}_t^{1-\alpha}v(t) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_a^t \frac{v(s)}{(t-s)^{\alpha}}\,ds, \quad t > a.$$
(8.2)

Furthermore, the corresponding left-sided Caputo derivatives of order  $\mu \in (0, 1)$  is obtained as

$$\binom{C}{a}\mathcal{D}_t^{\alpha}v(t) = \binom{RL}{a}\mathcal{I}_t^{1-\alpha}\frac{dv}{dx}(x) = \frac{1}{\Gamma(1-\alpha)}\int_a^t \frac{v'(s)}{(t-s)^{\alpha}}\,ds, \quad t > a.$$
(8.3)

The definitions of Riemann-Liouville and Caputo derivatives are linked by the following relationship, which can be derived by a direct calculation

$$\binom{RL}{a}\mathcal{D}_t^{\alpha}v(t) = \frac{v(a)}{\Gamma(1-\alpha)(t-a)^{\alpha}} + \binom{C}{a}\mathcal{D}_t^{\alpha}v(t),$$
(8.4)

which denotes that the definition of the aforementioned derivatives coincide when dealing with homogeneous Dirichlet initial/boundary conditions.

We now introduce the Cauchy problem to be solved in this work and its corresponding wellposedness (see Theorem 3.25(i) [310] with n = 1). Let  $C(\Omega)$  be the space of continuous functions u(t) in  $\Omega = [a, b]$  with the norm:

$$||u||_{C(\Omega)} = \max_{t \in \Omega} |u(t)|$$

Also, let  $0 < \alpha < 1$  and  $\gamma \in \mathbb{R}^+$ , with  $\gamma \leq \alpha$ . We define  $C_{\gamma}(\Omega)$  to be the following weighted space of continuous functions:

$$C_{\gamma}(\Omega) = \{g(t) | (t-a)^{\gamma} g(t) \in C(\Omega), ||g||_{C_{\gamma}} = ||(t-a)^{\gamma} g(t)||_{C} \},\$$
Let *G* be an open set in  $\mathbb{R}$ , and let a function  $f(t, u(t)) : (a, b] \times G \to \mathbb{R}$ , such that  $f(t, u(t)) \in C_{\gamma}(\Omega)$ and is Lipschitz continuous with respect to any  $u(t) \in G$ . Let the fractional Cauchy problem of interest given by:

$${}^{C}_{a}\mathcal{D}^{\alpha}_{t}u(t) = f(t, u(t)), \quad u(a) = u_{0}.$$
 (8.5)

Given the aforementioned conditions, there exists a unique solution for (8.5) in the following space of functions:

$$\mathbf{C}^{\alpha}_{\gamma}(\Omega) = \{ u(t) \in C(\Omega) | \ ^{C}_{a} \mathcal{D}^{\alpha}_{t} u(t) \in C_{\gamma}(\Omega) \}.$$

The corresponding solution with respect to u(t) equivalent to the following Volterra integral equation of second kind:  $u(t) = u_0 + \frac{1}{\Gamma(\alpha)} \int_a^t \frac{f(s,u(s))}{(t-s)^{1-\alpha}} ds$ , with  $a \le t \le b$ . We remark that for other particular forms of (8.5), the corresponding Volterra equation of second kind contains Mittag-Leffler functions  $E_{\alpha}(z)$ , which are defined through infinite sums and thus are not computationally-friendly. Therefore, we choose to work with the presented form, since the developed self-singularity-capturing framework can be extended for other FDEs in a straightforward way, without resorting to computationally expensive hyper-geometric functions. Furthermore, although the existence and uniqueness of Cauchy problems has been investigated [108, 310–312], yet, there is no comprehensive framework to understand the singular behavior of the solution given any general  $f(t, u(t)) \in C_{\gamma}(\Omega)$ . The developed formulation in this work is suitable for problems where a few initial discrete data points are known from u(t) and f(t, u(t)).

Due to the employed finite-difference discretization over the RL derivative in this work (see Section 8.3.1.2), we choose to rewrite (8.5) using (8.4) to obtain:

$${}^{RL}_{a}\mathcal{D}^{\alpha}_{t}u(t) = f(t,u(t)) - \frac{u_{0}}{\Gamma(1-\alpha)(t-a)^{\alpha}}.$$
(8.6)

As will be shown in the next sections, the developed scheme is able to capture singularities with a minimal number of time-steps, *i.e.* with restricted data for a short period of time.

# 8.3 Two-Stage Time-Integration Framework

In this section, we develop the two-stage framework for efficient time-integration of FDEs. We start with Stage-I, where the singularity-self-capturing scheme is presented for *S* singularities,



Figure 8.1: In Stage-I, the scheme captures the singularities for the short time-domain  $\tilde{\Omega}$ , given the short initial data. In Stage-II, the framework uses the singularities obtained in Stage-I for full time-integration of the FDE over  $\Omega$ .

computed over a small number of initial data points denoted by  $\tilde{N}$ . Then, after the multi-singular solution behavior is learned, we present the developed solution for FDEs in Stage-II, where the subsequent full time-integration of the FDE is carried out over N time steps (see Figure 8.1).

## 8.3.1 Stage-I: Self-singularity-capturing stage

We develop the self-singularity-capturing framework, starting with M correction terms for the initial time-steps  $\tilde{N}$ , at which data is available. We then utilize the developed algorithm in a self-capturing approach, through a hierarchical and iterative fashion.

## 8.3.1.1 Minimization method

Let  $t \in \tilde{\Omega}$ , with  $\tilde{\Omega} = [t_0, t_{\tilde{N}}]$ , where  $\tilde{N}$  denotes the number of initial short data points, such that  $\tilde{N} \ge M$ , and let  $\sigma \in \mathbb{R}^M$  be the following correction-power (singularity) vector:

$$\boldsymbol{\sigma} = [\sigma_1, \ \sigma_2, \ \dots, \ \sigma_M]^T$$

We define an error function  $E : \mathbb{R}^M \to \mathbb{R}^+$ , given by:

$$E(\boldsymbol{\sigma}) = \sum_{n=1}^{\tilde{N}} \left( u_n^{data} - u_n^N(\boldsymbol{\sigma}) \right)^2,$$
(8.7)

where  $u_n^N(\sigma)$  denotes the  $\sigma$ -dependent numerical solution of u(t) at  $t = t_n$ , and  $u_n^{data}$  represents the known initial shot-time data. Figure 8.1 illustrates the integration domain  $\tilde{\Omega}$  for Stage-I, where the error function (8.7) is evaluated for a short time. We apply an iterative gradient descent scheme in order to find  $\sigma^*$  that minimizes (8.7). Let  $\sigma^k$  be known at the *k*-th iteration. We compute the updated value  $\sigma^{k+1}$  for iteration k + 1 in the following fashion [313]:

$$\boldsymbol{\sigma}^{k+1} = \boldsymbol{\sigma}^k - \boldsymbol{\gamma}^k \nabla E(\boldsymbol{\sigma}^k),$$

where  $\gamma^k$  denotes the following two-point step size for the *k*-th iteration, given by [314]:

$$\gamma^{k} = \frac{\left(\sigma^{k} - \sigma^{k-1}\right)^{T} \left[\nabla E(\sigma^{k}) - \nabla E(\sigma^{k-1})\right]}{\left|\left|\nabla E(\sigma^{k}) - \nabla E(\sigma^{k-1})\right|\right|_{L^{2}(\mathbb{R}^{M})}^{2}}.$$
(8.8)

The gradient  $\nabla E : \mathbb{R}^+ \to \mathbb{R}^M$  of the error function is given by  $\nabla E(\sigma) = [\partial E/\partial \sigma_1, \ \partial E/\partial \sigma_2, \ \dots, \ \partial E/\partial \sigma_M]^T$ , where, instead of obtaining a closed form for the derivatives (which would implicitly involve the differentiation of  $u_i^N$ ), we utilize complex-step differentiation. Therefore, let  $\mathbf{e}_j = [0, 0, \dots, 1, \dots, 0]^T$ be a vector in  $\mathbb{R}^M$  of zeros, with a unit value in the *j*-th entry. Therefore, we have the following:

$$\nabla E(\boldsymbol{\sigma})_j \approx \frac{Im(E(\boldsymbol{\sigma}+i\Delta\sigma\mathbf{e}_j))}{\Delta\sigma}, \quad j=1,\,2,\,\ldots,\,M, \quad i=\sqrt{(-1)},\tag{8.9}$$

which only requires the additional evaluation of the error function perturbed by  $\Delta \sigma$ , which can be taken, *e.g.*, as  $10^{-14}$ . Given two numerical tolerances  $\epsilon$  and  $\epsilon_1$ , we iterate and find a new  $\sigma^{k+1}$  while both criteria  $E(\sigma^{k+1}) > \epsilon$  and  $||\nabla E(\sigma^k)|| > \epsilon_1$  are true. The latter criterion is introduced to minimize our error function, while the former is used for error control in our self-capturing scheme. As will be shown in the next sections, the criterion  $||\nabla E(\sigma^k)|| < \epsilon_1$  is satisfied for small  $\epsilon_1$  even when M < S, but the criterion  $E(\sigma^{k+1}) < \epsilon$  will only be satisfied when we use enough correction terms (see Section 8.3.1.3) to fully capture the *S* number of power-law singularities.

### 8.3.1.2 Numerical scheme for short-time integration

In the singularity-capturing scheme, given  $\sigma$ , in order to compute the error in (8.7) and the gradient (due to the error perturbation) (8.9), we need to compute the numerical solution  $u_n^N$  for  $n = 1, ..., \tilde{N}$  initial data points over time-intervals  $\Delta t$ . For this purpose, we employ the finite-difference discretization with corrections presented in [86] for the fractional RL derivative. Including correction terms, the discretization of the left-sided RL fractional derivative of order  $\alpha$ ,

evaluated at time  $t = t_n$ , with initial time a = 0, has the following form:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}u(t)|_{t=t_{n}}\approx {}^{RL}_{0}\mathcal{D}^{(\alpha,M)}_{t}u^{N}(t)|_{t=t_{n}}.$$

The above approximation is augmented by the *so-called* Lubich's correction terms, which is given by:

$${}^{RL}_{0}\mathcal{D}^{(\alpha,M)}_{t}u^{N}(t)|_{t=t_{n}} = {}^{RL}_{0}\mathcal{D}^{\alpha}_{t}u^{N}(t)|_{t=t_{n}} + \sum_{j=1}^{M}W_{j,n}(\sigma)\left(u_{j}^{N}-u_{0}\right),$$
(8.10)

with  $n = 1, ..., \tilde{N}$ . The term  $W_{j,n}(\sigma)$  denotes the correction weights, which depend on the correction powers  $\sigma \in \mathbb{R}^M$ . We assume a power-law solution singularity about t = 0, driven by the power-law kernel of the RL fractional derivative, *i.e.*,  $u|_{nearby} \approx \sum_{k=1}^M c_k t^{\sigma_k}$ . If  $\sigma = \{\sigma_k\}_{k=1}^M$  are known, the RL fractional derivative of each singular term,  $t^{\sigma_k}$ , can be obtained by:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}(t^{\sigma_{k}})|_{t=t_{n}} + \sum_{j=1}^{M} W_{j,n}t_{j}^{\sigma_{k}} = \frac{\Gamma(1+\sigma_{k})}{\Gamma(1+\sigma_{k}-\alpha)}t_{n}^{\sigma_{k}-\alpha}, \quad k=1,\ldots,M,$$
(8.11)

where the first term on the left-hand side of (8.11) denotes the discretized RL fractional derivative of  $t^{\sigma_k}$ , while the right-hand side represents the exact fractional derivative of  $t^{\sigma_k}$ , evaluated at  $t = t_n$ . Equation (8.11) can be written as:

$$\sum_{j=1}^{M} V_{k,j} W_{j,n} = \frac{\Gamma(1+\sigma_k)}{\Gamma(1+\sigma_k-\alpha)\Delta t^{\alpha}} n^{\sigma_k-\alpha} - \frac{1}{\Delta t^{\sigma_k}} \frac{RL}{0} \mathcal{D}_t^{\alpha}(t^{\sigma_k})|_{t=t_n},$$
(8.12)

with k = 1, ..., M, where  $V_{k,j} = j^{\sigma_k}$  denotes a Vandermonde matrix with size  $M \times M$ . Therefore, to obtain the starting weights  $W_{j,n}$ , the above linear system has to be solved for all  $n = 1, ..., \tilde{N}$ .

Substituting (8.10) into (8.6), we obtain the following discrete form for the FDE:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}u^{N}(t)|_{t=t_{n}} + \sum_{j=1}^{M} W_{j,n}(\sigma)\left(u_{j}^{N} - u_{0}\right) - \frac{u_{0}}{\Gamma(1-\alpha)t_{n}^{\alpha}} = f_{n}^{data},$$
(8.13)

with  $n = 1, \ldots, \tilde{N}$ .

In order to discretize  ${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}u^{N}(t)$ , we follow the difference scheme developed in [5], which is based on a second-order interpolation of u(t) for the fractional RL integral (8.1), similar to the L1-2 scheme for fractional Caputo derivatives developed in [30]. Therefore, when evaluating (8.1) at  $t = t_n$ , we split it into local  $\mathcal{L}$  and history  $\mathcal{H}$  parts as follows:

$${}^{RL}_{0}\mathcal{I}^{\alpha}_{t}u^{N}(t)|_{t=t_{n}} = \underbrace{\int_{t_{n-1}}^{t_{n}} k(t_{n}-s)u^{N}(s)\,ds}_{\mathcal{L}(u,t_{n})} + \underbrace{\sum_{k=0}^{n-2} \int_{t_{k}}^{t_{k+1}} k(t_{n}-s)u^{N}(s)\,ds}_{\mathcal{H}(u,t_{n})}, \tag{8.14}$$

with the kernel  $k(t) = t^{\alpha-1}/\Gamma(\alpha)$ . The function  $u^N(t)$  is approximated in an implicit fashion using Lagrange interpolands  $l_j^{(p)}(t)$  of order *p*:

$$u^{N}(t_{n}) \approx I^{(p)}u_{n}^{N} = \sum_{j=0}^{p} l_{j}^{(p)}(t)u_{n+j-p}^{N}, \quad \text{with} \quad l_{j}^{(p)}(t) = \prod_{\substack{i=0\\i\neq j}}^{p} \frac{t-t_{i}}{t_{j}-t_{i}}$$
(8.15)

Substituting (8.15) into (8.14), and evaluating the convolution integrals, we obtain the following approximations for the local and history parts, respectively, as

$$\mathcal{L}^{(n,\alpha)}u^{N} = \sum_{j=0}^{p} d_{j}^{(p)} u_{n+j-p}^{N}, \qquad (8.16)$$

$$\mathcal{H}^{(n,\alpha)}u^{N} = \sum_{j=0}^{n-p} \left( b_{n-1-j}^{(1)}u_{j}^{N} + b_{n-1-j}^{(2)}u_{j+1}^{N} + b_{n-1-j}^{(3)}u_{j+2}^{N} \right), \tag{8.17}$$

where the corresponding  $\alpha$ - and  $\Delta t$ - dependent coefficients  $d_j^{(p)}$  and  $b_j^{(1)}$ ,  $b_j^{(2)}$ ,  $b_j^{(3)}$  are presented in E.1. In our computations, we make use of p = 1 (piece-wise linear approximation) for the local part  $\mathcal{L}^{(1,\alpha)}u$ , when n = 1 (first time-step), and p = 2 for n > 1 (subsequent time-steps). The fractional RL derivative can be obtained from the above discretization by setting  $-1 < \alpha < 0$ . Therefore:

$${}^{RL}_{0}\mathcal{D}^{\alpha}u^{N}(t)|_{t=t_{n}} \approx \mathcal{L}^{(n,-\alpha)}u^{N} + \mathcal{H}^{(n,-\alpha)}u^{N}.$$
(8.18)

Finally, substituting (8.18) into (8.13), and recalling (8.16), we obtain the discretized form for our FDE:

$$\sum_{j=0}^{p} d_{j}^{(p)} u_{n+j-p}^{N} + \mathcal{H}^{(n,-\alpha)} u^{N} + \sum_{j=1}^{M} W_{j,n}(\sigma) \left( u_{j}^{N} - u_{0} \right) - \frac{u_{0}}{\Gamma(1-\alpha)t_{n}^{\alpha}} = f_{n}^{data},$$
(8.19)

with  $n = 1, \ldots, \tilde{N}$ .

**Remark 8.3.1.** Among a variety of available schemes, adopted the discretization of fractional operators introduced in [5] using Lubich's correction terms. However, in [5], the authors did not

perform a fully implicit computation of the second term on the left-hand-side of (8.13) when M > 1. Instead, they obtained the solutions for n = 1, ..., M using a fine, uniform time-grid with time-step size  $\tau = \Delta t^2$  and M = 1 correction term. We observe that using such a fine initial time-grid might be computationally expensive and ineffective when strong singularities are present (e.g.  $u(t) = t^{\sigma^*}$ , with  $0 < \sigma^* < 1 - \alpha$ ). In our developed scheme, we treat such term in a fully implicit fashion, where we solve a small linear system with M unknowns to obtain  $u_n^N$  for n = 1, ..., M. This ensures a proper inclusion of all M singularities in all time-steps near t = 0.

We present here the developed finite-difference scheme to solve the discretized FDE (8.19) for the particular case of M = 3. Here, we solve a small linear system for the fully-implicit computation at the first 3 time-steps, that is,  $t = \{\Delta t, 2\Delta t, 3\Delta t\}$ , which is obtained by expanding (8.19) for each of the time-steps, where we use p = 1 for the first one, with  $\mathcal{H}^{(1,-\alpha)}u^N = 0$ , and p = 2 for the subsequent ones. The expansions are presented as follows:

**First time-step**  $t = \Delta t$ :

$$\underbrace{\left(d_{1}^{(1)}+W_{1,1}\right)}_{A_{11}}u_{1}^{N}+\underbrace{\left(W_{2,1}\right)}_{A_{12}}u_{2}^{N}+\underbrace{\left(W_{3,1}\right)}_{A_{13}}u_{3}^{N}=f_{1}^{data}-r_{1}u_{0},$$
(8.20)

with,

$$r_1 = d_0^{(1)} - \left( W_{1,1} + W_{2,1} + W_{3,1} + \frac{\Delta t^{-\alpha}}{\Gamma(1-\alpha)} \right).$$

**Second time-step**  $t = 2\Delta t$ :

$$\underbrace{\left(d_{1}^{(2)}+b_{0}^{(2)}+W_{1,2}\right)u_{1}^{N}+\left(d_{2}^{(2)}+b_{0}^{(3)}+W_{2,2}\right)u_{2}^{N}+\underbrace{\left(W_{3,2}\right)u_{3}^{N}}_{A_{23}}}_{A_{23}}$$
$$=f_{2}^{data}-r_{2}u_{0},$$
(8.21)

with,

$$r_2 = d_0^{(2)} + b_0^{(1)} - \left( W_{1,2} + W_{2,2} + W_{3,2} + \frac{(2\Delta t)^{-\alpha}}{\Gamma(1-\alpha)} \right).$$

**Third time-step**  $t = 3\Delta t$ :

$$\underbrace{\left(d_{0}^{(2)}+b_{0}^{(1)}+b_{1}^{(2)}+W_{1,3}\right)}_{A_{31}}u_{1}^{N}+\underbrace{\left(d_{1}^{(2)}+b_{0}^{(2)}+b_{1}^{(3)}+W_{2,3}\right)}_{A_{32}}u_{2}^{N}$$

$$+\underbrace{\left(d_{2}^{(2)}+b_{0}^{(3)}+W_{3,3}\right)}_{A_{33}}u_{3}^{N}=f_{3}^{data}-r_{3}u_{0},$$
(8.22)

with,

$$r_3 = b_1^{(1)} - \left( W_{1,3} + W_{2,3} + W_{3,3} + \frac{(3\Delta t)^{-\alpha}}{\Gamma(1-\alpha)} \right).$$
(8.23)

Therefore, from (8.20)-(8.23), we solve the following linear system for  $n \leq 3$ :

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} u_1^N \\ u_2^N \\ u_3^N \end{bmatrix} = \begin{bmatrix} f_1^{data} \\ f_2^{data} \\ f_3^{data} \end{bmatrix} - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} u_0, \quad \text{if } n \le 3.$$
(8.24)

**Remark 8.3.2.** To obtain the solutions for M = 2, we only need to remove the third row/column of the coefficient matrix **A**, and set  $W_{1,3} = W_{3,1} = W_{2,3} = W_{3,2} = 0$  in (8.20)-(8.23). Also, we observe that the correction terms lead to a full matrix of coefficients, which is reduced to a lower-triangular form for the uncorrected case.

For the remaining time-steps (n > 3),  $u_1^N$ ,  $u_2^N$ ,  $u_3^N$  are known and we solve for  $u_n^N$  in the usual (but still implicit) time-stepping fashion, as follows:

$$u_n^N = \left( f_n^{data} - \sum_{j=0}^{1} d_j^{(2)} u_{n-2+j}^N - \mathcal{H}^{(n,-\alpha)} u^N - \sum_{j=1}^{M} W_{j,n} (u_j^N - u_0) + \frac{u_0 t_n^{-\alpha}}{\Gamma(1-\alpha)} \right) / d_2^{(2)}, \text{ if } 3 < n \le \tilde{N}.$$
(8.25)

**Remark 8.3.3.** The current formulation can be extended for a larger number of correction terms; however, using M > 9 will incur in an ill-conditioned system for (8.11). This fact was first analyzed by Diethelm .et.al [307] and later numerically shown by Zeng .et.al [87], which would incur in significant errors when computing the weights  $W_{n,j}$  and consequently propagate the errors to the operator discretization. In that sense, we choose M = 3 to capture the most critical singularities while keeping a small condition number and small residual for the linear system (8.11).

## 8.3.1.3 Stage-I algorithm

The Stage-I framework is described in Algorithm 8.1, which learns about the singularities of the solution using small  $\tilde{N}$ . The *M* captured singularities  $\sigma$  are utilized to initialize an FDE solver in Stage-II (see Section 8.3.2).

Algorithm 8.2 summarizes the main steps for the numerical scheme to capture the singularities of  $u^{data}$ ,  $f^{data}$  for diminutive times at fixed *M*.

## 8.3.1.4 Computational complexity of stage-I

We recall that in the presented scheme, the error function (8.7) is evaluated  $N_{it}$  times, which is the number of iterations until convergence of the minimization scheme. The complexity of this error function is dominated by the time-integration of the numerical solution  $u^N$  over  $\tilde{N}$  time-steps. For the first M time-steps, we use (8.24) and solve the corresponding linear system, which costs  $O(M^3)$ . For the remaining  $\tilde{N} - M$  time-steps we use (8.25), where the dominant cost is due to the direct numerical evaluation of the fractional derivatives, that is,  $O((\tilde{N} - M)^2)$ . Therefore, the computational complexity of the entire scheme is  $O((M^3 + (\tilde{N} - M)^2)N_{it})$ . However, here we use  $M \leq 3$ , and therefore the asymptotic complexity becomes  $O(\tilde{N}^2N_{it})$ . Furthermore,  $\tilde{N}$  is assumed to be small due to the short-time data, and we show in Section 8.4 that we are able to capture singularities with  $\tilde{N} = O(M)$ , which makes the presented scheme numerically efficient, as long as a large number of iterations for convergence is not required.

**Remark 8.3.4.** We observe that since  $\tilde{N}$  is small, there is no need to use fast time-stepping schemes in Stage-I, since the break-even point between fast and direct schemes usually lies in a range of moderate number of time-steps (e.g. about  $O(10^4)$  for the fast scheme in [5]). Therefore, for

Algorithm 8.1: Stage-I Self-Singularity-Capturing Scheme for FDEs.

1: Known data about  $u^{data}$ ,  $f^{data}$  for  $\tilde{N}$  time-steps of size  $\Delta t$ . 2: Set M = 1, initial guess  $\sigma^{(0)} = 0$  and numerical tolerances  $\epsilon, \epsilon_1$ . 3: while  $M \leq 3$  do Estimate  $\sigma_i^{(k)}$ , i = 1, ..., M using Algorithm 8.2 and obtain the error  $E(\sigma^{(k)})$ . 4: if  $E(\sigma^{(k)}) < \epsilon$  then 5: The singularities were captured within the specified tolerance  $\epsilon$ . 6: break 7: else 8: Additional correction terms needed: Set M = M + 1. 9: 10: if M == 2 then Set initial guess  $\sigma^{(0)} = [0, \sigma_1^{(k)}]^T$ . 11: else if M == 3 then 12: Set initial guess  $\sigma^{(0)} = [\sigma_1^{(k)}, \sigma_2^{(k)}, (\sigma_1^{(k)} + \sigma_2^{(k)})/2]^T$ . 13: end if 14: end if 15: 16: end while 17: return  $M, \sigma, E(\sigma)$ .

Algorithm 8.2: Stage-I Singularity Capturing Algorithm (with M correction terms).

1: Initial guess  $\sigma^0$ ,  $\gamma^0$ , compute  $W_{n,i}$  using (8.11) and  $E(\sigma^0)$  using (8.7), (8.24), (8.25).

2: while  $E(\sigma^k) > \epsilon$  and  $||\nabla E(\sigma^k)|| > \epsilon_1$  do

3: Compute the perturbation  $\sigma^k + i\Delta\sigma \mathbf{e}_j$  for j = 1, 2, ..., M.

- 4: Compute  $\nabla E(\sigma^k)$  using (8.9), (8.11), (8.7), (8.24), (8.25).
- 5: Compute  $\gamma^k$  using (8.8) and update  $\sigma^{k+1} = \sigma^k \gamma^k \nabla E(\sigma^k)$ .
- 6: end while
- 7: return  $\sigma$ ,  $E(\sigma)$ .

Algorithm 8.3: Complete solution framework for FDEs.

- 1: Stage-I: Self-Singularity-Capturing
- 2: Given data for  $u^{data}$ ,  $f^{data}$  for  $\tilde{N}$  time-steps, capture  $\sigma$  using Algorithm 8.1.
- 3: Stage-II: Numerical solution of the FDE
- 4: Let N be the total number of time-steps. Compute  $W_{n,j}$  using (8.12).
- 5: Solve  $u_n^N$  for n = 1, ..., M using (8.24).
- 6: **for** n = 4 until N **do**
- 7: Solve for  $u_n^N$  using (8.25).
- 8: end for

small  $\tilde{N}$ , fast schemes would decrease the performance of Stage-I, and would only be beneficial for

Stage-II.

#### **8.3.2** Stage-II: Integration of FDEs with the captured singularities

Once the multi-singular behavior of the solution is captured through the framework presented in Section 8.3.1.3 and Algorithm 8.1, a variety of numerical methods for FDEs can be implemented (*e.g.* other finite-difference and fast convolution schemes), incorporating the captured singularities. Here, to solve the FDE (8.6), we use the developed implicit finite-difference scheme presented in Section 8.3.1.2, and given by expressions (8.24) and (8.25) for  $t \in \Omega = [t_0, t_N]$ , using N time-steps of size  $\Delta t$  (not necessarily the same time-step size as Stage-I). The solution procedure is described in Algorithm 8.3.

The computational complexity of Stage-II depends exclusively on the employed numerical discretization for the FDE. We utilize the same time-integration scheme as in Stage-I, for *N* time-steps. Therefore, recalling (8.24) and (8.25), we have a complexity of  $O(M^3 + (N - M)^2)$ . However, since  $M \ll N$ , the asymptotic computational complexity of Stage-II becomes  $O(N^2)$ .

## 8.4 Numerical Results

We start with Stage-I with a computational analysis of the correction weights (see Section 8.4.1), followed by the capturing scheme for particular case of a single time-step and correction term (see Section 8.4.2). Then, we test the singularity-capturing Algorithm 8.2 for M = 1, 2 and the self-capturing Algorithm 8.1 for M = 3 (see Section 8.4.3). We also utilize the two-stage framework with random singularities and compare the accuracy of the entire time-integration framework with the captured singularities against *ad-hoc* choices through a comparison between the obtained error functions  $E(\sigma)$  (see Section 8.4.1). In all aforementioned tests, if not stated otherwise, we use the method of fabricated solutions, that is, we take  $u^{data} = u^{ext}$  and  $f^{data} = f^{ext}$ , where we assume the following solution:

$$u^{ext}(t) = \sum_{j=1}^{S} t^{\sigma_j^*}, \quad \sigma_j^* \in \mathbb{R}^+,$$
 (8.26)

with homogeneous initial condition  $u^{ext}(0) = 0$ . The term *S* denotes the number singularities/terms in  $u^{ext}(t)$ , and  $\sigma_j^*$  represents prescribed singularities to be captured. From the defined analytical solution, we obtain the forcing term using a direct calculation, given by [31]:

$$f^{ext}(t) = \sum_{j=1}^{S} \frac{\Gamma(1 + \sigma_j^*)}{\Gamma(1 + \sigma_j^* - \alpha)} t^{\sigma_j^* - \alpha}.$$
(8.27)

The numerical examples in this work are presented for verification of the developed framework, where  $u^{ext}$  and  $f^{ext}$  represent synthetic data for the Cauchy problem. In practice, only Stage-I of the framework utilizes experimental data for diminutive time to capture the multi-singularities, and Stage-II utilizes the captured singularities for the full time-integration of the FDE.

Furthermore, we test Stage-I of the framework for a multi-term FDE (see Section 8.4.4.2) and the two-stage framework for a one-term FDE with a *singular-oscillatory* solution (see Section 8.4.5). Finally, we test the developed framework against a nonlinear FDE and demonstrate its effectiveness when the solution data is sampled from a fine time-grid nearby the initial time (see Section 8.4.6). The developed algorithms were implemented in MATLAB R2018b, and were run in a laptop with Intel Core i7-8650U CPU with 1.90 GHz, 16 GB RAM and Windows 10 operating system.

#### 8.4.1 Numerical behavior of correction weights

We investigate the behavior of the initial correction weights  $W_{n,j}$  and the condition number for the Vandermonde matrix V presented in (8.12). Figure 8.2a illustrates the condition numbers for  $V_{M\times M}$  using different choices for  $\sigma_k$ , namely  $\sigma_k = \alpha k$  when the regularity of u(t) is known, and  $\sigma_k = 0.1k$  when it is unknown. We also illustrate the behavior of the correction weights using M = 1 with respect to the time-step size  $\Delta t$  and fractional order  $\alpha$  (corresponding to fractional differentiation/integration) in Figures 8.2b and 8.3. We observe that for  $\alpha = 0.5$  (fractional differentiation),  $W_{1,1}$  increases in magnitude as  $\Delta t$  decreases. On the other hand, for  $\alpha = 0.5$ (fractional integration), it starts with  $W_{1,1} \approx 0.2$  for  $\Delta t = 1$ , and decreases with  $\Delta t$ . For fractional integration, only positive correction weights are observed, that decrease slower with respect to n, but with all values decreasing to zero as  $\Delta t$  decreases.



Figure 8.2: (a) Condition numbers for different choices of powers  $\sigma_k$ . We observe that the choice  $\sigma_k = 0.1k$  for unknown regularity of u(t) [5] leads to the highest condition number, where at most M = 9 correction terms can be used with double precision arithmetic. (b) First correction weight  $W_{1,1}$  with respect to  $\Delta t$ .



Figure 8.3: Initial weights  $W_{1,n}$  for different time-step sizes  $\Delta t$ , with corrections for fractional differentiation/integration (*a*)  $\alpha = 0.5$  (fractional differentiation), where the initial weights have a larger magnitude that quickly decreases in the first time-steps, indicating that they are most relevant near t = 0. (*b*)  $\alpha = -0.5$  (fractional integral).

#### 8.4.2 Single time-step and correction term

We present the numerical results for a particular case of Stage-I in E.2 for S = 1 singularity and M = 1 correction term, with a closed-form for the correction weights (see (E.8)). Let the time domain  $\tilde{\Omega} = [0, \Delta t]$ , with fractional-order and time-step size kept constant, respectively, at  $\alpha = 0.5$  and  $\Delta t = 0.01$  in this section. Figure 8.4 presents the convergence behavior for  $\sigma_1^* = 0.5$ , and



Figure 8.4: Convergence behavior with  $\sigma^* = 0.5$  and initial guesses  $\sigma^{(0)} = \{0.0001, 1.05\}$  and time-step size  $\Delta t = 0.01$ .



Figure 8.5: Convergence behavior with  $\sigma^* = 0.1$  and initial guesses  $\sigma^0 = \{0.0001, 1.1\}$  and time-step size  $\Delta t = 0.01$ .

Figure 8.5 illustrates the obtained results using  $\sigma_1^* = 0.1$ . We observe that in both cases, the scheme captures the power  $\sigma_1^*$  from the analytical solution, with a relatively small number of iterations. Furthermore, we observe an overshooting in the iterative procedure for initial guess  $\sigma^{(0)} = 1.1$ , but nevertheless, the scheme still converges within machine precision. Figures 8.6 and 8.7 show, respectively, the results for S = 2 with  $\sigma_1^* = 0.1$ ,  $\sigma_2^* = 0.2$  and S = 3 with  $\sigma_1^* = 0.1$ ,  $\sigma_2^* = 0.3$ ,  $\sigma_3^* = 0.5$ . We observe that the converged values for  $\sigma$  are closer to  $\sigma_1^*$ , which is the most critical singularity for the chosen  $u^{ext}(t)$ .

Since the converged values for  $\sigma$  captured intermediate values between the defined singularities



Figure 8.6: Convergence behavior with  $\sigma_1^* = 0.1$ ,  $\sigma_2^* = 0.2$ , initial guesses  $\sigma^{(0)} = \{0.001, 0.5\}$  and time-step size  $\Delta t = 0.01$ . The converged value for the singularity  $\sigma \approx 0.1377$  is between  $\sigma_1^*, \sigma_2^*$ .



Figure 8.7: Convergence behavior with  $\sigma_1^* = 0.1$ ,  $\sigma_2^* = 0.3$ ,  $\sigma_3^* = 0.5$ , initial guesses  $\sigma^{(0)} = \{0.001, 0.5\}$  and time-step size  $\Delta t = 0.01$ . The converged value for the singularity is  $\sigma \approx 0.1856$ .

 $\sigma_1^*, \sigma_2^*, \sigma_3^*$  for the choice of  $\Delta t = 0.01$ , we analyze the convergence behavior of  $\sigma$  with respect to  $\Delta t$ . We present the obtained results in Figure 8.8 for two different sets of singular values, and we observe for the defined range of  $\Delta t$ , that  $\sigma$  lies between the singularities  $\sigma_1^*, \sigma_2^*, \sigma_3^*$ , and converge to the strongest singularity (in this case  $\sigma_1^*$ ) as  $\Delta t \to 0$ .



Figure 8.8: Converged values for the singularity  $\boldsymbol{\sigma}$  vs time-step size  $\Delta t$  with two choices of  $\boldsymbol{\sigma}^* = \begin{bmatrix} \sigma_1^*, \sigma_2^*, \sigma_3^* \end{bmatrix}^T$ .

## **8.4.3** Singularity capturing for *M* correction terms

We systematically test the capturing Algorithm 8.2 for multiple correction terms M = 1, 2, 3and multiple defined singularities S = 1, 2, 3 in  $u^{ext}$ . The tests are presented in an incremental fashion for M, where we show the capabilities of Algorithm 8.2 to capturing/approximating the singularities. We then demonstrate how the self-capturing framework defined in Algorithm 8.1 successfully determines the singularities for S = 3 and M = 3, where we compare the obtained errors with *ad-hoc* choices for  $\sigma$  using random strong singularities. Throughout this section, we keep the fractional order fixed at  $\alpha = 0.5$ , as well as short time-domain  $\tilde{\Omega} = [0, 1]$ , and perturbation  $\Delta \sigma = 10^{-14}$  for the complex step differentiation. For all cases, we define a tolerance  $\epsilon = 10^{-15}$  for  $E(\sigma)$  and unless stated otherwise,  $\epsilon_1 = 10^{-14}$  for  $||\nabla E(\sigma)||$ . We choose a smaller tolerance for the norm of the error gradient (since the  $E(\sigma)$  is defined with the norm  $||.||_2^2$ ) to make sure that  $E(\sigma)$ is always minimized before we introduce additional correction terms in the self-capturing Stage-I. We also use  $\gamma^0 = 10^{-3}$  for initialization in Algorithm 8.2. For cases where M = S, we compute the component-wise relative error of the converged  $\sigma^k$ , which we define as:

$$E_j^{\sigma} = \frac{|\sigma_j^* - \sigma_j^{(k)}|}{|\sigma_j^*|}, \quad j = 1, \dots, M,$$

where k denotes the iteration number when convergence is achieved, *i.e.*,  $E(\sigma^{(k)}) < \epsilon$ .



Figure 8.9: Second-order asymptotic convergence behavior for M = 1 correction term, S = 1 singularity with value  $\sigma_1^* = 0.1$ . The obtained relative error for the converged  $\sigma_1$  is  $E_1^{\sigma} = 2.290 \times 10^{-8}$ .

#### 8.4.3.1 One correction term

We consider M = 1 and  $\tilde{N} = 100$  initial data-points. Figures 8.9, 8.10 and 8.11 present the obtained results, respectively, for S = 1, 2, 3 singularities, using Algorithm 8.2. We observe that, when S = M, we can capture singularities within machine precision. When M < S, we are still able to find a minimum for  $E(\sigma)$  with an intermediate value for  $\sigma_1$ , similar to the results obtained for the simplified case in Section 8.4.2. Furthermore, when  $S \ge 2$ , or the initial guess  $\sigma^{(0)}$  is far from the true singularity, the iterative procedure assumes the typical zig-zag behavior of the gradient descent scheme.

#### 8.4.3.2 Two correction terms

We consider M = 2, where we first analyze the behavior of the error function  $E(\sigma)$  using S = 2 singularities (*see Figure 8.12*). Then, we use Algorithm 8.2 to capture the singularities  $\sigma^* = [0.1, 0.3]^T$  (*see Figure 8.13*), where we observe a more pronounced zig-zag behavior for convergence, compared to M = 1. We also obtain estimates of  $\sigma_1$ ,  $\sigma_2$  when dealing with S = 3 singularities, namely  $\sigma^* = [0.1, 0.3, 0.5]^T$  (*see Figure 8.14*). Of particular interest, we observe that the obtained singularities lie in the range of the true singularities, which are useful observations to define initial



Figure 8.10: Convergence behavior for M = 1, S = 2 with  $\sigma^* = [0.1, 0.3]^T$ . With the plateau in error and  $\sigma$  due to gradient convergence within the tolerance  $\epsilon_1$ . The scheme converges to an "*intermediate*" value  $\sigma \approx 0.153$ , between the true singularities.



Figure 8.11: Convergence behavior for M = 1, S = 3 with  $\sigma^* = [0.1, 0.3, 0.5]^T$ . In for both initial guesses, the scheme converges to an "*intermediate*" value  $\sigma \approx 0.184$ , which is closer to the strongest true singularity  $\sigma_1^* = 0.1$ .

guesses for cases with three correction terms and singularities.

## 8.4.3.3 Three correction terms

We test the case for M = 3, using S = 1, 2, 3. In this analysis, we use  $\tilde{N} = 3$  initial data points. Figures 8.15 and 8.16 illustrate, respectively, the obtained results for S = 1, 2 using Algorithm 8.2. We observe a quadratic convergence rate for S = 1, similar to Fig.8.9, but with a few more iterations.



Figure 8.12: Error function  $E(\sigma)$  for M = 2, S = 2, with  $\sigma_1^* = 0.1$ ,  $\sigma_2^* = 0.3$ . Two minima occur at  $\sigma^* = [0.1, 0.3]^T = [0.3, 0.1]^T$ , corresponding to the true singularities. We set  $\sigma_1 \neq \sigma_2$  to avoid a singular matrix in linear system (8.11).



Figure 8.13: Two correction terms M = 2 and two singularities S = 2, with  $\sigma^* = [0.1, 0.3]^T$ . The obtained converged values are  $\sigma = [0.299974, 0.099990]^T$ , which correspond to component-wise relative errors  $E^{\sigma} = [8.61, 9.94]^T \times 10^{-5}$ .

Furthermore, for M = 2, we observed a small change in the final value of  $\sigma_3$ , but nevertheless, capturing the two singularities  $\sigma_1^*$ ,  $\sigma_2^*$  is sufficient to minimize  $E(\sigma)$  when S = 2.

The numerical convergence of Algorithm 8.2 towards the correct singularities  $\sigma^*$  becomes much more difficult when using S = M = 3. Therefore, we make use of the self-capturing approach summarized in Algorithm 8.1, which incrementally solves the minimization problem using M = 1, 2, 3 and use the respective output singularities as initial guesses for the subsequent



Figure 8.14: Two correction terms M = 2 and three singularities S = 3, with  $\sigma^* = [0.1, 0.3]^T$  and  $\epsilon_1 = 10^{-11}$ . The converged values are  $\sigma = [0.112635, 0.420495]^T$ , which are closer to the stronger singularities  $\sigma_1 = 0.1$  and  $\sigma_3 = 0.5$ . The approximate singularities still lead to an approximation error of  $1.47 \times 10^{-11}$ .



Figure 8.15: Results for M = 3, S = 1. The obtained relative error for  $\sigma_1$  is  $E_1^{\sigma} = 4.869 \times 10^{-8}$ . The components  $\sigma_1$ ,  $\sigma_2$  remained practically constant.

number of correction terms M = M + 1. We present the obtained results in Fig.8.17. We observe that the scheme converges to the true singularities with errors for  $\sigma$  up to 0.024, but nevertheless, they yield an approximation error for  $u^N$  of  $10^{-15}$ .

We also test the influence of the number of initial data points  $\tilde{N}$  in Stage-I over the number of iterations  $N_{it}$  and number of corrections terms M. For this purpose, we set S = 3 singularities with values  $\sigma^* = [0.1, 0.3, 0.5]^T$  and we fix  $\Delta t = 0.1 [s]$ ,  $\alpha = 0.5$ ,  $\epsilon = 10^{-13}$ ,  $\epsilon_1 = 10^{-10}$ .



Figure 8.16: Results for M = 3, S = 2.

The obtained converged values are  $\sigma$  =  $[0.099997, 0.299995, 0.939015]^T$ , where  $\sigma_1$ ,  $\sigma_2$  captured the singularities, respectively with errors  $E_1^{\sigma} = 3.07 \times 10^{-5}$  and  $E_2^{\sigma} = 1.65 \times 10^{-5}$ .



Figure 8.17: Results for M = 3, S = 3 using  $\epsilon = 10^{-15}$ . The converged values are  $\sigma = [0.099, 0.498, 0.293]^T$ , which correspond to component-wise relative errors  $E^{\sigma} =$  $[0.014, 0.005, 0.024]^T$ .

We then vary  $\tilde{N}$  in Algorithm 8.1 and analyze the convergence behavior and computational time, which are presented in Table 8.1. We observe that the variation of  $\tilde{N}$  did not affect the number of captured singularities M, but the choice  $\tilde{N} = 3^7$  significantly increased the number of iterations. We also observe that despite the similar number of iterations  $N_{it}$  obtained for  $3^1 \leq \tilde{N} \leq 3^6$ , the computational time increases with  $\tilde{N}$  due to the computational complexity of Stage-I. Therefore, we consider  $\tilde{N} = O(M)$  an appropriate choice, as the singularities  $\sigma^*$  are captured with less

Ñ	М	N <sub>it</sub>	Computation Time [s]	$E(\sigma)$
3 <sup>1</sup>	3	74	0.217	$9.863015 \times 10^{-14}$
3 <sup>2</sup>	3	44	0.293	$2.101287 \times 10^{-14}$
3 <sup>3</sup>	3	51	0.617	$9.433562 \times 10^{-14}$
3 <sup>4</sup>	3	62	2.251	$9.037342 \times 10^{-14}$
35	3	98	11.346	$9.101754 \times 10^{-14}$
36	3	52	180.719	$1.550662 \times 10^{-14}$
3 <sup>7</sup>	3	445	1275.168	$8.823108 \times 10^{-14}$

computational cost, which is suitable when diminutive initial data is available.

Table 8.1: Influence of  $\tilde{N}$  in Stage-I of the developed framework.

## 8.4.4 Random singularities

We perform two numerical tests involving random power-law singularities, where we define three strong singularities  $\sigma_1^*$ ,  $\sigma_2^*$ ,  $\sigma_3^*$  randomly sampled from a uniform distribution  $\mathcal{U}(0, 1/2)$ . We employ the self-singularity-capturing procedure in the context of single- and multi- term FDEs.

#### **8.4.4.1** FDEs with random singularities

We test the two-stage framework for efficient time-integration of (8.6). We then compute  $u^{ext}(t)$  and  $f^{ext}(t)$ , respectively using (8.26) and (8.27), and use the self-capturing framework presented in Algorithm 8.1. We then compare the approximation error  $E(\sigma)$  with the choice  $\sigma_k = 0.1k$  defined in [5] when the singularities are unknown. Although our framework has no explicit information about the generated random singularities, we present them for verification purposes, which are given by:

$$\sigma^* = [0.0172230402514543, 0.219372179828199, 0.190779228546504]^T$$
.

We set  $\tilde{N} = 3$  with  $\Delta t = 1/3$ , and therefore,  $\tilde{\Omega} = [0, 1]$ ,  $\epsilon = 10^{-15}$ , and  $\epsilon_1 = 10^{-13}$  to Algorithm 8.3. Stage-I of the framework (Algorithm 8.1) converges with  $E(\sigma^{(k)}) = 2.96 \times 10^{-16}$  with M = 2 correction terms, with obtained values:

$$\boldsymbol{\sigma} = [0.0187990387914248, \ 0.206944449676742]^T, \tag{8.28}$$



Figure 8.18: Comparison of error vs time for long time-integration between the captured singularities and  $\sigma_k = 0.1k$  for different values of time-step size  $\Delta t$ .

with elapsed computational time of 0.169 [s]. After capturing the singularities within the desired precision  $\epsilon$ , we enter Stage-II and compute the numerical solution  $u^{N}(t)$  using the captured  $\sigma$  for multiple, longer time-integration domains  $\Omega$ . We remark that when using an *ad-hoc* choice of fixed  $\sigma_{k} = 0.1k$  with 4 correction terms, that is,

$$\boldsymbol{\sigma} = [0.1, \ 0.2, \ 0.3, \ 0.4]^T, \tag{8.29}$$

we obtain an approximation error  $E(\sigma) = 5.25 \times 10^{-5}$  over N = 4 time-steps. We use the captured powers (8.28) and the predefined ones (8.29) for longer time-integration. The obtained results are presented in Figure 8.18, where we observe how using 3 time-steps to capture the singularities leads to precise long time-integration with a large time-step size  $\Delta t = 1/3$  (blue curve). On the other hand, the errors for  $\sigma_k = 0.1k$  are much larger, and also do not improve with smaller  $\Delta t$  due to the presence of very strong singularities.

## 8.4.4.2 Multi-term FDEs with random singularities

In this section we show how the scheme in Stage-I can be applied for multi-term fractional differential equations. Let the following multi-term FDE:

$$\sum_{l=1}^{N_{\alpha}} {}^{RL}_{0} \mathcal{D}_{t}^{\alpha_{l}} u(t) = f(t, u(t)), \quad u(0) = u_{0}, \quad 0 < \alpha_{l} < 1.$$
(8.30)

where  $\alpha_l$  denotes the  $N_{\alpha}$  multi-fractional orders with  $l = 1, ..., N_{\alpha}$ . Using the approximation (8.10), and assuming the same powers  $\sigma$  for the correction weights for all fractional derivatives, we obtain:

$$\sum_{l=1}^{N_{\alpha}} {}^{RL}_{0} \mathcal{D}_{t}^{\alpha_{l}} u^{N}(t)|_{t=t_{n}} + \sum_{j=1}^{M} \left( \sum_{l=1}^{N_{\alpha}} W_{j,n}^{(\alpha_{l})}(\boldsymbol{\sigma}) \right) \left( u_{j}^{N} - u_{0} \right) = f_{n}^{\delta},$$
(8.31)

where we use the superscript  $(\alpha_l)$  in  $W_{j,n}^{(\alpha_l)}$  to denote the distinct sets of correction weights due to the fractional order  $\alpha_l$  through (8.12). The entire minimization scheme is identical, since it depends on the solution data for u(t). In order to solve (8.31) with the developed scheme in Stage-I, due to the linearity of (8.30), we only need to replace the initial correction weights  $W_{n,j}$ , and  $\alpha$ -dependent coefficients  $d_j$ ,  $b_j$  in (8.24) and (8.25) with the following summations:

$$\tilde{W}_{n,j} = \sum_{l=1}^{N_{\alpha}} W_{n,j}^{(\alpha_l)}, \quad \tilde{d}_j^{(p)} = \sum_{l=1}^{N_{\alpha}} d_j^{(p,\alpha_l)}, \quad \tilde{b}_j^{(k)} = \sum_{l=1}^{N_{\alpha}} b_j^{(k,\alpha_l)}, \quad k = 1, 2, 3$$

We utilize the fabricated solution (8.26) in (8.30), which yields the following force term:

$$f^{ext}(t) = \sum_{\alpha_l}^{N_{\alpha}} \sum_{j=1}^{S} \frac{\Gamma(1+\sigma_j^*)}{\Gamma(1+\sigma_j^*-\alpha_l)} t^{\sigma_j^*-\alpha_l}.$$
(8.32)

We set  $N_{\alpha} = 3$  fractional orders  $\{\alpha_1, \alpha_2, \alpha_3\} = \{0.3, 0.5, 0.7\}$ , and identically to Section 8.4.4.1, we sample the following random singularities from  $\mathcal{U}(0, 1/2)$ :

$$\boldsymbol{\sigma}^* = [0.13924910943352420, \ 0.2734407596024919, \ 0.4787534177171488]^T$$

Also, we set  $\tilde{N} = 3$  with  $\Delta t = 1/3$  and  $\tilde{\Omega} = [0, 1]$ ,  $\epsilon = 5 \times 10^{-15}$ , and  $\epsilon_1 = 10^{-14}$ , with  $\gamma^0 = 10^{-3}$  to Algorithm 8.1, where the scheme converges with the following approximate singularities:

$$\sigma = [0.1469249923105880, 0.4869203803691072, 0.3066386453671829]^{T}$$

Figure 8.19 presents the obtained results for each *M* in the self-capturing procedure, where we observe that the scheme does not fully capture the true singularities, but provides sufficiently good approximations to obtain errors as low as  $E(\sigma) = 2.31 \times 10^{-15}$ . The elapsed computational time is 10.65 [*s*], due to the larger number of iterations  $N_{it}$  required for convergence of Stage-I.



Figure 8.19: Singularities  $\sigma$  vs iteration number for a multi-term FDE with  $N_{\alpha} = 3$  in Stage-I for each M in Algorithm 8.1. (a) M = 1, with error  $E(\sigma) = 1.10 \times 10^{-5}$ , (b) M = 2, with error  $E(\sigma) = 3.83 \times 10^{-13}$ , and (c) M = 3 with convergence at  $E(\sigma) = 2.31 \times 10^{-15}$ . The black horizontal lines correspond to the true random singularities in the solution.

## 8.4.5 Singular-oscillatory solutions

We also test the two-stage framework sampling data points from a fabricated solution for (8.6), defined as the following multiplicative coupling between a power-law and oscillatory parts:

$$u^{ext}(t) = t^{\sigma^*} \cos(\omega t), \tag{8.33}$$

with homogeneous initial condition  $u^{ext}(0) = 0$ . The corresponding right-hand-side is analytically obtained as:

$$f^{ext}(t) = c_1 t^{\sigma^* - \alpha} \left[ c_{2p} \tilde{F}_q(a^{(1)}; b^{(1)}; c_4 t^2) + c_3 c_4 t^2{}_p \tilde{F}_q(a^{(2)}; b^{(2)}; c_4 t^2) \right],$$
(8.34)

with  $c_1 = -2^{\alpha - \sigma^* - 4} \pi \Gamma(1 + \sigma^*)$ ,  $c_2 = 8 (\alpha - \sigma^* - 1)$ ,  $c_3 = -4(1 + \sigma^*)(2 + \sigma^*)$  and  $c_4 = -\omega^2/4$ . Also,  ${}_p \tilde{F}_q$  represents the regularized, generalized hypergeometric function given by [315]:

$${}_p\tilde{F}_q(a_1,\ldots,a_p;b_1,\ldots,b_q;z) = \frac{pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;z)}{\Gamma(b_1)\ldots\Gamma(b_q)},$$

where, for the particular case (8.34), we have:

$$\begin{cases} a^{(1)} = \{\frac{(1+\sigma^*)}{2}, \frac{(2+\sigma^*)}{2}\}, \quad b^{(1)} = \{\frac{1}{2}, \frac{(2-\alpha+\sigma^*)}{2}, \frac{(3-\alpha+\sigma^*)}{2}\}, \\\\ a^{(2)} = \{\frac{(3+\sigma^*)}{2}, \frac{(4+\sigma^*)}{2}\}, \quad b^{(2)} = \{\frac{3}{2}, \frac{(4-\alpha+\sigma^*)}{2}, \frac{(3-\alpha+\sigma^*)}{2}\}. \end{cases}$$

We fix the fractional order  $\alpha = 0.5$ , frequency  $\omega = 10\pi$  and randomly sample  $\sigma^*$  from a uniform distribution  $\mathcal{U}(0, 1/3)$  and obtain a value  $\sigma^* = 0.242648195440154$ . For Stage-I, we consider  $\tilde{N} = 3$  data points with  $\tilde{\Omega} = [0, 0.01]$ , with  $\Delta t = 3/100 [s]$ . Furthermore, we set  $\epsilon = 10^{-11}$ ,  $\epsilon_1 = 10^{-14}$  and  $\gamma^0 = 10^{-3}$ . Using Algorithm 8.1 with a slight initial guess modification for  $\sigma^{(0)}$  when M = 2 in line 11 to  $\sigma^{(0)} = [1, \sigma_1^{(k)}]^T$  (since the developed framework is mainly oriented to strong singularities), we capture the following two singularities:

# $\boldsymbol{\sigma} = [0.2427452349772425, \ 2.220682758797950]^T,$

where the first converged singularity is an approximation to the randomly sampled value for  $\sigma^*$ . To understand the second captured singularity  $\sigma_2$ , let the series expansion of (8.33) around  $\omega t$ :

$$u^{ext}(t) = t^{\sigma^*} \cos(\omega t) = t^{\sigma^*} \left( 1 - \frac{\omega^2}{2} t^2 + O(t^4) \right) = t^{\sigma^*} - \frac{\omega^2}{2} t^{2+\sigma^*} + O(t^{4+\sigma^*}).$$
(8.35)

Therefore, the captured  $\sigma_2$  is an approximation of the second term  $2 + \sigma^*$  of the above series expansion. Although capturing the third singularity  $4 + \sigma^*$  is possible, we would need to set higher values for the initial guesses in the self-capturing algorithm, and finding the corresponding minimum becomes more difficult, since such higher-order, weaker singularities have less influence in the accuracy of the solution.

After capturing the singularities in Stage-I, with elapsed computational time of 0.149 [s], we apply them in Stage-II for a convergence test with T = 1 [s], with  $\Omega = [0, T]$ , and compare the approximate solution  $u^{N}(t)$  with the exact one (8.35) through the relative error defined as

$$E_{L^{2}} = \frac{||\mathbf{u}^{N} - \mathbf{u}^{ext}||_{L^{2}(\Omega)}}{||\mathbf{u}^{ext}||_{L^{2}(\Omega)}}.$$
(8.36)

between the two-stage framework other *ad-hoc* choices for  $\sigma$ , and also without corrections (see Figure 8.20a). We observe that capturing M = 2 singularities leads to the theoretical accuracy  $O(\Delta t^{3-\alpha})$  of the employed discretization, and also to errors about 2 orders of magnitude lower than the choice  $\sigma_k = 0.1k$  with M = 4 for the singularities in the observe range for  $\Delta t$ . We also compare the exact and approximate solutions over T = 25 [s] with N = 4096 time-steps of size  $\Delta t \approx 6.10 \times 10^{-3}$ , and observe that we fully capture the singular and oscillatory behaviors of the solution, with elapsed computational time of 0.426 [s].



Figure 8.20: (a) Convergence analysis comparing the accuracy of the captured singularities in Stage-I with *ad-hoc* choices for time-integration with T = 1 [s] in Stage-II. The term q denotes the convergence rate. The self-captured case uses M = 2 correction terms, while for  $\sigma_k = 0.1k$  and  $\sigma_k = \alpha k$  we use M = 4. (b) Exact and approximate solutions for u(t) using the captured singularities for longer time-integration over T = 25 [s].

## 8.4.6 Nonlinear FDE

Finally, we apply the developed framework for a nonlinear right-hand-side of the FDE (8.6), now given by:

$${}_{0}^{C}\mathcal{D}_{t}^{\alpha}u(t) = C_{1}u(t)^{2}\exp(-C_{2}t) + 1, \quad u(0) = 0,$$
(8.37)

where we set  $C_1 = 1$  and  $C_2 = 5$ . Differently from the previous examples, where the diminutive data points were sampled from a known solution  $u^{ext}(t)$ , here, we sample  $u^{data}(t)$  from a benchmark solution obtained through a fine-grid nearby t = 0. The right-hand-side is evaluated explicitly. Our procedure follows:

- I) Set the short time-domain  $\tilde{\Omega} = [0, 0.01]$  and numerically obtain the approximate solution of (8.37) using  $\Delta t = 10^{-5} [s]$ .
- II) Sample  $\tilde{N} = 100$  benchmark solution data points and utilize the singularity capturing algorithm (Stage-I) with  $\Delta t = 10^{-4}$  and  $\epsilon_1 = 10^{-14}$  over  $\tilde{\Omega}$  to obtain **e**. The value of  $\epsilon$  is chosen according to the employed fractional order  $\alpha$ .

• III) We utilize the captured singularities and the RHS of (8.37) evaluated explicitly for full time-integration (Stage-II) over  $\Omega = [0, 1]$ , using  $\Delta t = 10^{-4} [s]$ , and compare the results with the benchmark solution integrated through  $\Omega$ .

We perform two tests: In the first, we set  $\alpha = 0.2$ ,  $\epsilon = 1.1 \times 10^{-5}$  in Stage-I, and capture  $\sigma = 2.158080327840559 \times 10^{-1}$ . In the second one, we set  $\alpha = 0.25$ ,  $\epsilon = 7.5 \times 10^{-5}$  and capture  $\sigma = 7.602862102264105 \times 10^{-2}$ . Figure 8.21 illustrates the obtained results for full time-integration. We observe that the self-captured solution matches the benchmark case for the entire time-integration domain, including nearby t = 0, demonstrating that the developed scheme is effective for nonlinear FDEs with unknown solutions. The obtained computational times for the self-capturing framework are: 0.07 [s] for fine grid solution and sampling, 0.15 [s] for Stage-I and 0.86 [s] for Stage-II, yielding a total computational time of 1.08 [s], compared to 48.58 [s] for the benchmark solution. Therefore, the fine grid sampling at diminutive time had minimal influence on the computational cost.



Figure 8.21: Self-captured and benchmark solutions *versus* time for full time-integration of a nonlinear FDE.

#### **CHAPTER 9**

## IMPLICIT-EXPLICIT TIME INTEGRATION SCHEMES FOR NONLINEAR FRACTIONAL DIFFERENTIAL EQUATIONS

# 9.1 Background

Fractional differential equations (FDEs) have been widely applied in a variety of scientific fields, where the observed data presents the trademark of power-laws/heavy-tailed statistics across many length/time scales. Some applications include, *e.g.*, anomalous models for bio-tissues [8, 42, 43], food rheology [24, 44, 45] and earth sciences [316]. Regarding nonlinear FDEs for anomalous transport/materials, we outline fractional Navier-Stokes equations [317], fractional phase-field equations [318], fractional subgrid-scale modeling [225], complex constitutive laws applied to structural problems undergoing large deformations/strains [1, 75] as well as nonlinear vibrations of beams [319].

Obtaining closed forms for linear FDEs can be challenging, especially for any general form of f(t). In the few instances when the corresponding solution u(t) is known, it is usually impractical to be numerically evaluated. Furthermore, obtaining analytical solutions becomes impossible in the presence of nonlinearities. Therefore, a series of numerical methods for FDEs were developed since the 80's, with several significant contributions summarized in Figure 9.1. In such schemes it is fundamental to incorporate the history effects arising from the fractional operators. The pioneering works are attributed to Lubich [86, 88], on *discretized fractional calculus* in the sense of fractional multi-step and finite-difference (FD) schemes. Later on, Tang [89] developed a superlinear convergent FD scheme, followed by a numerical quadrature approach for fractional derivatives introduced by Diethelm [90]. In the 2000's, Diethelm developed a predictor-corrector approach in addition to a fractional Adams method [94, 108]. Later on, Lin and Xu [91] developed a FD discretization with order  $2 - \alpha$ , which was applied to the time-fractional diffusion equation. More recently, Garrappa [82] developed trapezoidal methods for fractional multi-step approaches, Zeng *et* 



Figure 9.1: Research timeline on significant and diverse numerical schemes for time-fractional differential equations.

*al.* [92] developed a second-order scheme for time-fractional diffusion equations, while Li *et al.* [93] developed a high-order scheme with order  $3-\alpha$ . Spectral methods were also developed in the context of FDEs/FPDEs [95–101, 297, 299], and distributed-order differential equations [260, 261, 266]. In particular, Zayernouri and Karniadakis [96] developed an exponentially-accurate spectral element method for FDEs and Lischke *et al.* [102] developed a fast, *tunably-accurate* spectral method.

It is known that time-fractional operators possess power-law kernels with a singularity nearby the initial time, which produces non-smooth solutions that deteriorate the accuracy of many existing numerical schemes. In order to handle such problem, Lubich [86] introduced the *so-called* correction method, which was later applied to a series of direct/multi-step schemes for linear/nonlinear FDEs [87, 106, 113, 114], and also employed in a *self-singularity-capturing* approach by Suzuki and Zayernouri [177]. In the aforementioned works, the correct determination of singularity powers leads to global high accuracy of the numerical schemes. The idea of *graded meshes* was also introduced with the same objectives by Brunner [320], who developed a spline collocation scheme

for Volterra integro-differential equations, where the graded meshes correspond to non-uniform time-grids which are simple to incorporate in existing FD schemes. Graded meshes were later applied to nonlinear Volterra integral equations [321]. An implicit FD approach was developed in the context of graded meshes by Yuste and Quintana-Murillo [83]. More recently, stability issues of existing/new FD approaches were addressed by Zhang *et al.* [84] for the time-fractional diffusion equation, and also by Stynes *et al.* [85] for a reaction-diffusion problem, where, in the latter, an optimal mesh grading parameter was obtained. For a comparison between the performance of Lubich's corrections and graded meshes, we refer the readers to [106].

The main computational challenge of direct FD schemes for time-integration of FDEs is the evaluation of the history term, which usually leads to a computational complexity of  $O(N^2)$  and memory storage of O(N), where N represents the total number of time-steps. To address such issues, fast schemes were developed, starting with the first-order fast convolution method by Lubich and Schädle [103], which reduced the computational complexity to  $O(N \log N)$ , and memory requirements to  $O(\log N)$ . The main idea of the scheme is to approximate the power-law kernel via numerical inverse Laplace transforms and split the integral operator (but not the time-grid) into exponentially increasing time steps. Later on, Schädle et al. [104] extended the developed fast convolution for nonlinear FDEs. A third-order extension was developed by Yu et al. [105] and applied to the time-integration for 3D simulation of a class of time-fractional PDEs. Zeng et al. [106] developed an improved version of the fast-convolution approach, which considers real-valued integration contours with the order  $3 - \alpha$ . Of particular interest, fast matrix-based schemes were also developed, such as the fast-inversion approach by Lu et al. [322], the kernel compression method by Baffet and Hesthaven [107] and the KPS preconditioner by Zhou et al. [323]. The main idea of such approaches is to represent the time-stepping equation in a global linear system and exploit the resulting Toeplitz-like structure through Fast-Fourier-Transforms (FFTs).

In addition to the aforementioned challenges, dealing with stiff/nonlinear problems further deteriorates the accuracy and might pose stability issues to existing numerical schemes. Fractional linear multi-step approaches become interesting alternatives to handle such issues. Diethelm and Ford [108] developed a predictor-corrector scheme and later analyzed the error of a family of fractional Adams-Bashforth/Moulton schemes [94]. Galeone and Garrappa studied the stability of implicit and explicit fractional multi-step methods [109, 110] and proposed new explicit schemes with larger stability regions. In addition, the stability analysis of fractional predictor-corrector schemes was studied by Garrappa [111]. Also in the context fractional multi-step schemes, Zayernouri and Matzavinos [112] developed a family of fractional Adams schemes for high-order explicit/implicit treatment of nonlinear problems, where a particular time-splitting preserved the original structure of integer-order Adams schemes. Larger stability regions can be obtained through semi-implicit schemes, where for instance, Cao *et al.* [113] developed two IMEX schemes for nonlinear FDEs, utilizing two distinct force extrapolation formulas and also analyzed the stability of the developed schemes. Recently, Zeng *et al.* [114] developed a new class of fast, second-order semi-implicit methods for nonlinear FDEs through new fast convolutions. Zhou *et al.* also developed and analyzed the convergence and stability of one-leg approaches [324] and a class of boundary value methods and their block version [325, 326] for stiff/nonlinear FDEs.

Although a significant amount of relevant works was developed, they usually address the aforementioned singularity/performance/stability issues for stiff/nonlinear problems separately. In this regard, there is still a need on numerical schemes for stiff/nonlinear FDEs that I) efficiently handle the numerical solution with low-regularity for both the solution u(t) and nonlinear term f(t, u(t)); II) present linear complexity with respect to the number of time-steps N; III) have larger stability regions compared to the existing numerical schemes; IV) mimick and generalize the structure of existing integer-order IMEX schemes, widely employed by the scientists and engineers to its fractional-order counterparts. The main contribution of the present work is to develop a class of IMEX methods for accurate time-integration of stiff/nonlinear FDEs. Specifically:

• We start with the linear multi-step FAMMs developed by Zayernouri and Matzavinos [112] in the sense of linear/nonlinear fractional Cauchy equations. For the linear problem, two sets of Lubich-like correction terms [86] are employed.

- We develop a class of new first- and second-order IMEX methods with the combination of Zayernouri and Matzavinos [112] FAMMs with two extrapolation methods for the nonlinear term. The obtained methods are denoted by IMEX(*p*), which is first-order accurate when *p* = 0, and second-order accurate when *p* = 1.
- The convergence and linear stability of the developed IMEX methods are proved and the corresponding regions of stability are shown to be larger for smaller values of the fractional order  $\alpha$ .
- The convolution nature of the fractional operators allows us to represent the corresponding IMEX methods in the language of global-in-time Toeplitz-like nonlinear systems, and employ the fast approximate inversion approach by Lu *et al.* [322]. Since the Toeplitz system is nonlinear, we utilize a Picard iteration scheme which takes  $N^p$  iterations until convergence with respect to a specified tolerance  $\epsilon^p$ . Under suitable conditions,  $N^p$  does not significantly increase with N.
- The corresponding *history load* for the developed IMEX schemes is given by hypergeometric functions, which are efficiently evaluated through a Gauss-Jacobi quadrature with a fixed number of *Q* integration points.
- The asymptotic computational complexity of the scheme is  $O(N \log N)$ , with memory storage of order O(N).

This paper is organized as follows: Section 9.2 follows a step-by-step procedure, starting with linear multi-step FAMMs for linear FDEs, up to nonlinear FDEs, when the developed IMEX methods will be introduced. In Section 9.3 we demonstrate the linear stability of the developed IMEX methods. In Section 9.4 we put the corresponding IMEX methods in the language of a global non-linear system of equations and employ a fast solver. The numerical results for linear/nonlinear/stiff FDEs with discussions are shown in Section 9.5.

# 9.2 Implicit-Explicit Time-Integration Methods

We develop two IMEX methods for efficient time-integration of nonlinear FDEs. In a step-bystep fashion, we start with the numerical solution of a fractional linear Cauchy problem, following the idea of FAMMs proposed by Zayernouri and Matzavions in [112]. To capture the singularity of the solution u(t) of the considered problem, we then develop two sets of appropriate correction terms by using Lubich's approach [86] for the resulting fractional operators. As a next step, we introduce a nonlinear forcing term f(t, u(t)) and develop two IMEX methods for the solution of the resulting nonlinear Cauchy problem, which also introduces two additional sets of correction weights due to f(t, u(t)).

## 9.2.1 Definitions

We start with some preliminary definitions for fractional calculus (see e.g. [327]). The left-sided Caputo fractional derivative of order  $\alpha$  (0 <  $\alpha$  < 1) is defined by

$${}_{t_{L}}^{C}D_{t}^{\alpha}u(t) = {}_{t_{L}}I_{t}^{1-\alpha}u'(t) = \frac{1}{\Gamma(1-\alpha)} \int_{t_{L}}^{t} \frac{u'(v)}{(t-v)^{\alpha}}dv, \quad t > t_{L},$$
(9.1)

where  $\Gamma(\cdot)$  denotes the usual gamma function. The operator  ${}_{tL}I_t^{\alpha}$  represents the  $\alpha$ -th order (0 <  $\alpha < 1$ ) left-sided fractional Riemann-Liouville (RL) integral operator, defined as

$${}_{t_{L}}I_{t}^{\alpha}u(t) = \frac{1}{\Gamma(\alpha)} \int_{t_{L}}^{t} \frac{u(v)}{(t-v)^{1-\alpha}} dv, \quad t > t_{L}.$$
(9.2)

The corresponding inverse operator of (9.2), *i.e.*, the left-sided Riemann-Liouville fractional derivative of order  $\alpha$  is denoted by

$${}^{RL}_{t_L}D^{\alpha}_t u(t) = \frac{d}{dt} \left[ {}_{t_L}I^{\alpha}_t u(t) \right] = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_{t_L}^t \frac{u(v)}{(t-v)^{\alpha}} dv, \quad t > t_L.$$
(9.3)

Moreover, the left-sided Caputo fractional derivative and the left-sided Riemann-Liouville fractional derivative are linked by the following relationship:

$${}^{RL}_{t_L} D^{\alpha}_t u(t) = \frac{u(t_L)}{\Gamma(1-\alpha)(t-t_L)^{\alpha}} + {}^{C}_{t_L} D^{\alpha}_t u(t).$$
(9.4)

## 9.2.2 Linear FDEs

Consider the numerical solutions of the following linear FDE:

$${}_{0}^{C}D_{t}^{\alpha}u(t) = \lambda u(t), \ \alpha \in (0,1], \ t \in (0,T]; \ u(0) = u_{0},$$
(9.5)

where  $\lambda \in \mathbb{C}$ ,  $u_0 \in \mathbb{R}^d$ . Now, we adopt the FAMMs developed in [112] to solve (9.5). Let h > 0be the time-step size with h = T/N ( $N \in \mathbb{N}$ ) and  $t_k = kh$  ( $0 \le k \le N$ ). By the definition of the Caputo fractional derivative (9.1), we can split the fractional operator in history and local parts:

$${}^{C}_{0}D^{\alpha}_{t}u(t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t_{k}} \frac{u'(v)}{(t-v)^{\alpha}} dv + \frac{1}{\Gamma(1-\alpha)} \int_{t_{k}}^{t} \frac{u'(v)}{(t-v)^{\alpha}} dv$$
  
$$:= H^{k}(t) + {}^{C}_{t_{k}}D^{\alpha}_{t}u(t).$$
(9.6)

Moreover, from (9.4), we have

$${}^{C}_{t_{k}}D^{\alpha}_{t}u(t) = {}^{C}_{t_{k}}D^{\alpha}_{t}[u(t) - u(t_{k}) + u(t_{k})] = {}^{C}_{t_{k}}D^{\alpha}_{t}[u(t) - u(t_{k})] = {}^{RL}_{t_{k}}D^{\alpha}_{t}[u(t) - u(t_{k})].$$
(9.7)

Then, by substituting (9.6) and (9.7) into (9.5), it holds that

$${}^{RL}_{t_k} D^{\alpha}_t [u(t) - u(t_k)] = \lambda u(t) - H^k(t), \quad \alpha \in (0, 1], \ t \in (0, T].$$
(9.8)

Applying the inverse operator  $t_k I_t^{\alpha}$  on the both sides of (9.8) and evaluating at  $t = t_{k+1}$ , we obtain

$$u(t_{k+1}) - u(t_k) = \left[ \lambda_{t_k} I_t^{\alpha} u(t) - \mathcal{H}^k(t) \right] \Big|_{t=t_{k+1}},$$
(9.9)

where  $\mathcal{H}^{k}(t)$  denotes the history load term, which is given by:

$$\mathcal{H}^{k}(t) = {}_{t_{k}}I^{\alpha}_{t}(H^{k}(t)) = \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_{t_{k}}^{t} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \int_{0}^{t_{k}} \frac{u'(s)}{(v-s)^{\alpha}} ds dv.$$
(9.10)

We follow the FAMMs from [112] and interpolate u(t) from  $t_k I_t^{\alpha} u(t) \Big|_{t=t_{k+1}}$  in an implicit fashion:

$${}_{t_k} I_t^{\alpha} u(t) \Big|_{t=t_{k+1}} \approx h^{\alpha} \sum_{j=0}^p \beta_j^{(p)} u(t_{k+1-j}), \quad p = 0, 1,$$
(9.11)

with the following fractional Adams-Moulton coefficients, respectively, for p = 0 and p = 1,

$$\beta_0^{(0)} = \frac{1}{\Gamma(\alpha+1)}; \quad \beta_0^{(1)} = \frac{1}{\Gamma(\alpha+2)}, \quad \beta_1^{(1)} = \frac{\alpha}{\Gamma(\alpha+2)}.$$

Moreover, these coefficients recover the standard Adams-Moulton method's coefficients in the limit case when  $\alpha = 1$ . To compute the history load term  $\mathcal{H}^k(t_{k+1})$ , on each small interval  $[t_j, t_{j+1}] (0 \le j \le k - 1)$ , we linearly interpolate u(t) when p = 0, as follows:

$$\Pi_{1,j}u(t) = \frac{t - t_{j+1}}{t_j - t_{j+1}}u(t_j) + \frac{t - t_j}{t_{j+1} - t_j}u(t_{j+1}),$$

therefore, we obtain the following form for the history load:

$$\mathcal{H}^{k}(t_{k+1}) \approx \mathcal{H}^{k}_{0}(t_{k+1}) = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k-1} \frac{u(t_{j+1}) - u(t_{j})}{h} \left(\mathcal{A}_{k,j} - \mathcal{A}_{k,j+1}\right), \tag{9.12}$$

where

$$\begin{aligned} \mathcal{A}_{k,j} &= \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} (v - t_j)^{1 - \alpha} dv = h \int_0^1 (1 - \theta)^{\alpha - 1} (k - j + \theta)^{1 - \alpha} d\theta \\ &= h \begin{cases} \frac{(k - j)^{1 - \alpha}}{\alpha} {}_2F_1 \left( \alpha - 1, 1; \alpha + 1; \frac{1}{j - k} \right), & 0 \le j < k, \\ \Gamma(\alpha) \Gamma(2 - \alpha), & j = k, \end{cases} \end{aligned}$$
(9.13)

in which  $_2F_1(a, b; c; z)$  denotes the hypergeometric function. Also, when p = 1, we utilize quadratic interpolation function  $\Pi_{2,j}u(t)$  to approximate u(t) on the interval  $[t_j, t_{j+1}]$  ( $0 \le j \le k - 1$ ) as follows:

$$\begin{split} \Pi_{2,j} u(t) = & \frac{(t-t_j)(t-t_{j+1})}{(t_{j-1}-t_j)(t_{j-1}-t_{j+1})} u(t_{j-1}) + \frac{(t-t_{j-1})(t-t_{j+1})}{(t_j-t_{j-1})(t_j-t_{j+1})} u(t_j) \\ & + \frac{(t-t_{j-1})(t-t_j)}{(t_{j+1}-t_{j-1})(t_{j+1}-t_j)} u(t_{j+1}), \end{split}$$

and therefore, the history load for the choice of p = 1 is given by

$$\mathcal{H}^{k}(t_{k+1}) \approx \mathcal{H}^{k}_{1}(t_{k+1}) = \mathcal{H}^{k}_{0}(t_{k+1}) + \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=1}^{k-1} \frac{u(t_{j+1}) - 2u(t_{j}) + u(t_{j-1})}{h^{2}} \left[ -\frac{h(\mathcal{A}_{k,j} + \mathcal{A}_{k,j+1})}{2} + \frac{\mathcal{B}_{k,j} - \mathcal{B}_{k,j+1}}{2-\alpha} \right], \quad (9.14)$$

where

$$\mathcal{B}_{k,j} = \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} (v - t_j)^{2 - \alpha} dv = h^2 \int_0^1 (1 - \theta)^{\alpha - 1} (k - j + \theta)^{2 - \alpha} d\theta$$
$$= h^2 \begin{cases} \frac{(k - j)^{2 - \alpha}}{\alpha} {}_2F_1 \left( \alpha - 2, 1; \alpha + 1; \frac{1}{j - k} \right), & 0 \le j < k, \\ \frac{\Gamma(\alpha) \Gamma(3 - \alpha)}{2}, & j = k. \end{cases}$$
(9.15)

Let  $u_k$  be the approximate solution of  $u(t_k)$   $(0 \le k \le N)$ , and denote

$$\mathcal{H}_{p}^{k} = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(p)} u_{j}, \quad p = 0, 1,$$
(9.16)

where the coefficients  $\gamma_{k,j}^{(p)}$  are presented in F.1. Then, we get the FAMMs for (9.9) have the following discrete form:

$$\frac{u_{k+1} - u_k}{h^{\alpha}} = \lambda \sum_{j=0}^p \beta_j^{(p)} u_{k+1-j} - \frac{1}{h^{\alpha}} \mathcal{H}_p^k, \quad p = 0, 1.$$
(9.17)

In order to lay the analytical basis for the convergence and linear stability analysis of the methods, we introduce several preparatory results through a series of lemmas, with their corresponding proofs given in F.2.

**Lemma 9.2.1.** The coefficients  $\{\gamma_{k,j}^{(p)}\}$  in (9.16) have the following properties for  $0 \le j \le k$ ,  $0 \le k \le N$  and p = 0, 1:

• 
$$\gamma_{k,j}^{(0)} < 0 \ (0 \le j \le k - 1), \ 0 < \gamma_{k,k}^{(0)} \le C_1;$$
  
•  $\gamma_{k,j}^{(1)} < 0 \ (0 \le j \le k - 3), \ \left| \gamma_{k,j}^{(1)} \right| \le C_1 \ (j = k - 2, \ k - 1 \ or \ k);$   
•  $\sum_{j=0}^k \gamma_{k,j}^{(0)} = 0, \ \sum_{j=0}^k \gamma_{k,j}^{(1)} = 0,$ 

where  $C_1 > 0$  is a constant.

**Lemma 9.2.2.** Let  $u(t) = t^{\sigma}$  ( $\sigma \ge 0$ ). Then there exists a constant  $C_2 > 0$  independent of h such that

$$\left| t_k I_t^{\alpha} u(t) \right|_{t=t_{k+1}} - h^{\alpha} \sum_{j=0}^p \beta_j^{(p)} u(t_{k+1-j}) \right| \le C_2 h^{\alpha+p+1} t_{k+1}^{\sigma-p-1}.$$
**Lemma 9.2.3.** Let  $u(t) = t^{\sigma}$  ( $\sigma \ge 0$ ). Then there exists a constant  $C_3 > 0$  independent of h such that

$$\left|\mathcal{H}^{k}(t_{k+1}) - \mathcal{H}^{k}_{p}(t_{k+1})\right| \leq C_{3} \left(h^{\sigma+\alpha+1}t_{k+1}^{-\alpha-1} + h^{\alpha+p+1}t_{k+1}^{\sigma-\alpha-p-1} + h^{p+1}\right).$$

## 9.2.3 Correction terms

It is well-known that the solutions of (9.5) usually exhibit weak singularity at the initial time and it can be written as the summation of regular and singular parts (see e.g. [94, Theorem 2.1]):

$$u(t) = \psi(t) + \sum_{\nu=1}^{\hat{\nu}} \hat{c}_{\nu} t^{\nu \alpha} + \sum_{\nu=1}^{\tilde{\nu}} \tilde{c}_{\nu} t^{1+\nu \alpha}, \qquad (9.18)$$

where  $\hat{v} = \lceil 2/\alpha \rceil - 1$ ,  $\tilde{v} = \lceil 1/\alpha \rceil - 1$ ,  $\psi \in C^2[0, T]$ ,  $\hat{c}_1, \hat{c}_2, \dots, \hat{c}_{\hat{v}} \in \mathbb{R}$  and  $\tilde{c}_1, \tilde{c}_2, \dots, \tilde{c}_{\tilde{v}} \in \mathbb{R}$ . Hence, the optimal convergence rates of the above discussed numerical methods cannot be achieved (see Lemma 9.2.2 and 9.2.3). To improve the accuracy near the initial time, we follow Lubich's idea (cf. [86]) by adding correction terms to the resulting fractional operators of (9.9). From (9.18), we assume that the solution u(t) of (9.5) has the form (*see e.g. [87, 94, 113] for more discussions on the regularity of FDEs*):

$$u(t) - u(0) = \sum_{r=1}^{m+1} d_r t^{\sigma_r} + \zeta(t) t^{\sigma_{m+2}}, \quad 0 < \sigma_r < \sigma_{r+1},$$
(9.19)

where  $d_1, d_2, \ldots, d_{m+1} \in \mathbb{R}$  are some constants, *m* is a positive integer and  $\zeta(t)$  is a uniformly continuous function for  $t \in [0, T]$ . The term  $\{\sigma_r\}$  represents positive correction powers which is usually uniquely determined by the considered equation. We will now introduce the correction approach for each term of the right-hand-side of (9.9).

I) We start with the term  $_{t_k} I_t^{\alpha} u(t) \Big|_{t=t_{k+1}}$ . It follows from Lemma 9.2.2 that

$$\begin{split} t_{k} I_{t}^{\alpha} u(t) \Big|_{t=t_{k+1}} &= t_{k} I_{t}^{\alpha} \left( u(t) - u(0) \right) \Big|_{t=t_{k+1}} + t_{k} I_{t}^{\alpha} u(0) \Big|_{t=t_{k+1}} \\ &= h^{\alpha} \sum_{j=0}^{p} \beta_{j}^{(p)} \left( u(t_{k+1-j}) - u_{0} \right) \\ &+ h^{\alpha} \sum_{j=1}^{mu} W_{k,j}^{(\alpha,\sigma,p)} \left( u(t_{j}) - u_{0} \right) + \frac{h^{\alpha}}{\Gamma(\alpha+1)} u_{0} + R_{k+1}^{u} \\ &= h^{\alpha} \sum_{j=0}^{p} \beta_{j}^{(p)} u(t_{k+1-j}) + h^{\alpha} \sum_{j=1}^{mu} W_{k,j}^{(\alpha,\sigma,p)} \left( u(t_{j}) - u_{0} \right) + R_{k+1}^{u} \\ &:= h^{\alpha} I_{mu}^{\alpha,\sigma,p} u(t_{k+1}) + R_{k+1}^{u}, \end{split}$$
(9.20)

with  $R_{k+1}^u = O(h^{\alpha+p+1}t_{k+1}^{\sigma_{m_u+1}-p-1})$ . The correction weights  $\{W_{k,j}^{(\alpha,\sigma,p)}\}$  are chosen such that (9.20) is exact for  $u(t) = t^{\sigma_r}$   $(1 \le r \le m_u)$ , and therefore are obtained through the following linear system of order  $m_u \times m_u$  to be solved for k = 0, 1, ..., N - 1 time steps:

$$\sum_{j=1}^{m_u} W_{0,j}^{(\alpha,\sigma,p)} j^{\sigma_r} = \frac{\Gamma(\sigma_r+1)}{\Gamma(\sigma_r+\alpha+1)} - \sum_{j=0}^{p} \beta_j^{(p)} (1-j)^{\sigma_r}, \quad 1 \le r \le m_u,$$
(9.21)

$$\sum_{j=1}^{m_{u}} W_{k,j}^{(\alpha,\sigma,p)} j^{\sigma_{r}} = \frac{k^{\sigma_{r}}}{\Gamma(\alpha+1)} {}_{2}F_{1}\left(-\sigma_{r}, 1; \alpha+1; -\frac{1}{k}\right) - \sum_{j=0}^{p} \beta_{j}^{(p)} (k+1-j)^{\sigma_{r}},$$

$$1 \le k \le N-1, \quad 1 \le r \le m_{u}.$$
(9.22)

II) For the history load  $\mathcal{H}^k(t_{k+1})$ , we introduce the correction terms as follows. Substituting (9.19) into (9.10) and using Lemma 9.2.3 yield

$$\mathcal{H}^{k}(t_{k+1}) = \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \int_{0}^{t_{k}} \frac{[u(s)-u(0)]'}{(v-s)^{\alpha}} ds dv + \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \int_{0}^{t_{k}} \frac{u'(0)}{(v-s)^{\alpha}} ds dv = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(p)} u(t_{j}) + \sum_{j=1}^{\tilde{m}u} \tilde{W}_{k,j}^{(\alpha,\sigma,p)} \left(u(t_{j})-u_{0}\right) + \tilde{R}_{k+1}^{u} := \mathcal{H}_{\tilde{m}u}^{\alpha,\sigma,p} u(t_{k+1}) + \tilde{R}_{k+1}^{u},$$
(9.23)

with  $\tilde{R}_{k+1}^{u} = O(h^{\sigma_{\tilde{m}u+1}+\alpha+1}t_{k+1}^{-\alpha-1}) + O(h^{\alpha+p+1}t_{k+1}^{\sigma_{\tilde{m}u+1}-\alpha-p-1}) + O(h^{p+1})$ . The history load correction weights  $\{\tilde{W}_{k,j}^{(\alpha,\sigma,p)}\}$  are chosen such that (9.23) is exact for  $u(t) = t^{\sigma_{r}}$   $(1 \le r \le m_{\tilde{u}})$ . However, we remark that it is very difficult to obtain the analytical solution of  $\mathcal{H}^{k}(t_{k+1})$ , given  $u(t) = t^{\sigma_{r}}$ . Fortunately, we know from [328] that (9.9) is also equivalent to

$$u(t_{k+1}) = u(t_k) + \frac{\lambda}{\Gamma(\alpha)} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} u(v) dv + \frac{\lambda}{\Gamma(\alpha)} \int_0^{t_k} \left[ (t_{k+1} - v)^{\alpha - 1} - (t_k - v)^{\alpha - 1} \right] u(v) dv.$$
(9.24)

Comparing (9.9) with (9.24) and using (9.5), we can obtain

$$\mathcal{H}^{k}(t_{k+1}) = -\frac{\lambda}{\Gamma(\alpha)} \int_{0}^{t_{k}} \left[ (t_{k+1} - v)^{\alpha - 1} - (t_{k} - v)^{\alpha - 1} \right] u(v) dv$$
$$= -\frac{1}{\Gamma(\alpha)} \int_{0}^{t_{k}} \left[ (t_{k+1} - v)^{\alpha - 1} - (t_{k} - v)^{\alpha - 1} \right]_{0}^{C} D_{t}^{\alpha} u(v) dv.$$
(9.25)

Therefore, we have the following linear system of size  $\tilde{m}_u \times \tilde{m}_u$  to be solved for k = 1, 2, ..., N - 1 time steps:

$$\sum_{j=1}^{\tilde{m}_{\mathcal{U}}} \tilde{W}_{k,j}^{(\alpha,\sigma,p)} j^{\sigma_{r}} = k^{\sigma_{r}} - \frac{\Gamma(\sigma_{r}+1)}{\Gamma(\alpha)\Gamma(\sigma_{r}-\alpha+1)} (k+1)^{\sigma_{r}} B\left(\frac{k}{k+1}; \sigma_{r}-\alpha+1, \alpha\right) - \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(p)} j^{\sigma_{r}}, \quad 1 \le k \le N-1, \quad 1 \le r \le \tilde{m}_{\mathcal{U}}, \tag{9.26}$$

where B(z; a, b) denotes the incomplete beta function, which is defined by

$$B(z; a, b) = \int_0^z v^{a-1} (1-v)^{b-1} dv.$$

Substituting (9.20) and (9.23) into (9.9) yields

$$u(t_{k+1}) = u(t_k) + \lambda h^{\alpha} I_{m_u}^{\alpha,\sigma,p} u(t_{k+1}) - \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u(t_{k+1}) + R_{k+1}^u + \tilde{R}_{k+1}^u, \quad p = 0, 1.$$
(9.27)

Dropping the truncation errors  $R_{k+1}^u$  and  $\tilde{R}_{k+1}^u$  in (9.27) and replacing  $u(t_k)$  with approximate solution  $u_k$ , we obtain the following FAMMs with correction terms for solving (9.5):

$$\frac{u_{k+1} - u_k}{h^{\alpha}} = \lambda I_{m_u}^{\alpha,\sigma,p} u_{k+1} - \frac{1}{h^{\alpha}} \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u_{k+1}, \quad p = 0, 1,$$
(9.28)

with  $I_{m_u}^{\alpha,\sigma,p}u_{k+1}$  and  $\mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p}u_{k+1}$  given, respectively, by:

$$I_{m_{u}}^{\alpha,\sigma,p}u_{k+1} = \sum_{j=0}^{p} \beta_{j}^{(p)}u_{k+1-j} + \sum_{j=1}^{m_{u}} W_{k,j}^{(\alpha,\sigma,p)}\left(u_{j} - u_{0}\right),$$
(9.29)

and

$$\mathcal{H}_{\tilde{m}_{u}}^{\alpha,\sigma,p}u_{k+1} = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(p)}u_{j} + \sum_{j=1}^{\tilde{m}_{u}} \tilde{W}_{k,j}^{(\alpha,\sigma,p)}\left(u_{j} - u_{0}\right).$$
(9.30)

## 9.2.4 Nonlinear FDEs

Having defined the discretization and corrections for the linear case, we now consider the numerical solutions of the following nonlinear FDE:

$${}_{0}^{C}D_{t}^{\alpha}u(t) = \lambda u(t) + f(t,u), \ \alpha \in (0,1], \ t \in (0,T]; \ u(0) = u_{0},$$
(9.31)

where the nonlinear function  $f : (0, T] \times \mathbb{R}^d \to \mathbb{R}^d$  satisfies the Lipschitz condition with constant L > 0:

$$\|f(t,u) - f(t,\hat{u})\|_{\infty} \le L \, \|u - \hat{u}\|_{\infty}, \quad t \in (0,T], \ u, \hat{u} \in \mathbb{R}^d,$$
(9.32)

where  $\|\cdot\|_{\infty}$  denotes the usual maximum norm on  $\mathbb{R}^d$ . Under these assumptions, it has been proved by Diethelm and Ford [108, Theorem 2.1 and 2.2] that problem (9.31) has a unique solution on the interval (0, *T*].

By the same token, we adopt the FAMMs developed in [112] to solve (9.31), and in a similar fashion as Section 9.2.2, but with the addition of the nonlinear term f(t, u), we have:

$$u(t_{k+1}) - u(t_k) = \left[ \lambda_{t_k} I_t^{\alpha} u(t) + {}_{t_k} I_t^{\alpha} f(t, u) - \mathcal{H}^k(t) \right] \Big|_{t=t_{k+1}}.$$
(9.33)

Therefore, the FAMMs for (9.33) is given by:

$$\frac{u_{k+1} - u_k}{h^{\alpha}} = \sum_{j=0}^p \beta_j^{(p)} \left( \lambda u_{k+1-j} + f_{k+1-j} \right) - \frac{1}{h^{\alpha}} \mathcal{H}_p^k, \quad p = 0, 1,$$
(9.34)

where  $f_{k+1-j} = f(t_{k+1-j}, u_{k+1-j})$ .

# **9.2.4.1** Corrections terms for f(t, u)

The regularity of f(t, u) is related to the regularity of u(t). If u(t) satisfies (9.19), we know from (9.31) that

$$f(t, u) - f(0, u(0)) = -\lambda \sum_{r=1}^{m+1} d_r t^{\sigma_r} + \sum_{r=1}^{m+1} d_r \frac{\Gamma(\sigma_r + 1)}{\Gamma(\sigma_r - \alpha + 1)} t^{\sigma_r - \alpha} + \dots$$
$$:= \sum_{r=1}^{l+1} h_r t^{\delta_r} + \hat{\zeta}(t) t^{\delta_l + 2}, \quad \delta_r < \delta_{r+1}, \tag{9.35}$$

where  $\hat{\zeta}(t)$  is a uniformly continuous function for  $t \in [0, T]$  and  $\delta_r \in {\sigma_l} \cup {\sigma_l - \alpha}$ . Similar to (9.20) and by using Lemma 9.2.2, we have

$$t_{k} I_{t}^{\alpha} f(t, u) \Big|_{t=t_{k+1}} = h^{\alpha} \sum_{j=0}^{p} \beta_{j}^{(p)} f(t_{k+1-j}, u(t_{k+1-j}))$$

$$+ h^{\alpha} \sum_{j=1}^{m_{f}} W_{k,j}^{(\alpha,\delta,p)} \left( f(t_{j}, u(t_{j})) - f(0, u_{0}) \right) + R_{k+1}^{f}$$

$$:= h^{\alpha} I_{m_{f}}^{\alpha,\delta,p} f(t_{k+1}, u(t_{k+1})) + R_{k+1}^{f},$$

$$(9.36)$$

where  $R_{k+1}^f = O(h^{\alpha+p+1}t_{k+1}^{\delta_m f+1-p-1})$ , and  $\{W_{k,j}^{(\alpha,\delta,p)}\}$  with k = 0, 1, ..., N-1 and  $j = 1, 2, ..., m_f$  are given by:

$$\sum_{j=1}^{m_f} W_{0,j}^{(\alpha,\delta,p)} j^{\delta r} = \frac{\Gamma(\delta_r + 1)}{\Gamma(\delta_r + \alpha + 1)} - \sum_{j=0}^{p} \beta_j^{(p)} (1-j)^{\delta r}, \quad 1 \le r \le m_f,$$
(9.37)

$$\sum_{j=1}^{m_{f}} W_{k,j}^{(\alpha,\delta,p)} j^{\delta_{r}} = \frac{k^{\delta_{r}}}{\Gamma(\alpha+1)} {}_{2}F_{1}\left(-\delta_{r}, 1; \alpha+1; -\frac{1}{k}\right) - \sum_{j=0}^{p} \beta_{j}^{(p)} (k+1-j)^{\delta_{r}},$$

$$1 \le k \le N-1, \quad 1 \le r \le m_{f}.$$
(9.38)

Inserting (9.20), (9.23) and (9.36) into (9.33) yields

$$u(t_{k+1}) = u(t_k) + \lambda h^{\alpha} I_{m_u}^{\alpha,\sigma,p} u(t_{k+1}) + h^{\alpha} I_{m_f}^{\alpha,\delta,p} f(t_{k+1}, u(t_{k+1})) - \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u(t_{k+1}) + R_{k+1}^u + R_{k+1}^f + \tilde{R}_{k+1}^u, \quad p = 0, 1.$$
(9.39)

Therefore, we obtain the following FAMMs with correction terms for solving (9.31):

$$\frac{u_{k+1} - u_k}{h^{\alpha}} = \lambda I_{m_u}^{\alpha,\sigma,p} u_{k+1} + I_{m_f}^{\alpha,\delta,p} f_{k+1} - \frac{1}{h^{\alpha}} \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u_{k+1}, \quad p = 0, 1,$$
(9.40)

with  $I_{m_u}^{\alpha,\sigma,p}u_{k+1}$ ,  $\mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p}u_{k+1}$  and  $I_{m_f}^{\alpha,\delta,p}f_{k+1}$  given, respectively, by (9.29), (9.30) and

$$I_{m_f}^{\alpha,\delta,p} f_{k+1} = \sum_{j=0}^{p} \beta_j^{(p)} f_{k+1-j} + \sum_{j=1}^{m_f} W_{k,j}^{(\alpha,\delta,p)} \left( f_j - f_0 \right).$$
(9.41)

In order to obtain the IMEX methods, we follow the idea from Cao et al. [113], and employ an extrapolation to linearize the nonlinear force term  $f(t_{k+1}, u(t_{k+1}))$  in (9.39), which is given by:

$$f(t_{k+1}, u(t_{k+1})) = E_k^p f(t_k, u(t_k)) + \sum_{j=1}^{m_f} W_{k,j}^{(\delta,p)}(f(t_j, u(t_j)) - f(0, u_0)) + \tilde{R}_{k+1}^f,$$
(9.42)

where

$$E_k^p f(t_k, u(t_k)) = \begin{cases} f(t_k, u(t_k)), & p = 0, \\ 2f(t_k, u(t_k)) - f(t_{k-1}, u(t_{k-1})), & p = 1, \end{cases}$$
(9.43)

and  $\tilde{R}_{k}^{f} = O(h^{p+1}t_{k+1}^{\delta \tilde{m}_{f}+1-p-1})$ . In addition, the  $\tilde{m}_{f} \times \tilde{m}_{f}$  linear system for correction weights is given by:

$$\sum_{j=1}^{\tilde{m}_{f}} W_{k,j}^{(\delta,0)} j^{\delta r} = (k+1)^{\delta r} - k^{\delta r}, \quad 1 \le r \le \tilde{m}_{f},$$
(9.44)

$$\sum_{j=1}^{\tilde{m}_f} W_{k,j}^{(\delta,1)} j^{\delta r} = (k+1)^{\delta r} - 2k^{\delta r} + (k-1)^{\delta r}, \quad 1 \le r \le \tilde{m}_f.$$
(9.45)

Inserting (9.42) into (9.39) yields

$$u(t_{k+1}) = u(t_k) + \lambda h^{\alpha} I_{m_u}^{\alpha,\sigma,p} u(t_{k+1}) + h^{\alpha} I_{m_f}^{\alpha,\delta,p} f(t_{k+1}, u(t_{k+1})) + h^{\alpha} \beta_0^{(p)} \Biggl[ -f(t_{k+1}, u(t_{k+1})) + E_k^p f(t_k, u(t_k)) + \sum_{j=1}^{\tilde{m}_f} W_{k,j}^{(\delta,p)}(f(t_j, u(t_j)) - f(0, u_0)) \Biggr] - \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u(t_{k+1}) + R_{k+1}^u + R_{k+1}^f + \tilde{R}_{k+1}^u + h^{\alpha} \beta_0^{(p)} \tilde{R}_{k+1}^f, \quad p = 0, 1.$$
(9.46)

Finally, we obtain the IMEX(p) methods in the following form:

$$\frac{u_{k+1} - u_k}{h^{\alpha}} = \lambda I_{m_u}^{\alpha,\sigma,p} u_{k+1} + I_{m_f}^{\alpha,\delta,p} f_{k+1} + \beta_0^{(p)} \left[ -f_{k+1} + E_k^p f_k + \sum_{j=1}^{\tilde{m}_f} W_{k,j}^{(\delta,p)}(f_j - f_0) \right] - \frac{1}{h^{\alpha}} \mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p} u_{k+1}, \quad p = 0, 1,$$
(9.47)

with  $I_{m_u}^{\alpha,\sigma,p}u_{k+1}$ ,  $\mathcal{H}_{\tilde{m}_u}^{\alpha,\sigma,p}u_{k+1}$ ,  $I_{m_f}^{\alpha,\delta,p}f_{k+1}$  and  $E_k^p f_k$  given, respectively, by (9.29), (9.30), (9.41) and

$$E_k^p f_k = \begin{cases} f_k, & p = 0, \\ 2f_k - f_{k-1}, & p = 1. \end{cases}$$
(9.48)

**Remark 9.2.4.** If  $\alpha = 1$ , the history load term for (9.31) is zero and we don't need to add the correction terms to solve (9.31). Moreover, (9.47) recovers the standard IMEX methods.

In the following, we will present the convergence results for the IMEX(p) methods (9.47). For this purpose, we first introduce some preparatory results. Both of the proofs will be given in F.2.

**Lemma 9.2.5.** The correction weights  $W_{k,j}^{(\alpha,\sigma,p)}$ ,  $\tilde{W}_{k,j}^{(\alpha,\sigma,p)}$ ,  $W_{k,j}^{(\alpha,\delta,p)}$  and  $W_{k,j}^{(\delta,p)}$  in (9.20), (9.23), (9.36) and (9.42), respectively, satisfy

$$\begin{split} \left| W_{k,j}^{(\alpha,\sigma,p)} \right| &= O((k+1)^{\sigma_{m_u}-p-1}), \quad \left| W_{k,j}^{(\alpha,\delta,p)} \right| = O((k+1)^{\delta_m f^{-p-1}}), \\ \left| \tilde{W}_{k,j}^{(\alpha,\sigma,p)} \right| &= O((k+1)^{-\alpha-1}) + O((k+1)^{\sigma_{\tilde{m}u}-p-1}), \quad \left| W_{k,j}^{(\delta,p)} \right| = O((k+1)^{\delta_{\tilde{m}f}-p-1}). \end{split}$$

**Theorem 9.2.6.** Suppose that the Lipschitz condition (9.32) holds.

If  $\sigma_{\tilde{m}_u} \leq p+1$ ,  $\sigma_{m_u}, \delta_{m_f}, \delta_{\tilde{m}_f} \leq p+\alpha+1$ , then, for the IMEX(p) methods (9.47), there exists a constant  $C_4 > 0$  independent of h such that

$$\max_{0 \le k \le N} \|u(t_k) - u_k\|_{\infty} \le C_4 \left( \sum_{j=1}^M \|u(t_j) - u_j\|_{\infty} + h^q \right), \tag{9.49}$$

where  $M = \max \left\{ m_u, m_f, \tilde{m}_u, \tilde{m}_f \right\}$  and

$$q = \min\left\{p+1, \sigma_{\tilde{m}u+1}+p, \sigma_{mu+1}+\alpha+p, \delta_{m_f+1}+\alpha+p, \delta_{\tilde{m}_f+1}+\alpha+p\right\}.$$

# **9.3** Linear Stability of IMEX(*p*) Methods

In this section, we investigate the linear stability of the proposed IMEX(p) methods (9.47) by considering the following usual scalar test equation

$${}_{0}^{C}D_{t}^{\alpha}u(t) = \lambda u(t) + \rho u(t), \ \alpha \in (0,1], \ t \ge 0, \ \lambda, \rho \in \mathbb{C}; \ u(0) = u_{0}.$$
(9.50)

For this, the following result from [329] is useful to determine the stability regions of the obtained numerical schemes.

**Lemma 9.3.1.** (cf. [329]) Assume that the sequence  $\{g_k\}$  is convergent and that the quadrature weights  $w_k (k \ge 1)$  satisfy

$$w_k = \frac{k^{\alpha-1}}{\Gamma(\alpha+1)} + v_k$$
, where  $\sum_{k=1}^{\infty} |v_k| < \infty$ ,

then the stability region of the convolution quadrature  $u_k = g_k + \hat{h} \sum_{j=0}^k w_{k-j} u_j$  is

$$S = \left\{ \hat{h} \in \mathbb{C} : 1 - \hat{h} w^{\alpha}(\xi) \neq 0, \ |\xi| \le 1 \right\}, \text{ where } w^{\alpha}(\xi) = \sum_{j=0}^{\infty} w_j \xi^j,$$

where  $\hat{h} = h^{\alpha}(\lambda + \rho)$  or  $\hat{h}$  is some function of  $h^{\alpha}(\lambda + \rho)$ .

We first consider the linear stability of the IMEX(0) for the test equation (9.50), it holds that

$$u_{k+1} = u_k + \frac{\lambda h^{\alpha}}{\Gamma(\alpha+1)} u_{k+1} + h^{\alpha} \left( \lambda \sum_{j=1}^{m_u} W_{k,j}^{(\alpha,\sigma,0)} + \rho \sum_{j=1}^{m_f} W_{k,j}^{(\alpha,\delta,0)} \right) (u_j - u_0) + \frac{\rho h^{\alpha}}{\Gamma(\alpha+1)} \left[ u_k + \sum_{j=1}^{\tilde{m}_f} W_{k,j}^{(\delta,0)} (u_j - u_0) \right] - \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(0)} u_j - \sum_{j=1}^{\tilde{m}_u} \tilde{W}_{k,j}^{(\alpha,\sigma,0)} (u_j - u_0) = u_k + \frac{h^{\alpha}}{\Gamma(\alpha+1)} (\lambda u_{k+1} + \rho u_k) - \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(0)} u_j + \sum_{j=1}^{M} W_{k,j} (u_j - u_0),$$
(9.51)

where

$$\begin{split} \sum_{j=1}^{M} W_{k,j}(u_j - u_0) = \lambda h^{\alpha} \sum_{j=1}^{m_u} W_{k,j}^{(\alpha,\sigma,0)}(u_j - u_0) + \rho h^{\alpha} \sum_{j=1}^{m_f} W_{k,j}^{(\alpha,\delta,0)}(u_j - u_0) \\ &+ \frac{\rho h^{\alpha}}{\Gamma(\alpha+1)} \sum_{j=1}^{\tilde{m}_f} W_{k,j}^{(\delta,0)}(u_j - u_0) - \sum_{j=1}^{\tilde{m}_u} \tilde{W}_{k,j}^{(\alpha,\sigma,0)}(u_j - u_0). \end{split}$$

Since  $\sum_{j=1}^{M} W_{k,j}(u_j - u_0)$  does not affect the stability analysis, so we don't give the exact expression of  $W_{k,j}$ . Denote  $U(\xi) = \sum_{k=0}^{\infty} u_k \xi^k$ ,  $|\xi| \le 1$ . Then it follows from (9.51) that

$$\begin{split} \sum_{k=0}^{\infty} u_{k+1} \xi^k &= \sum_{k=0}^{\infty} u_k \xi^k + \frac{\lambda h^{\alpha}}{\Gamma(\alpha+1)} \sum_{k=0}^{\infty} u_{k+1} \xi^k + \frac{\rho h^{\alpha}}{\Gamma(\alpha+1)} \sum_{k=0}^{\infty} u_k \xi^k \\ &- \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{k=0}^{\infty} \left( \sum_{j=0}^k \gamma_{k,j}^{(0)} u_j \right) \xi^k + \sum_{k=0}^{\infty} \sum_{j=1}^M W_{k,j} (u_j - u_0) \xi^k, \end{split}$$

which leads to

$$\frac{1}{\xi}(U(\xi) - u_0) = U(\xi) + \frac{\lambda h^{\alpha}}{\Gamma(\alpha + 1)\xi} (U(\xi) - u_0) + \frac{\rho h^{\alpha}}{\Gamma(\alpha + 1)} U(\xi) - \frac{1}{\Gamma(\alpha)\Gamma(2 - \alpha)} \gamma_k^{(0)}(\xi) U(\xi) + \sum_{k=1}^{\infty} \sum_{j=1}^{M} W_{k,j}(u_j - u_0)\xi^k,$$
(9.52)

where  $\gamma_k^{(0)}(\xi) = \sum_{j=0}^{\infty} \gamma_{k,j}^{(0)} \xi^j$ . We simplify (9.52) as

$$\left[1-\xi-\frac{\lambda h^{\alpha}}{\Gamma(\alpha+1)}-\frac{\rho h^{\alpha}}{\Gamma(\alpha+1)}\xi+\frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)}\gamma_{k}^{(0)}(\xi)\xi\right]U(\xi)=H(\xi),$$

where

$$H(\xi) = \sum_{k=0}^{\infty} H_k \xi^k = \left[ 1 - \frac{\lambda h^{\alpha}}{\Gamma(\alpha+1)} \right] u_0 + \sum_{k=1}^{\infty} \sum_{j=1}^m W_{k,j} (u_j - u_0) \xi^{k+1}.$$

By using Lemma 9.2.5, when

$$\sigma_{m_u}, \delta_{m_f}, \delta_{\tilde{m}_f} < 1, \quad \sigma_{\tilde{m}_u} < \alpha + 1,$$

we can obtain that  $\{H_k\}$  is a convergent sequence. Moreover, we know from Lemma 9.2.1 that  $\sum_{j=0}^{\infty} |\gamma_{k,j}^{(0)}| < \infty$ . Then it follows from Lemma 9.3.1 that method IMEX(0) is stable if

$$1 - \xi - \frac{\lambda h^{\alpha}}{\Gamma(\alpha+1)} - \frac{\rho h^{\alpha}}{\Gamma(\alpha+1)} \xi + \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \gamma_k^{(0)}(\xi) \xi \neq 0, \quad \forall |\xi| \le 1.$$

Similarly, we can obtain the stability region of the method IMEX(1). Then we have the following theorem.

**Theorem 9.3.2.** Let  $\rho = \kappa \lambda$  and  $\hat{h} = \lambda h^{\alpha}$ . Then for  $\sigma_{m_u}, \delta_{m_f}, \delta_{\tilde{m}_f} , <math>\sigma_{\tilde{m}_u} < \alpha + p + 1$ , we have the stability region of IMEX(0):

$$S_0 = \mathbb{C} \setminus \left\{ \hat{h} : \hat{h} = \frac{\Gamma(\alpha+1)}{1+\kappa\xi} \left( 1 - \xi + \frac{\gamma_k^{(0)}(\xi)\xi}{\Gamma(\alpha)\Gamma(2-\alpha)} \right), \ |\xi| \le 1 \right\}.$$

and the stability region of IMEX(1):

$$S_1 = \mathbb{C} \setminus \left\{ \hat{h} : \hat{h} = \frac{\Gamma(\alpha+2)}{(1+\kappa)(\alpha\xi+1)-\kappa(\xi-1)^2} \left( 1 - \xi + \frac{\gamma_k^{(1)}(\xi)\xi}{\Gamma(\alpha)\Gamma(2-\alpha)} \right), \ |\xi| \le 1 \right\},$$

where  $\gamma_k^{(1)}(\xi) = \sum_{j=0}^{\infty} \gamma_{k,j}^{(1)} \xi^j$ .

In Figure 9.2 (a)-(c), we plot the stability regions of the method IMEX(0) with  $\alpha = 0.2, 0.5, 0.8$ and  $\rho = 0.5\lambda$ , respectively. We also plot the stability regions of the method IMEX(1) with  $\alpha = 0.2, 0.5, 0.8$  and  $\rho = 0.5\lambda$  in Figure 9.2 (d). As the functions  $\gamma_k^{(p)}(\xi) = \sum_{j=0}^{\infty} \gamma_{k,j}^{(p)} \xi^j$  is not explicitly known, so in all these figures we take  $k = 10^5$ .

# **9.4** The Fast Implementation of IMEX(*p*) Methods

The step-by-step numerical solution of (9.47) for *N* time-steps requires  $O(N^2)$  evaluations of the time-dependent coefficients given by the hypergeometric functions, making the scheme expensive. Hence, we rewrite (9.47) as the matrices form, where the corresponding convolution matrices of coefficients have the Toeplitz structure and thus we leverage the use of FFTs to obtain the solution of the problem with complexity  $O(N \log N)$ . For simplicity and objectivity, we demonstrate the procedure only for the IMEX(0) scheme, for which we start by introducing the notations

$$U = (u_1, u_2, \dots, u_N)^T$$
,  $F(U) = (f_1, f_2, \dots, f_N)^T$ ,

where U denotes the unknown solution vector. Then IMEX(0) can be written in a compact form:

$$(A \otimes I_d - \lambda B \otimes I_d)U = h^{\alpha}(B \otimes I_d + C \otimes I_d)F(U) + D, \qquad (9.53)$$



Figure 9.2: (a) Stability region of IMEX(0) with  $\alpha = 0.2$  and  $\rho = 0.5\lambda$ ; (b) Stability region of IMEX(0) with  $\alpha = 0.5$  and  $\rho = 0.5\lambda$ ; (c) Stability region of IMEX(0) with  $\alpha = 0.8$  and  $\rho = 0.5\lambda$ ; (d) Stability region of the IMEX(1) with different  $\alpha$  and  $\rho = 0.5\lambda$ .

where  $\otimes$  denotes the Kronecker product and  $I_d$  represents the  $d \times d$  identity matrix. Here the value of *d* can represents, for instance, the number of equations for a system of nonlinear FDEs.

Furthermore, we have:

$$A = \begin{bmatrix} 1 & & & \\ -1 + \frac{\gamma_{1,1}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & 1 & & \\ \frac{\gamma_{2,1}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & -1 + \frac{\gamma_{2,2}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & 1 & \\ \vdots & \vdots & \ddots & \ddots & \\ \frac{\gamma_{N-1,1}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & \frac{\gamma_{N-1,2}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & \cdots & -1 + \frac{\gamma_{N-1,N-1}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)} & 1 \end{bmatrix} \in \mathbb{R}^{N \times N}, \quad (9.54)$$

$$B = \frac{1}{\Gamma(\alpha+1)}I_N, \quad C = \frac{1}{\Gamma(\alpha+1)} \begin{bmatrix} -1 & & \\ 1 & -1 & & \\ 0 & 1 & -1 & \\ \vdots & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -1 \end{bmatrix} \in \mathbb{R}^{N \times N}, \quad (9.55)$$

and *D* is a vector related to the corrections and solutions for the initial steps, in the following way:

$$D = \lambda h^{\alpha} (W_{m_{u}} \otimes I_{d}) U_{m_{u}} + h^{\alpha} (W_{m_{f}} \otimes I_{d}) F(U_{m_{f}}) - (W_{\tilde{m}_{u}} \otimes I_{d}) U_{\tilde{m}_{u}}$$
  
+ 
$$\frac{h^{\alpha}}{\Gamma(\alpha+1)} (W_{\tilde{m}_{f}} \otimes I_{d}) F(U_{\tilde{m}_{f}}) + (a_{0} \otimes I_{d}) u_{0} + h^{\alpha} (b_{0} \otimes I_{d}) f_{0},$$
(9.56)

where the correction weights  $W_{\hat{M}}$  ( $\hat{M} = m_u, m_f, \tilde{m}_u, \tilde{m}_f$ ) are denoted by the  $N \times \hat{M}$  matrices with the element  $W_{k,j}^{(\alpha,\sigma,0)}, W_{k,j}^{(\alpha,\sigma,0)}, \tilde{W}_{k,j}^{(\alpha,\sigma,0)}$  and  $\tilde{W}_{k,j}^{(\delta,0)}$ , respectively, for k = 0, 1, ..., N - 1 and  $j = 1, 2, ..., \hat{M}$ . We also have,

$$a_{0} = \left(1, \frac{\gamma_{1,0}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)}, \frac{\gamma_{2,0}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)}, \dots, \frac{\gamma_{N-1,0}^{(0)}}{\Gamma(\alpha)\Gamma(2-\alpha)}\right)^{T} \in \mathbb{R}^{N},$$
  
$$b_{0} = \left(\frac{1}{\Gamma(\alpha+1)}, 0, \dots, 0\right)^{T} \in \mathbb{R}^{N}, \quad U_{\hat{M}} = \left(u_{1} - u_{0}, u_{2} - u_{0}, \dots, u_{\hat{M}} - u_{0}\right)^{T}.$$

From (9.13), we observe that  $\mathcal{A}_{k+1,j+1} = \mathcal{A}_{k,j}$ , and therefore A is a lower-triangular Toeplitz matrix.

In what follows, we will analyze the unique solvability of the IMEX(0) scheme. For this purpose, we introduce the mapping  $\Phi_h : \mathbb{R}^{Nd} \to \mathbb{R}^{Nd}$  as follows:

$$\Phi_h(X) := h^{\alpha} \left[ (A - \lambda B)^{-1} (B + C) \otimes I_d \right] F(X) + \left[ (A - \lambda B)^{-1} \otimes I_d \right] D,$$

and therefore, we have the following result.

Theorem 9.4.1. Suppose that Lipschitz condition (9.32) holds and

$$h^{\alpha}L\|(A - \lambda B)^{-1}(B + C)\|_{\infty} < 1.$$
(9.57)

Then the method IMEX(0) has a unique solution  $U \in \mathbb{R}^{Nd}$ .

*Proof.* Let  $X = (x_1^T, x_2^T, \dots, x_N^T)^T$ ,  $\hat{X} = (\hat{x}_1^T, \hat{x}_2^T, \dots, \hat{x}_N^T)^T$  be two arbitrary vectors in  $\mathbb{R}^{Nd}$ . It follows from the Lipschitz condition (9.32) that

$$\begin{split} \left\| \Phi_h(X) - \Phi_h(\hat{X}) \right\|_{\infty} &\leq h^{\alpha} \left\| (A - \lambda B)^{-1} (B + C) \right\|_{\infty} \left\| F(X) - F(\hat{X}) \right\|_{\infty} \\ &\leq h^{\alpha} L \left\| (A - \lambda B)^{-1} (B + C) \right\|_{\infty} \left\| X - \hat{X} \right\|_{\infty}. \end{split}$$

If condition (9.57) holds, we know that  $\Phi_h(X)$  is a contraction mapping with contraction factor  $h^{\alpha}L\|(A-\lambda B)^{-1}(B+C)\|_{\infty}$ . Moreover, it is well known that space  $\mathbb{R}^{Nd}$  with norm  $\|\cdot\|_{\infty}$  is complete. Hence, according to the Banach contraction mapping principle (see e.g. [330]), mapping  $\Phi_h(X)$  has a unique fixed point in  $\mathbb{R}^{Nd}$ . Namely, the method IMEX(0) has a unique solution  $U \in \mathbb{R}^{Nd}$ .

**Remark 9.4.2.** It should be pointed that, the coefficient matrices A for IMEX(1) is not the Toeplitz matrices, but we can choose the first column  $a_1$  of A as

$$\hat{a}_1 = \left(1, -1 + \frac{\gamma_{2,2}^{(1)}}{\Gamma(\alpha)\Gamma(2-\alpha)}, \frac{\gamma_{3,2}^{(1)}}{\Gamma(\alpha)\Gamma(2-\alpha)}, \dots, \frac{\gamma_{N,2}^{(1)}}{\Gamma(\alpha)\Gamma(2-\alpha)}\right)^T \in \mathbb{R}^N.$$

Then A will be a Toeplitz matrix. Moreover, if we do this, the corresponding vector D for IMEX(1) will be change by adding the term  $[(\hat{a}_1 - a_1) \otimes I_d] U$ .

## 9.4.1 Fast approximate inversion scheme

In order to obtain a fast solution to the Toeplitz system (9.53), we employ the scheme developed in [322], which approximates the lower-triangular Toeplitz matrix  $K^{-1}$ . In particular, we have  $K = (A \otimes I_d - \lambda B \otimes I_d)$  for the method IMEX(0) in (9.53). The first step involves approximating the matrix *K* by the following block  $\epsilon$ -circulant matrix:

$$K_{\epsilon} = \begin{bmatrix} K_{0} & \epsilon K_{N-1} & \dots & \epsilon K_{2} & \epsilon K_{1} \\ K_{1} & K_{0} & \epsilon K_{N-1} & \dots & \epsilon K_{2} \\ \vdots & K_{1} & K_{0} & \ddots & \vdots \\ K_{N-2} & \dots & \ddots & \ddots & \epsilon K_{N-1} \\ K_{N-1} & K_{N-2} & \dots & K_{1} & K_{0} \end{bmatrix},$$
(9.58)

with  $\epsilon > 0$ . It is reported by Lu *et al.* [322] that the accuracy of the fast inversion is  $O(\epsilon)$ , where mathematically  $\epsilon$  can be taken arbitrarily small. However, for double-precision arithmetic,  $\epsilon$  cannot be set too small due to rounding errors. Numerical experiments demonstrated the smallest practical value to be  $\epsilon = 5 \times 10^{-9}$ . It is also shown in [322] that  $K_{\epsilon}^{-1}$  is also a block  $\epsilon$ -circulant matrix, and therefore the solution to system (9.53) can be written in the following way:

$$U \approx K_{\epsilon}^{-1} R,$$

where R denote the right-hand side of (9.53).

Let  $D_{\varrho} = \text{diag}(1, \varrho, \dots, \varrho^{N-1})$ , with  $\varrho = \epsilon^{1/N}$  be a diagonal matrix and  $F_N$  be a  $N \times N$  Fourier matrix. We then have the following spectral decomposition:

$$K_{\epsilon}^{-1} = \left[ (D_{\varrho}^{-1} F_N^*) \otimes I_d \right] \operatorname{diag} \left( \Lambda_0^{-1}, \Lambda_1^{-1}, \dots, \Lambda_{N-1}^{-1} \right) \left[ (F_N D_{\varrho}) \otimes I_d \right],$$

with

$$\begin{bmatrix} \Lambda_{0} \\ \Lambda_{1} \\ \vdots \\ \Lambda_{N-1} \end{bmatrix} = \begin{bmatrix} (\sqrt{N}F_{N}D_{\varrho}) \otimes I_{d} \end{bmatrix} \begin{bmatrix} K_{0} \\ K_{1} \\ \vdots \\ K_{N-1} \end{bmatrix}.$$
(9.59)

Finally, the approximate solution for *U* becomes:

$$U \approx \left[ (D_{\varrho}^{-1} F_N^*) \otimes I_d \right] \operatorname{diag} \left( \Lambda_0^{-1}, \Lambda_1^{-1}, \dots, \Lambda_{N-1}^{-1} \right) \left[ (F_N D_{\varrho}) \otimes I_d \right] R, \tag{9.60}$$

where in practical implementations, we replace the Fourier matrices  $F_N$  in (9.59) and (9.60) with FFT operations in order to achieve a computational complexity of  $O(N \log N)$ . The other operations to form R do not require FFTs, since matrices B and C are sparse, lower-Toeplitz nature, and the vector D is formed through the multiplication of tall matrices with small vectors.

**Remark 9.4.3.** Note that (9.60) is a nonlinear system, therefore iterative solver should be applied to solve this problem. As is known, the Newton iteration method may be the most popular solver for a general system of nonlinear equations G(x) = 0. However, the disadvantages of the Newton iteration method is that, at each iteration step, it requires the explicit form of the  $N \times N$  Jacobian matrix  $G'(x^{(n)})$ , where  $x^{(n)}$  denotes the nth-approximation to x. So the computation of the Newton iteration method could be much more expensive. In order to overcome this disadvantage, Picard iteration method has been used to solve the system (9.60), where, for a given iteration n, we have:

$$U^{(n+1)} = K_{\epsilon}^{-1} R(U^{(n)}), \tag{9.61}$$

until  $||U^{(n+1)} - U^{(n)}|| > \epsilon^p$ , where  $U^{(n)}$  denotes the nth-approximation to U and  $\epsilon^p$  represents the tolerance of the Picard iteration scheme.

## 9.4.2 Fast computation of hypergeometric functions

Accurate and efficient computations of the Gauss hypergeometric function  ${}_{2}F_{1}(a, b; c; z)$  is also fundamental to the developed scheme. From [331], we know that there is no simple answer for this problem, and different methods are optimal for different parameter regimes. When  $\Re(c) > \Re(a) > 0$  or  $\Re(c) > \Re(b) > 0$ , the Gauss-Jacobi quadrature method is effective. As stated in [332], when  $|\arg(1-z)| < \pi$ , we have

$${}_{2}F_{1}(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_{0}^{1} (1-zt)^{-a} w_{b,c}(t)dt, \quad \Re(c) > \Re(b) > 0, \tag{9.62}$$

where  $w_{b,c}(t) = (1-t)^{c-b-1}t^{b-1}$ . The parameters *a* and *b* in (9.62) can be interchanged due to the basic power series definition of the hypergeometric function. Transforming  $t \rightarrow \frac{\tilde{t}+1}{2}$ , we can obtain that

$$\begin{split} \int_{0}^{1} (1-zt)^{-a} w_{b,c}(t) d\tilde{t} &= \frac{1}{2^{c-1}} \int_{-1}^{1} \left( 1 - \frac{1}{2}z - \frac{1}{2}z\tilde{t} \right)^{-a} (1-\tilde{t})^{c-b-1} (1+\tilde{t})^{b-1} dt \\ &= \sum_{j=1}^{Q} w_{j}^{GJ} \left( 1 - \frac{1}{2}z - \frac{1}{2}zt_{j}^{GJ} \right)^{-a} + E_{Q}(a,b,z), \end{split}$$

where  $t_j^{GJ}$  and  $w_j^{GJ}$  are the Gauss-Jacobi nodes and weights on [-1, 1], and Q is the number of mesh points. Error bounds for this method are discussed in [333].

# **9.4.3** Algorithm of IMEX(*p*) methods

We present the main stages of the developed fast IMEX(p) methods for efficient time-integration of nonlinear FDEs in Algorithm 9.1. The algorithm particularly described the IMEX(0) approach, but the main steps remain the same for IMEX(1), with slight modifications regarding the number of sets of correction weights and forms for the nonlinear system matrices. The operators  $\mathcal{F}(\cdot)$  and  $\mathcal{F}^{-1}(\cdot)$  represent, respectively, the forward and inverse Fast Fourier Transforms.

**Remark 9.4.4.** For the FAMMs (9.17), (9.34) and the FAMMs with correction terms (9.28), (9.40), we also can use the fast implementation proposed in this section to construct the corresponding fast methods.

# 9.5 Numerical Tests

We present several numerical examples to verify our theoretical analysis presented in the previous sections. In all presented numerical examples, we utilize a numerical tolerance  $\epsilon = 5 \times 10^{-9}$  for the fast inversion step. For all hypergeometric functions involved in the evaluation of correction weights and history load term, we utilize Q = 200 Gauss-Jacobi quadrature points. One exception is the incomplete beta function evaluated for the history load correction in (9.26). For this case, the argument  $\frac{k}{k+1}$  approaches 1 as N increases, and a numerical quadrature becomes a poor choice due

Algorithm 9.1: Fast IMEX(0) Integration Scheme for Nonlinear FDEs.

- 1: Known database:
- 2: Initial parameters  $h, N, \epsilon, \epsilon^p, \lambda$ , number of correction terms and powers  $\sigma, \delta$ .
- 3: Compute the first column  $a_1$  of A defined in (9.54). Compute B and C defined in (9.55) with sparse allocation.
- 4: Compute corrections using (9.21)-(9.22), (9.26), (9.37)-(9.38) and (9.44) (or (9.45)) for all *N* time-steps.
- 5: Compute  $D_{\rho}$ . Assemble the first column  $K_{\epsilon,1}$  of  $K_{\epsilon}$  in (9.58).
- 6: Compute  $\Lambda = \mathcal{F}((D_{\varrho} \otimes I_d)K_{\epsilon,1})$  to obtain (9.59).
- 7: **Picard Iteration:** Initial guess  $U^{(0)}$ .
- 8: while  $e > \epsilon^p$  do
- 9: Compute  $D(U^{(n)})$  using (9.56). Compute  $F(U^{(n)})$ .
- 10: Compute  $R(U^{(n)})$  using (9.53)

11: Compute 
$$r_{\epsilon} = \mathcal{F}\left( (D_{\varrho} \otimes I_d) R(U^{(n)}) \right)$$

- 12: Solve  $\tilde{r}_{\epsilon} = \Lambda^{-1} r_{\epsilon}$
- 13: Compute the updated solution vector  $U^{(n+1)} = D_0^{-1} \mathcal{F}^{-1}(\tilde{r}_{\epsilon})$ .
- 14: Compute  $e = ||U^{(n+1)} U^{(n)}||$ .
- 15: n = n + 1
- 16: end while
- 17: return  $U^{(n+1)}$

to singularities. In that sense we evaluate the incomplete beta function using the native MATLAB implementation. Furthermore, given  $\Omega = (0, T]$ , we utilize the following quantities:

$$\operatorname{err}_{N}(h) = \frac{\|u(t_{N}) - u_{N}\|_{\infty}}{\|u(t_{N})\|_{\infty}}, \quad \operatorname{err}(h) = \frac{\max_{0 \le k \le N} \|u(t_{k}) - u_{k}\|_{\infty}}{\max_{0 \le k \le N} \|u(t_{k})\|_{\infty}}$$
$$\operatorname{Order}_{1} = \log_{2} \left[ \frac{\operatorname{err}_{N}(h)}{\operatorname{err}_{N}(h/2)} \right], \quad \operatorname{Order}_{2} = \log_{2} \left[ \frac{\operatorname{err}(h)}{\operatorname{err}(h/2)} \right]$$

to denote the error at the endpoint *T*, the global error on the solution interval  $\Omega$  and convergence order of the used method at the endpoint *T* and on the solution interval  $\Omega$ , respectively. The developed framework was implemented in MATLAB R2019a and was run in a desktop computer with Intel Core i7-6700 CPU with 3.40 GHz, 16 GB RAM and Ubuntu 18.04.2 LTS operating system.

**Example 6.** Linear FDE (see e.g. [112]):

$${}_{0}^{C}D_{t}^{\alpha}u(t) = f(t), \ \alpha \in (0,1], \ t \in (0,1]; \ u(0) = 0.$$
(9.63)



Figure 9.3: Computational time *versus* number of time steps *N* for the original (red curves) and the developed, fast (blue curves) FAMMs.

The exact solution of (9.63) is  $u(t) = t^{p+\alpha}$  for p = 1, 2. Therefore the corresponding force term is  $f(t) = \frac{\Gamma(\alpha+p+1)}{\Gamma(p+1)}t^p$ . Recalling Remark 9.4.4, we can employ the fast inversion scheme directly to the FAMM (9.17) in order to obtain a fast FAMM. Therefore, in this example we compare the performance between the fast and original FAMMs (9.17), where we verify the computational complexity and accuracy of both original and fast schemes.

Table 9.1 presents the obtained results for the implemented FAMMs at the endpoint T = 1 and no correction terms. Similar to the results in [112], we observe that the convergence order is independent of the fractional order  $\alpha$ , preserving the accuracy of the integer-order methods. For the case of  $\alpha = 0.9$  and p = 0, the scheme required a smaller time-step size  $h = 2^{-13}$  to achieve a linear convergence rate with  $Order_1 = 0.9967$  and error  $err_N(h) = 1.9520e-06$ . The computational times for the original and fast FAMMs are illustrated in Figure 9.3. We observe the computational complexity of  $O(N \log N)$  for the developed fast FAMMs. A break-even point at N = 4 is observed between both methods, which makes the fast method more computationally efficient when N > 4time-steps.

Example 7. Stiff FDE (see e.g. [113]):

$${}_{0}^{C}D_{t}^{\alpha}u(t) = Pu(t) + Su(t) + g(t), \ \alpha \in (0,1], \ t \in (0,10]; \ u(0) = [1, 1, 1]^{T},$$
(9.64)

		The	e fast FAMM wi	$i\mathbf{th} p = 0.$			
$\alpha = 0.1$			$\alpha = 0.$	.5	$\alpha = 0.9$	$\alpha = 0.9$	
h	$\operatorname{err}_N(h)$	Order <sub>1</sub>	$\operatorname{err}_N(h)$	Order <sub>1</sub>	$\operatorname{err}_N(h)$	Order <sub>1</sub>	
$2^{-3}$	5.2795e-03	_	9.7878e-03	_	1.0461e-03	_	
$2^{-4}$	2.6031e-03	1.0202	5.0535e-03	0.9537	6.0576e-04	0.7883	
$2^{-5}$	1.2912e-03	1.0115	2.5658e-03	0.9779	3.3733e-04	0.8446	
$2^{-6}$	6.4272e-04	1.0064	1.2925e-03	0.9892	1.8357e-04	0.8778	
$2^{-7}$	3.2058e-04	1.0035	6.4866e-04	0.9947	9.8414e-05	0.8994	

Table 9.1: The errors at the endpoint and convergence orders of the FAMMs for (9.63) with p = 0 (upper table) and p = 1 (lower table).

The fast FAMM with p = 1.

	$\alpha = 0$	.1	$\alpha = 0$	.5	$\alpha = 0.9$	)
h	$\operatorname{err}_N(h)$	Order <sub>1</sub>	$\operatorname{err}_N(h)$	Order <sub>1</sub>	$\operatorname{err}_N(h)$	Order <sub>1</sub>
$2^{-3}$	2.1934e-05	_	4.0975e-04	_	4.9840e-04	_
$2^{-4}$	5.5334e-06	1.9869	9.6888e-05	2.0804	1.2210e-04	2.0292
$2^{-5}$	1.4102e-06	1.9723	2.3574e-05	2.0391	2.9761e-05	2.0366
$2^{-6}$	3.5857e-07	1.9756	5.8150e-06	2.0193	7.2452e-06	2.0383
$2^{-7}$	8.9586e-08	2.0009	1.4452e-06	2.0085	1.7663e-06	2.0363

where

$$P = \begin{bmatrix} -1 & 0 & 0.001 \\ -0.0005 & -0.0008 & -0.0002 \\ 0.001 & 0 & -0.001 \end{bmatrix}, \quad S = \begin{bmatrix} -0.006 & 0 & 0.002 \\ -0.001 & -0.002 & 0 \\ 0 & -0.005 & -0.008 \end{bmatrix}$$
$$g(t) = \begin{pmatrix} a_1\Gamma_1 t^{\sigma_1 - \alpha} + a_2\Gamma_2 t^{\sigma_2 - \alpha} \\ a_3\Gamma_3 t^{\sigma_3 - \alpha} + a_4\Gamma_4 t^{\sigma_4 - \alpha} \\ a_5\Gamma_5 t^{\sigma_5 - \alpha} + a_6\Gamma_6 t^{\sigma_6 - \alpha} \end{pmatrix} - (P + S) \begin{pmatrix} a_1 t^{\sigma_1} + a_2 t^{\sigma_2} + 1 \\ a_3 t^{\sigma_3} + a_4 t^{\sigma_4} + 1 \\ a_5 t^{\sigma_5} + a_6 t^{\sigma_6} + 1 \end{pmatrix},$$

with  $\Gamma_k = \frac{\Gamma(\sigma_k+1)}{\Gamma(\sigma_k+1-\beta)}$ ,  $1 \le k \le 6$ . Therefore, the exact solution for the stiff FDE (9.64) is given by:

$$u(t) = \left(a_1 t^{\sigma_1} + a_2 t^{\sigma_2} + 1, \ a_3 t^{\sigma_3} + a_4 t^{\sigma_4} + 1, \ a_5 t^{\sigma_5} + a_6 t^{\sigma_6} + 1\right)^T,$$

where, as in [113], we consider  $\sigma_1 = \alpha$ ,  $\sigma_2 = 2\alpha$ ,  $\sigma_3 = 1 + \alpha$ ,  $\sigma_4 = 5\alpha$ ,  $\sigma_5 = 2$ ,  $\sigma_6 = 2 + \alpha$ , and  $a_1 = 0.5$ ,  $a_2 = 0.8$ , and  $a_3 = a_4 = a_5 = a_6 = 1$ . For the numerical solution of (9.64), we take f(t, u) = Su(t) + g(t) and employ the IMEX(p) scheme with  $\alpha = 0.3$ , utilizing a Picard iteration

tolerance of  $\epsilon^p = 5 \times 10^{-7}$ . We remark that the coefficients of P and S are taken as small enough values in order to satisfy the Lipschitz condition for the Picard iteration scheme, and nevertheless, the choice of such values still makes (9.64) stiff. The obtained results are presented in Table 9.2, where we obtain first-order convergence for the IMEX(0) method without using correction terms. On the other hand, for IMEX(1), we obtain second-order convergence when using M = 3 correction terms with correction powers  $\sigma = \{\alpha, 2\alpha, 1 + \alpha\}$  and  $\delta = \{2\alpha, 1 + \alpha, 5\alpha\}$ .

Table 9.2: The global errors and convergence orders of the methods IMEX(*p*) for (9.64) with p = 0 (upper table) and p = 1 (lower table) and  $\alpha = 0.3$ .

		IMEX(	0)	
	M = 0	0	M = 1	
h	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>
$2^{-3}$	1.9340e-02	_	1.9271e-02	_
$2^{-4}$	9.7036e-03	0.9950	9.6793e-03	0.9935
$2^{-5}$	4.8614e-03	0.9972	4.8518e-03	0.9964
$2^{-6}$	2.4334e-03	0.9984	2.4294e-03	0.9979
$2^{-7}$	1.2175e-03	0.9991	1.2157e-03	0.9988

#### IMEX(1)

	M = 0	0	<i>M</i> =	1	M = 1	2	M = 3	3
h	err( <i>h</i> )	Order <sub>2</sub>						
$2^{-3}$	6.5717e–04	_	4.3931e-04	_	2.4945e-04	_	2.1176e-04	_
$2^{-4}$	3.8296e-04	0.7791	1.5083e-04	1.5424	6.2702e-05	1.9922	5.6167e-05	1.9146
$2^{-5}$	2.3992e-04	0.6746	5.5600e-05	1.4397	1.5730e-05	1.9950	1.4606e-05	1.9431
$2^{-6}$	1.5407e-04	0.6390	2.1541e-05	1.3680	4.0658e-06	1.9519	3.7593e-06	1.9581
$2^{-7}$	9.9312e-05	0.6335	8.5481e-06	1.3334	1.7074e-06	1.2517	9.6316e-07	1.9646

**Example 8.** *Nonlinear FDE (cf. [113, 114]):* 

$${}_{0}^{C}D_{t}^{\alpha}u(t) = \lambda u(t) + f(t, u(t)), \ \alpha \in (0, 1], \ t \in \Omega; \ u(0) = u_{0}.$$
(9.65)

*We consider the following cases for* (9.65)*:* 

• Case I) Let  $\lambda = -0.2$ , f(t, u(t)) = 0 and  $u_0 = 1$ . The corresponding analytical solution is given by  $u(t) = E_{\alpha}(-0.2t^{\alpha})$ , where  $E_{\alpha}(t)$  represents the Mittag-Leffler function (cf. [171]).

• Case II) Let  $\lambda = -1$ ,  $f(t, u(t)) = -0.1u^2 + g(t)$ ,  $u_0 = 1$  and choose g(t) such that the exact solution of (9.65) is given by  $u(t) = 1 + t + t^2/2 + t^3/3 + t^4/4$ .

• Case III) Let 
$$\lambda = -1$$
,  $f(t, u(t)) = 0.01u(1 - u^2) + 2\cos(2\pi t)$  and  $u_0 = 1$ .

We start with **Case I**), for which we consider  $\Omega = (0, 40]$  and a tolerance  $\epsilon^p = 10^{-7}$  for the Picard iteration, with varying number of correction terms M and  $\alpha = 0.4$ . The obtained results are presented in Table 9.3 for the methods IMEX(p), where the CPU time (CPU) measured in seconds represent the running time of the methods. We observe the linear convergence rate when using M = 2 correction terms for IMEX(0). The convergence rates also improve for IMEX(1), however, we attain the accuracy limit of the scheme when using M = 4. Such accuracy limit is determined by the value of  $\epsilon = 5 \times 10^{-9}$  utilized for the fast inversion approach discussed in Section 9.4.1.

Table 9.3: The global errors and convergence orders of the methods IMEX(*p*) for solving Case I) with  $\alpha = 0.4$ , varying *h* and correction terms *M* with corresponding powers  $\sigma_k = \delta_k = k\alpha$ .

h	М	IM	EX(0)		М	IM	EX(1)	
		err( <i>h</i> )	Order <sub>2</sub>	CPU		err( <i>h</i> )	Order <sub>2</sub>	CPU
$2^{-2}$		7.6111e-03	_	0.21		5.9001e-03	_	0.37
$2^{-3}$		5.7608e-03	0.4019	0.37		4.6835e-03	0.3352	0.68
$2^{-4}$	0	4.3450e-03	0.4069	0.75	0	3.6810e-03	0.3475	1.37
$2^{-5}$		3.2724e-03	0.4090	1.35		2.8698e-03	0.3591	2.65
$2^{-6}$		2.4640e-03	0.4093	2.65		2.2231e-03	0.3684	5.32
$2^{-2}$		1.9406e-03	_	0.22		2.1673e-05	_	1.06
$2^{-3}$		1.2144e-03	0.6762	0.35		1.0252e-05	1.0800	2.13
$2^{-4}$	1	7.4541e-04	0.7042	0.73	2	4.7644e-06	1.1055	4.03
$2^{-5}$		4.5062e-04	0.7261	1.36		2.1831e-06	1.1259	7.95
$2^{-6}$		2.6918e-04	0.7433	2.66		9.8961e-07	1.1415	16.04
$2^{-2}$		3.2061e-04	_	0.56		1.4155e-07	_	1.74
$2^{-3}$		1.7125e-04	0.9047	1.10		5.0125e-08	1.4978	3.32
$2^{-4}$	2	9.0232e-05	0.9244	1.97	4	2.5470e-08	0.9767	6.49
$2^{-5}$		4.7019e-05	0.9404	3.91		2.7468e-08	_	13.07
$2^{-6}$		2.4284e-05	0.9532	7.85		3.6517e-08	_	26.02

For **Case II**), we let  $\Omega = (0, 1]$  and  $\epsilon^p = 10^{-7}$ . The obtained results are presented in Table 9.4, where we observe that both schemes achieve the theoretical convergence rates for the global error.

			INIEA(U)				
	$\alpha = 0.$	.2	$\alpha = 0$	.5	$\alpha = 0.3$	8	
h	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>	
2 <sup>-6</sup>	1.9855e-02	_	1.8557e-02	_	1.7421e-02	_	
$2^{-7}$	9.9111e-03	1.0024	9.2800e-03	0.9998	8.7136e-03	0.9994	
$2^{-8}$	4.9517e-03	1.0011	4.6425e-03	0.9992	4.3602e-03	0.9989	
$2^{-9}$	2.4750e-03	1.0005	2.3226e-03	0.9991	2.1821e-03	0.9987	
$2^{-10}$	1.2373e-03	1.0002	1.1619e-03	0.9992	1.0921e-03	0.9986	
			IMEX(1)				
	$\alpha = 0.$	.2	$\alpha = 0$	.5	$\alpha = 0.8$		
h	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>	
2 <sup>-6</sup>	5.3875e-04	_	4.4167e-04	-	3.7370e-04	_	
$2^{-7}$	1.3610e-04	1.9849	1.1153e-04	1.9856	9.4359e-05	1.9856	
$2^{-8}$	3.4206e-05	1.9924	2.8033e-05	1.9922	2.3740e-05	1.9909	
$2^{-9}$	8.5751e-06	1.9960	7.0286e-06	1.9958	5.9679e-06	1.9920	
$2^{-10}$	2.1498e-06	1.9960	1.7586e-06	1.9988	1.4862e-06	2.0056	

Table 9.4: The global errors and convergence orders of the methods IMEX(*p*) for solving Case II) with no correction term for p = 0 and M = 2 correction terms for p = 1, with  $\sigma = \delta = \{1 - \alpha, 1\}$ .

For Case III), we consider  $\Omega = (0, 50]$ , and we set a numerical tolerance  $\epsilon^p = 10^{-6}$  for the Picard iteration. Figures 9.4 and 9.5a illustrate the obtained highly oscillatory solutions. We also perform a convergence analysis utilizing a benchmark solution with  $h = 2^{-11}$  and M = 3 correction terms and evaluate the global error. The obtained results are presented in Table 9.5, where the expected first- and second-order convergence rates are obtained, respectively, with p = 0 without correction terms, and p = 1 using M = 3 correction terms. The computational times for the developed IMEX schemes are illustrated in Figure 9.5b including the initial phase for computation of correction weights. We observe the computational complexity of  $O(N \log N)$  for the developed schemes even for nonlinear problems, with a small difference between the first- and second-order the developed IMEX(0) scheme with the direct, fully implicit L1 approach developed by Zeng et al. [106] with order  $O(h^{3-\alpha})$ . Therefore, we use the same problem setup and parameters, and use a Newton sub-iteration for the nonlinear problem. We compute the errors and convergence order without correction terms and varying fractional orders.



Figure 9.4: Solution *versus* time t for Case III) using h = 0.005 and M = 1 correction term.



Figure 9.5: (a) Solution versus time t for Case III) using h = 0.005 with M = 1 correction term. (b) Computational time versus number of time steps N for the developed IMEX schemes.

For  $\alpha = \{0.2, 0.5, 0.7\}$ , we obtained, respectively,  $err(h = 2^{-7}) = \{2.4581e-02, 1.5633e-02, 5.6208e-03\}$  and  $Order_2 = \{0.1233, 0.4930, 0.7524\}$ . We observe that although the L1 approach achieves similar error levels than the IMEX(0) scheme (Table 9.5, top), it is at most  $O(h^{\alpha})$  accurate for the tested values of h, while the IMEX(0) scheme is first-order accurate without the need of any correction terms and  $\alpha$ -independent.

			IMEX(0)			
	$\alpha = 0.$	2	$\alpha = 0$	.5	$\alpha = 0.$	7
h	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>	err( <i>h</i> )	Order <sub>2</sub>
2 <sup>-3</sup>	4.4883e-01	_	3.3552e-01	_	2.5798e-01	_
$2^{-4}$	2.2466e-01	0.9984	1.6681e-01	1.0082	1.3311e-01	0.9546
$2^{-5}$	1.1217e-01	1.0021	8.3553e-02	0.9975	6.7629e-02	0.9769
$2^{-6}$	5.6354e-02	0.9931	4.2141e-02	0.9875	3.4015e-02	0.9915
$2^{-7}$	2.8246e-02	0.9965	2.1163e-02	0.9937	1.7091e-02	0.9929
			INTEV(1)			
			INIEA(1)			
	$\alpha = 0$	.2	$\alpha = 0$	.5	$\alpha = 0.7$	7
h	$\frac{\alpha = 0}{\operatorname{err}(h)}$	.2 Order <sub>2</sub>	$\frac{\alpha = 0}{\operatorname{err}(h)}$	.5 Order <sub>2</sub>	$\frac{\alpha = 0.7}{\operatorname{err}(h)}$	7 Order <sub>2</sub>
$\frac{h}{2^{-3}}$	$\frac{\alpha = 0}{\operatorname{err}(h)}$ 3.3534e-01	.2 Order <sub>2</sub>	$\frac{\alpha = 0}{\text{err}(h)}$ 1.9664e-01	.5 Order <sub>2</sub>	$\frac{\alpha = 0.7}{\text{err}(h)}$	7 Order <sub>2</sub>
$\frac{h}{2^{-3}}$	$\frac{\alpha = 0}{\text{err}(h)}$ 3.3534e-01 9.5452e-02	.2 Order <sub>2</sub> - 1.8128	$\frac{\alpha = 0}{\text{err}(h)}$ 1.9664e-01 8.1541e-02	.5 Order <sub>2</sub> - 1.2699	$     \frac{\alpha = 0.7}{\text{err}(h)}     2.5260e-01     7.1427e-02   $	7 Order <sub>2</sub> - 1.8223
$ \frac{h}{2^{-3}} \\ 2^{-4} \\ 2^{-5} $	$\frac{\alpha = 0}{\text{err}(h)}$ 3.3534e-01 9.5452e-02 2.2387e-02	.2 Order <sub>2</sub> - 1.8128 2.0921	$\frac{\alpha = 0}{\text{err}(h)}$ $\frac{1.9664\text{e-}01}{8.1541\text{e-}02}$ $2.0062\text{e-}02$	5 Order <sub>2</sub> - 1.2699 2.0230		7 Order <sub>2</sub> - 1.8223 1.8007
$ \frac{h}{2^{-3}} \\ 2^{-4} \\ 2^{-5} \\ 2^{-6} $	$\frac{\alpha = 0}{\text{err}(h)}$ 3.3534e-01 9.5452e-02 2.2387e-02 5.4892e-03	.2 Order <sub>2</sub> - 1.8128 2.0921 2.0280	$\frac{\alpha = 0}{\text{err}(h)}$ $\frac{1.9664\text{e-}01}{8.1541\text{e-}02}$ $2.0062\text{e-}02$ $4.5814\text{e-}03$	5 Order <sub>2</sub> - 1.2699 2.0230 2.1306		7 Order <sub>2</sub> - 1.8223 1.8007 2.0705

Table 9.5: Convergence results for the IMEX(p) scheme solving Case III) without corrections for p = 0 and M = 3 correction terms for p = 1, with  $\sigma = \delta = \{\alpha, 2\alpha, 1 + \alpha\}$ .

### **CHAPTER 10**

### SUMMARY AND FUTURE WORKS

The main objective of this work was to develop a data-driven multi-scale framework for modeling and simulating the response of anomalous materials. Some multi-scale aspects in plasticity were presented, from fundamental molecular dynamics simulations to discrete dislocation dynamics, from which the emerging power-laws may be physically inform continuum viscoplastic models. An existence study for visco-elastic anomalous materials is performed with fractional linear/nonlinear visco-elasticity, which successfully captured the multi power-law behavior of urinary bladder tissue undergoing large strains. In order to model the failure of anomalous visco-plastic materials, we developed two fractional-order visco-elasto-plastic materials, followed by an extension of memory-dependent damage and novel fractional return-mapping schemes to solve the corresponding systems of equations. Later on a generalized return-mapping approach was developed for several linear/nonlinear fractional visco-elastic models. We also analyzed influence of varying fractional orders of visco-elasticity in the nonlinear vibration of cantilever beams. In order to address numerical issues with the family of multi-term FDEs resulting in the developed models, we develop a new research front of data-driven numerical methods for FDEs, where we learn the regularity of the solution. Furthermore, we develop efficient and accurate, fast IMEX schemes, which shows larger stability regions compared to existing schemes.

# **10.1 Concluding Remarks**

In **Chapter 2**, we performed a series of MD simulations on canonical pure and dislocationperturbed systems, in order to estimate a deterministic table of DDD parameters to carry dislocation dynamics simulations. The results of the DDD simulations were consistent with theoretical and experimental finding in the literature, showing the self-similar characteristics of dislocation systems that could be couple to the developed continuum models in this work and provide an insight on the physical interpretation of fractional orders in slip systems. In **Chapter 3** we developed a data-driven fractional modeling framework for linear and nonlinear viscoelasticity which was validated for the first time in the uniaxial relaxation of porcine urinary bladder tissue for a wide range of applied strains. Our approach employed fractional linear and quasi-linear visco-elastic models to account for anomalous power-law relaxation and large strains. Our main findings in this study were:

- Our existence study was able to relate the power-law features of specimens from five distinct bladder samples to the fractional orders in linear/quasi-linear fractional models, and is an interesting step towards an automated model selection framework.
- The bladder uniaxial relaxation data was obtained from consecutive and increasing step strain applications, indicating the presence of nonlinear, strain-dependent effects on the relaxation functions.
- Our obtained data is consistent with other bladder rheology studies, indicating higher stress levels for the trigone region, and an exponential-like stress-strain relationship.
- Among linear visco-elastic models employed for the first relaxation step (25% strains), the fractional Maxwell model was the most suited for all regional bladder samples, with two fractional orders, which dominate short- and long-times. More complex linear fractional models consistently recovered the FM, and the FKV model proved to be unfeasible since it recovers a SB element.
- The employed fractional quasi-linear viscoelastic model successfully captured the multi-step relaxation behavior with four material parameters and without any requirement of parameter recalibration, yielding a fractional order range  $\alpha = 0.25 0.30$  with root mean squared errors below 2%.
- Fractional calculus can be a interesting alternative to describe the linear/nonlinear behavior of porcine UB especially within a material model selection framework, since fractional models

potentially provide a reduced number of material parameters due to the presence of multiple power-laws in relaxation.

In **Chapter 4**, we developed two new fractional-order models for uniaxial large strains and visco-elasto-plastic behavior of materials in structural analysis. This generalized framework is amenable to modeling nonlinear and more complex effects namely *visco-elasto-plastic* response of materials. Two models, namely M1 and M2, were introduced with the following approaches for visco-plastic behavior:

- The model M1 was developed by modifying the classical rate-independent elasto-plasticity, with a rate-depen- dent yield function via the application of the time-fractional Caputo derivative on the accumulated plastic strain.
- The model M2 was developed as a fractional-order extension of the classical Duvaut-Lions elasto-visco-plastic model. In this sense, the time-fractional Caputo derivative was introduced in a visco-plastic regularization equation that solved for the visco-plastic strain when an overstress level was achieved.

Based on the adopted yield stress update procedure, both models assumed a fast transition from visco-plastic to visco-elastic regime when unloading the material. Nevertheless we performed cyclic strain tests with different relaxation times and strain rates for both models and determined that:

- The model M2 showed more rate-dependency in the visco-plastic range, and is suitable for materials with general relaxation times and strain rates, since it was naturally defined based on the classical Duvaut-Lions formulation.
- The model M1 proved to be more suitable for materials with lower relaxation times (less dissipative) and lower strain rates, since the enforcement of the consistency condition assumed a fast relaxation occurring during the time interval  $\Delta t$  under consideration.

An algorithm, called *fractional return-mapping*, was proposed to solve the nonlinear system of equilibrium equations resulted from the models. This algorithm seamlessly generalizes the standard return-mapping algorithm to its fractional counterpart, leading to an efficient framework for treating engineering applications involving visco-elasto-plastic materials. Most of the existing numerical methods for standard (integer-order) cases are not better than first-order accurate in time. Therefore, in our future work, we will also focus on developing further efficient numerical methods in terms of accuracy and computational costs.

A benchmark test performed with prescribed strains verified a linear convergence rate for the model M1. We observed a superlinear convergence rate for the model M2, since this model had no time integration of the plastic slip. We implemented the classical models of rate-independent elasto-plasticity and elasto-visco-plasticity of Duvaut-Lions type and verified that:

- Both models recover the classical elasto-plastic model with the choice of  $\beta_E \rightarrow 0$  and  $\beta_K \rightarrow 0$ , even for the snap-through problem where a large number of tension/compression cycles was observed.
- The model M2 recovered the classical Duvaut-Lions model for monotonic strains by setting  $\beta_E \rightarrow 0$  and  $\beta_K \rightarrow 1$ . We did not obtain the same result for the model M1 due to the adopted algorithmic procedure.

The application to a two-member truss showed the influence of dissipation and strain hardening effects on the structure according to the value of the fractional-orders for the visco-elastic and visco-plastic parts.

In **Chapter 5** we developed a thermodynamically consistent, fractional visco-elasto-plastic model with memory-dependent damage using fractional Helmholtz free-energies, visco-plastic/damage potentials and the Clausius-Duhem inequality. The damage energy release rate was derived from the visco-elastic free-energy to obtain a consistent bulk energy loss for anomalous materials.

A first-order, semi-implicit fractional return-mapping algorithm, which generalizes existing standard ones, was developed to solve the resulting nonlinear system of FDEs. We note that

255

most existing algorithms for standard plasticity models are not more accurate than ours. We also developed a new FD scheme with accuracy  $O(\Delta t^{2-\beta})$  for the free-energy/damage energy release, with computational complexity of  $O(N^2 \log N)$  through FFTs.

We also performed a set of numerical tests and observed that:

- The fractional orders  $\beta_E$  and  $\beta_K$  tune the competition between the plastic slip and damage energy release rate for damage evolution.
- Higher values of  $\beta_E$ ,  $\beta_K$  yielded lower damage levels for lower strain rates/cycles; However, the damage increased significantly faster than lower values of  $\beta_E$ ,  $\beta_k$  for higher strain rates/cycles.
- For the free-energy discretization, the break-even point between the original and fast schemes was low, about *N* = 200 time-steps.
- The developed discretization recovered the limit Hookean  $\beta \to 0$  and Newtonian  $\beta \to 1$  cases for the free-energy.

In **Chapter 6** we proposed a general return-mapping procedure for multiple power-law, timefractional visco-elasto-plastic materials. The developed framework provided a flexible way to integrate multiple known fractional visco-elastic models that are representative of soft materials rheology to power-law viscoplastic hardening and permanent strains. Furthermore, nonlinear viscoelasticity suitable for bio-tissues was considered through a fractional quasi-linear Fung's model, which allowed the possibility of plasticity onset after substantial amounts of visco-elastic strains. The main features of the proposed framework are:

- The trial states were taken after full discretization of stress and internal variables, which allowed a straightforward decomposition of the yield function into final and trial states.
- The developed return-mapping procedure is fully-implicit for linear viscoelastic models and semi-implicit for quasi-linear viscoelasticity, and for simplicity, the chosen numerical discretization for fractional derivatives was an L1 finite-difference approach.

- Our correction step for viscoplasticity had the same structure for all viscoelastic models, with the only difference being a scaling discretization constant.
- We carried out numerical experiments with analytical and reference solutions that demonstrated the  $O(\Delta t^{2-\beta})$  global accuracy, surprisingly even in some instances with general loading/unloading conditions.
- The developed return-mapping discretization was compared to an existing approach, and the difference between discretizations relied on cases with extensive plastic history and high strain rates.

Regarding the computational costs, the framework is computationally tractable since it does not involve history calculations for the plastic slip, and is therefore about 50% faster than the previously existing fractional framework, regardless of the employed numerical discretization for fractional derivatives. Extensions on fast numerical schemes of order  $O(N \log N)$  for the employed time-fractional derivatives would be straightforward to implement. We also note that the thermodynamics of all models in the developed framework can be analyzed through the approach developed in [75].

In **Chapter 7**, the anomalous nonlinear dynamics driven by the application of extraordinary materials was investigated. Our anomalous system is represented as a nonlinear fractional Kelvin-Voigt viscoelastic cantilever beam. A spectral method was employed for spatial discretization of the governing equation of motion, reducing it to a set of nonlinear fractional ODEs. The corresponding system was linearized and the time-fractional integration was carried out through a direct L1 finite-difference scheme, together with a Newmark method. For the nonlinear solution, a method of multiple scale was employed, and the time response of the beam subject to a base excitation was obtained. We performed a set of numerical experiments on the system response under varying fractional orders, representing different stages of material evolution, where we observed:

• Anomalous drift in peak amplitude response according to fractional orders, and the presence of a low-frequency critical point under linear forced vibration.

- Short-time and long-time anomalous behaviors under linear free vibration, respectively, for Riemann-Liouville and Caputo definitions.
- Super sensitivity of the amplitude response with respect to the fractional model parameters at free vibration.
- A critical behavior of the decay rate sensitivity with respect to  $\alpha$ , where increasing values of fractional order yielded higher decay rates (softening) before a critical value  $\alpha_{cr}$ . Lower decay rates (stress hardening) were observed beyond such critical value.
- A bifurcation behavior under steady-state amplitude at primary resonance case.

The choice of a fractional Kelvin-Voigt model in this work allowed us to describe a material in the intersection between anomalous and standard constitutive behavior, where the contribution of the SB element yields the power-law material response, while the Hookean spring reflects the instantaneous response of many engineering materials. In addition, the shifts in amplitude-frequency response with respect to the fractional order motivate future studies on the downscaling of fractional operators to the associated far-from-equilibrium dynamics (polymer caging/reptation, dislocation avalanches) in evolving heterogeneous microstructures [40]. In terms of modifications of the current model, different material distribution functions could be chosen, leading to application-based material design for a wide range of structural materials and anomalous systems, including microelectromechanical systems (MEMS). Finally, regarding numerical discretizations, one could utilize additional active vibration modes, as well as faster time-fractional integration methods, in order to better capture the fundamental dynamics of the presented system.

The developed model will be used in future to simulate the excitation of the outer hair cells inside the cochlea. The individual hair cells will be modeled as 'cantilever beams' with variable sizes along the basilar membrane. In addition to the nonlocal and history effects in hair cell biomechanics, the *mechanoelectrical transduction* of the hair cells will be incorporated into the model.

In **Chapter 8** we developed a two-stage framework for accurate and efficient solution of FDEs. It consists of: **I**) A self-singularity-capturing scheme, where the inputs were limited data for diminutive time, and the output was the captured power-law singular values of the solution. The limited data is either obtained experimentally or sampled from a fine time-grid nearby t = 0. We developed an implicit finite-difference algorithm for the FDE solution and employed a gradient optimization scheme. **II**) The captured singularities were then inputs of an implicit finite-difference scheme for FDEs with accuracy  $O(\Delta t^{3-\alpha})$ . Based on our numerical tests, we observed that:

- The scheme was able to fully capture *S* singularities using  $M \ge S$  correction terms. When S > M, the scheme still obtained approximations of the *M* singularities, which was useful for error control.
- When M = 1, an estimation of the most critical singularity was captured by the scheme, regardless of S.
- The developed scheme was used in a self-singularity-capturing framework, which determined the singularity values up to the desired tolerance *ε*.
- Once the singularities are captured in the first stage, we can successfully employ any known numerical scheme for more accurate and efficient solution of the corresponding FDE, when compared to the *ad-hoc* singularity choices done in [5].
- The scheme was able to capture two singularities from a solution using a strong power-law singularity coupled with an oscillatory smooth part, which allowed us to obtain the theoretical accuracy  $O(\Delta t^{3-\alpha})$  of the employed numerical discretization for the fractional derivative. Furthermore, by solving a nonlinear FDE, we demonstrate that the developed framework does not require the knowledge of any analytical solution.

The main advantage of the developed scheme over other works on correction methods [5, 86, 87] is the self-capturing of strong multi-singularities  $\sigma$  of the solution data in Stage-I instead of *ad-hoc* choices. This led to smaller solution errors while achieving the theoretical convergence rate of

the employed numerical integration schemes in Stage-II, with algorithmically minimal correction terms M, and consequently requiring less computational cost. The total computational complexity of the two-stage framework is  $O(\tilde{N}^2 N_{it} + N^2)$ , since the number of correction terms M is small.

In **Chapter 9** we developed two new first- and second-order IMEX schemes for accurate and efficient solution of stiff/nonlinear FDEs with singularities. Both of the schemes are based on the linear multi-step FAMM developed by Zayernouri and Matzavinos [112], followed by an extrapolation formula from which we obtain the *so-called* IMEX(p) scheme. In order to handle the inherent singularities of the FDEs, we introduced 4 sets of correction terms for the IMEX(p) schemes. The convergence and linear stability of the developed schemes is also analyzed. A fast solution for the developed schemes is attained by employing a fast-inversion approach developed by Lu *et al.* [322] on the resulting nonlinear Toeplitz system, leading to a computational complexity of  $O(N \log N)$ . Based on our computational results, we observed that:

- When considering a linear problem, the fast implementation of the scheme was significantly faster than the original FAMM by Zayernouri and Matzavinos [112], with a very low *break*even point at N = 4 time-steps.
- Both IMEX(p) schemes achieved global first- (for p = 0) and second-order (for p = 1) convergence rates for stiff/nonlinear, highly-oscillatory and singular solutions, given the choice of appropriate sets of correction terms.
- The computational performance was slightly better for the IMEX(0) scheme. We also remark that such scheme is simpler to implement and generally requires a smaller number of correction terms due to lower regularity requirements to attain first-order accuracy.

The main advantages of the developed IMEX schemes in comparison to other works are: larger stability regions when compared to the IMEX schemes developed by Cao *et al.* [113]; and also a fast solution alternative when compared to the original fractional Adams-Bashforth/Moulton methods developed by Zayernouri and Matzavinos [112], and the IMEX schemes by Cao *et al.* [113]. When compared to the matrix-based fast solver for FDEs developed by Lu [322], the developed framework

in this work handles the numerical solution of nonlinear and singular FDEs instead of only linear ones.

# **10.2 Future Works**

Following the modeling, numerical, and applied studies done in this work, we believe the the developed framework has viable applications towards the modeling of anomalous materials across a range of time-scales. Potential improvements of the framework could be done through upscaling studies from MD-DDD until macro-scale plasticity in order to identify the corresponding fractional orders for the plastic regime and also meso-scale studies to shed light on the physical meaning of fractional orders from the corresponding fractal dislocation networks. Uncertainty quantification studies on the developed fractional models would also aid towards a Bayesian model selection framework, and finally, multi-dimensional extensions of fractional visco-elasto-plasticity would also be an interesting direction to expand the functionality of the models towards large-scale applications.

APPENDICES

### **APPENDIX A**

# **DERIVATIONS IN CHAPTER 4**

# A.1 Solution of the Fractional-Order Differential Equations in Incremental Form

In this section we present the explicit expressions for the variables at time  $t_{n+1}$  after applying the finite-difference scheme for the Caputo time-fractional derivatives for both models. The trial stress is given by

$$\tau_{n+1}^{trial} = E^* \left( \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta E} \varepsilon - \varepsilon_{n+1}^{v p^{trial}} + \varepsilon_n^{v p} - \mathcal{H}^{\beta E} \varepsilon^{v p} \right), \tag{A.1}$$

where

$$E^* = \frac{E}{\Delta t^{\beta E} \Gamma(2 - \beta_E)},\tag{A.2}$$

where  $E^*$  has units of [*Pa*]. Recalling that  $\varepsilon_{n+1}^{vp^{trial}} = \varepsilon_n^{vp}$ , we can rewrite Eq.A.1 as

$$\tau_{n+1}^{trial} = E^* \left( \varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta E} \varepsilon - \mathcal{H}^{\beta E} \varepsilon^{\nu p} \right).$$
(A.3)

The associated trial yield function for the model M1 is explicitly given by

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - \left[\tau^{Y} + H\alpha_{n+1}^{trial} + K^{*}(\alpha_{n+1}^{trial} - \alpha_{n} + \mathcal{H}_{tp_{n}}^{\beta K}\alpha)\right],$$
(A.4)

with

$$K^* = \frac{K}{\Delta t^{\beta_K} \Gamma(2 - \beta_K)},\tag{A.5}$$

where K \* has units of [*Pa*]. Recalling that  $\alpha_{n+1}^{trial} = \alpha_n$ , we obtain

$$f_{n+1}^{trial} = |\tau_{n+1}^{trial}| - \left(\tau^Y + H\alpha_n + K^* \mathcal{H}_{tp_n}^{\beta K} \alpha\right).$$
(A.6)

Now we consider the solution for the plastic slip  $\Delta \gamma_{n+1}$ . Applying Eqs.4.41 and 4.46 to Eq.4.40 for the model M1, we obtain

$$\frac{E}{\Delta t^{\beta E} \Gamma(2-\beta_{E})} \left( \Delta \gamma_{n+1} - \Delta \gamma_{n} + \mathcal{H}^{\beta E} \Delta \gamma \right) 
+ \frac{K}{\Delta t^{\beta K} \Gamma(2-\beta_{K})} \left( \Delta \gamma_{n+1} - \Delta \gamma_{n} + \mathcal{H}^{\beta K}_{tp_{n+1}} \Delta \gamma \right) + H \Delta \gamma_{n+1} = f^{trial}_{n+1}.$$
(A.7)
Solving the above equation for the plastic slip at current time  $t_{n+1}$ , we obtain

$$\Delta \gamma_{n+1} = \frac{E^* \left( \Delta \gamma_n - \mathcal{H}^{\beta} E \, \Delta \gamma \right) + K^* \left( \Delta \gamma_n - \mathcal{H}^{\beta}_{tp_{n+1}} \Delta \gamma \right) + f^{trial}_{n+1}}{E^* + K^* + H}.$$
(A.8)

Applying the same procedure to Eq.4.35, we obtain the updated stress  $\tau_{n+1}$  for the model M1 given by

$$\tau_{n+1} = \tau_{n+1}^{trial} - E^* \left( \Delta \gamma_{n+1} - \Delta \gamma_n + \mathcal{H}^{\beta E} \Delta \gamma \right) \operatorname{sign} \left( \tau_{n+1}^{trial} \right).$$
(A.9)

Now we present the explicit expression for  $\varepsilon_{n+1}^{vp}$  from Eq.4.58 for the model M2. Therefore, we have

$$E^{*}\left(\varepsilon_{n+1}^{\nu p} - \varepsilon_{n}^{\nu p} + \mathcal{H}^{\beta E}\varepsilon^{\nu p}\right) + K^{*}\left(\varepsilon_{n+1}^{\nu p} - \varepsilon_{n}^{\nu p} + \mathcal{H}^{\beta K}_{tp_{n+1}}\varepsilon^{\nu p}\right) = E^{*}\left(\varepsilon_{n+1} - \varepsilon_{n} + \mathcal{H}^{\beta E}\varepsilon\right) - \operatorname{sign}\left(\tau_{n+1}^{trial}\right)\tau^{\gamma\prime}.$$
(A.10)

Solving for  $\varepsilon_{n+1}^{vp}$ , we obtain

$$\varepsilon_{n+1}^{\nu p} = \varepsilon_n^{\nu p} + \frac{E^* \left(\varepsilon_{n+1} - \varepsilon_n + \mathcal{H}^{\beta} E \varepsilon - \mathcal{H}^{\beta} K \varepsilon\right) - K^* \mathcal{H}_{tp_{n+1}}^{\beta K} \varepsilon^{\nu p} - \operatorname{sign}\left(\tau_{n+1}^{trial}\right) \tau^{\gamma \prime}}{E^* + K^*}.$$
 (A.11)

## A.2 Newmark Integration Scheme

We consider the equation of conservation of linear momentum in the discrete implicit form using a Newmark integration scheme without damping effects [206],

$$\mathbf{M}\mathbf{a}_{n+1} + \mathbf{R}_{n+1} = \mathbf{P}_{n+1}, \tag{A.12}$$

with the above terms already described in Section 4.4. The initial conditions at t = 0 are given by

$$\mathbf{u}_0 = \bar{\mathbf{u}}, \quad \mathbf{v}_0 = \bar{\mathbf{v}}. \tag{A.13}$$

The global accelerations and velocities are approximated as

$$\mathbf{a}_{n+1} = b_1 \left( \mathbf{u}_{n+1} - \mathbf{u}_n \right) - b_2 \mathbf{v}_n - b_3 \mathbf{a}_n \tag{A.14}$$

$$\mathbf{v}_{n+1} = b_4 \left( \mathbf{u}_{n+1} - \mathbf{u}_n \right) - b_5 \mathbf{v}_n - b_6 \mathbf{a}_n,$$
 (A.15)

with the following Newmark coefficients

$$b_1 = \frac{1}{g_1 \Delta t^2}, \quad b_2 = \frac{1}{g_1 \Delta t}, \qquad b_3 = \frac{1 - 2g_1}{2g_1}$$
$$b_4 = \frac{g_2}{g_1 \Delta t^2}, \quad b_5 = \left(1 - \frac{g_2}{g_1}\right), \quad b_6 = \left(1 - \frac{g_2}{2g_1}\right) \Delta t,$$

where it is usual to choose  $g_1 = 0.5$ ,  $g_2 = 0.25$  for unconditional stability.

#### **APPENDIX B**

## **DERIVATIONS IN CHAPTER 5**

# B.1 Proof of Lemma 5.3.1

We take the time derivative of the free-energy (5.10) and obtain:

$$\dot{\psi} = \int_0^\infty \tilde{E}(z) \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds \left(\frac{d}{dt} \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds\right) dz \tag{B.1}$$

with

$$\frac{d}{dt} \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds = \dot{\varepsilon}(t) - \int_0^t \frac{1}{z} \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds.$$
(B.2)

Substituting (B.2) into (B.1), we obtain:

$$\dot{\psi} = \left[ \int_0^\infty \tilde{E}(z) \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds \right) dz \right] \dot{\varepsilon} - \int_0^\infty \frac{\tilde{E}(z)}{z} \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds \right)^2 dz.$$
(B.3)

Let  $\mathbb{E}^* = \frac{\mathbb{E}}{\Gamma(1-\beta)\Gamma(\beta)}$ . Note that the term inside brackets in (B.3) equals:

$$\int_{0}^{\infty} \tilde{E}(z) \left( \int_{0}^{t} \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) \, ds \right) \, dz$$

$$= \int_{0}^{\infty} \frac{\mathbb{E}^{*}}{z^{\beta+1}} \left( \int_{0}^{t} \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) \, ds \right) \, dz$$

$$= \mathbb{E}^{*} \int_{0}^{t} \left[ \int_{0}^{\infty} z^{-(\beta+1)} \exp\left(-\frac{t-s}{z}\right) \, dz \right] \dot{\varepsilon}(s) \, ds$$

$$= \mathbb{E}^{*} \int_{0}^{t} \left[ \int_{0}^{\infty} \frac{u^{\nu-1}}{(t-s)^{\beta}} \exp(-u) \, du \right] \dot{\varepsilon}(s) \, ds$$

$$= \mathbb{E}^{*} \int_{0}^{t} \left[ \frac{\Gamma(\beta)}{(t-s)^{\beta}} \right] \dot{\varepsilon}(s) \, ds = \frac{\mathbb{E}}{\Gamma(1-\beta)} \int_{0}^{t} \frac{\dot{\varepsilon}(s)}{(t-s)^{\beta}} \, ds$$

$$= \mathbb{E}_{0}^{C} \mathcal{D}_{t}^{\beta} \left( \varepsilon \right). \tag{B.4}$$

Substituting (B.4) into (B.3), and the result into (5.9), we obtain:

$$\left[\tau - \mathbb{E}_{0}^{C}\mathcal{D}_{t}^{\beta}(\varepsilon)\right]\dot{\varepsilon} + \int_{0}^{\infty}\frac{\tilde{E}(z)}{z}\left(\int_{0}^{t}\exp\left(-\frac{t-s}{z}\right)\dot{\varepsilon}(s)ds\right)^{2}dz \ge 0.$$
(B.5)

Since the strain rate  $\dot{\varepsilon}$  is arbitrary, we set the argument inside brackets to zero without violating the above inequality, to obtain the stress-strain relationship for the SB model:

$$\tau = \mathbb{E}_{0}^{C} \mathcal{D}_{t}^{\beta} \left( \varepsilon \right).$$

Furthermore, the remainder of (B.5) represents an internal positive mechanical dissipation, given by:

$$\mathcal{D}_{mech}(\varepsilon) = \int_0^\infty \frac{\tilde{E}(z)}{z} \left( \int_0^t \exp\left(-\frac{t-s}{z}\right) \dot{\varepsilon}(s) ds \right)^2 dz \ge 0,$$

where the above inequality holds, since z and  $\tilde{E}(z)$  are positive.

## **B.2** Proof of Theorem 5.4.4

We recall the mechanical dissipation (5.26):

$$\tau \dot{\varepsilon}^{vp} - R\dot{\alpha} - Y\dot{D} + (1 - D)\left(\mathcal{D}_{mech}^{ve} + \mathcal{D}_{mech}^{vp}\right) \ge 0,\tag{B.6}$$

where we must prove that the above inequality holds. Substituting (5.31), (5.32) into (5.26) yields:

$$\tau \operatorname{sign}(\tau) \dot{\gamma} - R \dot{\gamma} - Y \dot{D} + (1 - D) \left( \mathcal{D}_{mech}^{ve} + \mathcal{D}_{mech}^{vp} \right) \ge 0,$$

Rearranging the above equation, we obtain:

$$\left[ |\tau| - \left( (1-D)\tau^Y + R \right) \right] \dot{\gamma} - Y\dot{D} + (1-D) \left( \tau^Y \dot{\gamma} + \mathcal{D}_{mech}^{ve} + \mathcal{D}_{mech}^{vp} \right) \ge 0,$$

where the first term is is related to the persistency condition [192]:

$$\left[\left|\tau\right| - \left((1-D)\tau^{Y} + R\left(\alpha\right)\right)\right]\dot{\gamma} = f(\tau, \alpha, D)\dot{\gamma} = 0,$$

and therefore,

$$(1-D)\left(\tau^{Y}\dot{\gamma} + \mathcal{D}_{mech}^{ve} + \mathcal{D}_{mech}^{vp}\right) - Y\dot{D} \ge 0.$$
(B.7)

We check the positiveness for each term of the above inequality. For the first term, since the damage is always positive, so is (1 - D). Also, we have  $\tau^Y > 0$  and  $\dot{\gamma} \ge 0$  [192]. From Lemma 5.3.1 the mechanical dissipations  $\mathcal{D}_{mech}^{ve}$  and  $\mathcal{D}_{mech}^{vp}$  are also positive. For the second term, -Y is positive and so is  $\dot{D}$ , since D is a monotonically increasing function. Therefore, inequality (B.7) holds, and thus the developed model is thermodynamic admissible.

## **B.3** Convexity of the Yield Function

*Proof.* Recalling (5.28), we have

$$f(\tau, \alpha, D) := |\tau| - \left[ (1-D)\tau^Y + R \right],$$

where  $R(\alpha, D) = (1 - D) \left[ \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha) + H\alpha \right]$ . We fix *D* since we are interested in showing the convexity of *f* with respect to  $\tau$  and *R*. Let  $x_1 = (\tau_1, R_1), x_2 = (\tau_2, R_2), \xi \in [0, 1]$ , with  $R_i = (\alpha_i, D) = \mathbb{K}_0^C \mathcal{D}_t^{\beta K}(\alpha) |_{\alpha = \alpha_i} + H\alpha_i$ . Therefore, we have:

$$\begin{split} f\left(\xi x_{1}+(1-\xi)x_{2}\right) &= |\xi\tau_{1}+(1-\xi)\tau_{2}|-(1-D)\tau^{Y}-\xi R_{1}-(1-\xi)R_{2},\\ &= |\xi\tau_{1}+(1-\xi)\tau_{2}|-\xi\left[(1-D)\tau_{Y}+R_{1}\right]\\ &-(1-\xi)\left[(1-D)\tau^{Y}+R_{2}\right],\\ &\leq \xi\left\{|\tau_{1}|-\left[(1-D)\tau^{Y}+R_{1}\right]\right\} (\text{by Jensen inequality})\\ &+(1-\xi)\left\{|\tau_{2}|-\left[(1-D)\tau^{Y}+R_{2}\right]\right\},\\ &= \xi f(x_{1})+(1-\xi)f(x_{2}). \end{split}$$

## **B.4** Local Truncation Error for the Free-Energy Discretization

We prove the local truncation error (5.47) for the discretized Helmholtz free-energy density. Before we prove it, we need the following result.

**Lemma B.4.1.** *Let*  $\beta \in (0, 1)$ *, then* 

$$\int_{t_i}^{t_{i+1}} \left[ (t_{n+1} - s)^{-\beta} - (2t_{n+1} - s)^{-\beta} \right] ds \le C_1 \Delta t^{1-\beta}, \quad 0 \le i \le n,$$
(B.8)

where  $C_1$  is a constant independent of  $\Delta t$ .

Proof. We can obtain

$$\begin{split} &\int_{t_i}^{t_{i+1}} \left[ (t_{n+1} - s)^{-\beta} - (2t_{n+1} - s)^{-\beta} \right] ds \\ &= -\frac{(t_{n+1} - s)^{1-\beta}}{1-\beta} \bigg|_{t_i}^{t_{i+1}} + \frac{(2t_{n+1} - s)^{1-\beta}}{1-\beta} \bigg|_{t_i}^{t_{i+1}} \\ &= \frac{\Delta t^{1-\beta}}{1-\beta} \left[ (n+1-i)^{1-\beta} - (n-i)^{1-\beta} + (2n+1-i)^{1-\beta} - (2n+2-i)^{1-\beta} \right]. \end{split}$$

Since

$$(n+1)^{1-\beta} - n^{1-\beta} = (1-\beta) \int_{-1}^{0} (n-s)^{-\beta} ds \le (1-\beta)n^{-\beta}, \quad n \ge 1,$$

then, when  $0 \le i \le n - 1$ , we have

$$\begin{split} \int_{t_i}^{t_{i+1}} \left[ (t_{n+1} - s)^{-\beta} - (2t_{n+1} - s)^{-\beta} \right] ds &\leq \Delta t^{1-\beta} \left[ \frac{1}{(n-i)^{\beta}} - \frac{1}{(2n+1-i)^{\beta}} \right] \\ &\leq \frac{\Delta t^{1-\beta}}{(n-i)^{\beta}}, \end{split}$$

for i = n, it holds that

$$\begin{split} \int_{t_n}^{t_{n+1}} \left[ (t_{n+1} - s)^{-\beta} - (2t_{n+1} - s)^{-\beta} \right] ds \\ &= \frac{\Delta t^{1-\beta}}{1-\beta} \left[ 1 + (n+1)^{1-\beta} - (n+2)^{1-\beta} \right] \\ &\leq \frac{\Delta t^{1-\beta}}{1-\beta} \left[ 1 - \frac{1-\beta}{(n+1)^{\beta}} \right] \leq \frac{\Delta t^{1-\beta}}{1-\beta}. \end{split}$$

Therefore this lemma is proved. Next, we prove the local truncation error for the free-energy discretization. From

$$\begin{split} \rho\psi(\varepsilon_{n+1}) = &\tilde{\mathbb{E}} \int_{0}^{t_{n+1}} \int_{0}^{t_{n+1}} \frac{\dot{\varepsilon}(s_1)\dot{\varepsilon}(s_2)}{(2t_{n+1} - s_1 - s_2)^{\beta}} ds_1 ds_2 \\ = &\tilde{\mathbb{E}} \sum_{i,j=0}^{n} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} \frac{\Delta\varepsilon_{i+1}\Delta\varepsilon_{j+1}}{\Delta t^2 (2t_{n+1} - s_1 - s_2)^{\beta}} ds_1 ds_2 + \tilde{r}_{\Delta t}^{n+1}, \end{split}$$

with 
$$\tilde{\mathbb{E}} = \frac{\mathbb{E}}{2\Gamma(1-\beta)}$$
 and  $\Delta \varepsilon_{k+1} = \varepsilon_{k+1} - \varepsilon_k$ . We know that  

$$\begin{aligned} \left| \vec{r}_{\Delta t}^{n+1} \right| &= \left| \tilde{\mathbb{E}} \sum_{i,j=0}^n \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \left[ \dot{\varepsilon}(s_1)\dot{\varepsilon}(s_2) - \frac{\Delta \varepsilon_{i+1}\Delta \varepsilon_{j+1}}{\Delta t^2} \right] ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \sum_{i,j=0}^n \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \left[ \dot{\varepsilon}(s_1)\dot{\varepsilon}(s_2) - \dot{\varepsilon}(s_1) \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right. \\ &+ \dot{\varepsilon}(s_1) \frac{\Delta \varepsilon_{j+1}}{\Delta t} - \frac{\Delta \varepsilon_{i+1}\Delta \varepsilon_{j+1}}{\Delta t^2} \right] ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \sum_{i,j=0}^n \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \left[ \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_2) - \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right) \right. \\ &+ \frac{\Delta \varepsilon_{j+1}}{\Delta t} \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) \right] ds_1 ds_2 \right| \\ &\leq \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_2) - \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &+ \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \dot{\varepsilon}(s_1) \left| \frac{\delta \varepsilon_{i+1}}{\Delta t} \right| ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right| \left| \frac{\delta \varepsilon_{i+1}}{\Delta t} \right| ds_1 ds_2 \right| \\ &= \left| \tilde{\mathbb{E}} \left| \frac{\delta \varepsilon_{i+1}}{\Delta t} \right| ds_1 ds_2 \right| ds_1 ds_2 \right| ds_1 ds_2 \right| ds_1 ds_2 ds_1$$

where

$$I_{1} = \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \int_{t_{i}}^{t_{i+1}} \int_{t_{j}}^{t_{j+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta} \dot{\varepsilon}(s_{1}) \left( \dot{\varepsilon}(s_{2}) - \frac{\Delta \varepsilon_{j+1}}{\Delta t} \right) ds_{1} ds_{2} \right|,$$

and

$$I_2 = \tilde{\mathbb{E}} \left| \sum_{i,j=0}^n \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} (2t_{n+1} - s_1 - s_2)^{-\beta} \left( \dot{\varepsilon}(s_1) - \frac{\Delta \varepsilon_{i+1}}{\Delta t} \right) ds_1 ds_2 \right|.$$

Assume  $\varepsilon(t) \in C^2[0, T]$ , then one can obtain that:

$$\varepsilon(t) \le C_2, \quad \dot{\varepsilon}(t) \le C_3, \ t \in [0, T].$$

On each small interval  $[t_i, t_{i+1}]$   $(0 \le i \le n)$ , denoting the linear interpolation function of  $\varepsilon(t)$  as  $\prod_i \varepsilon(t)$ :

$$\Pi_i \varepsilon(t) = \frac{t - t_{i+1}}{t_i - t_{i+1}} \varepsilon_i + \frac{t - t_i}{t_{i+1} - t_i} \varepsilon_{i+1},$$

it follows from the linear interpolation theory that

$$\varepsilon(t) - \prod_i \varepsilon(t) = \frac{\varepsilon''(\xi_i)}{2} (t - t_i)(t - t_{i+1}) \le c_i \Delta t^2, \quad t \in [t_i, t_{i+1}], \ \xi_i \in (t_i, t_{i+1}),$$

with  $0 \le i \le n$ , and here  $c_i$  is a constant independent of  $\Delta t$ .

For  $I_1$ , we have

$$\begin{split} I_{1} &= \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \int_{t_{j}}^{t_{j+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta} \left[ \varepsilon(s_{2}) - \Pi_{j}\varepsilon(s_{2}) \right]' ds_{1} ds_{2} \right| \\ &= \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \int_{t_{j}}^{t_{j+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta} d\left[ \varepsilon(s_{2}) - \Pi_{j}\varepsilon(s_{2}) \right] ds_{1} \right| \\ &= \beta \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \int_{t_{j}}^{t_{j+1}} \left[ \varepsilon(s_{2}) - \Pi_{j}\varepsilon(s_{2}) \right] (2t_{n+1} - s_{1} - s_{2})^{-\beta-1} ds_{1} ds_{2} \right| \\ &\leq \beta \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \int_{t_{j}}^{t_{j+1}} c_{j}\Delta t^{2} (2t_{n+1} - s_{1} - s_{2})^{-\beta-1} ds_{1} ds_{2} \right| \\ &\leq \beta \tilde{\mathbb{E}} C_{4}\Delta t^{2} \left| \sum_{i=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \int_{0}^{t_{n+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta-1} ds_{1} ds_{2} \right| \\ &= \tilde{\mathbb{E}} C_{3}C_{4}\Delta t^{2} \left| \sum_{i=0}^{n} \int_{t_{i}}^{t_{i+1}} \dot{\varepsilon}(s_{1}) \left[ (t_{n+1} - s_{1})^{-\beta} - (2t_{n+1} - s_{1})^{-\beta} \right] ds_{1} \right| \\ &\leq \tilde{\mathbb{E}} C_{3}C_{4}\Delta t^{2} \left| \sum_{i=0}^{n} \int_{t_{i}}^{t_{i+1}} \left[ (t_{n+1} - s_{1})^{-\beta} - (2t_{n+1} - s_{1})^{-\beta} \right] ds_{1} \right|, \end{split}$$

where  $C_4 = \max_{0 \le j \le n} c_j$ . For  $I_2$ , it holds that

$$\begin{split} I_{2} &= \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_{i}}^{t_{i+1}} \int_{t_{j}}^{t_{j+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta} \left[ \varepsilon(s_{1}) - \Pi_{i} \varepsilon(s_{1}) \right]' ds_{1} ds_{2} \right| \\ &= \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_{j}}^{t_{j+1}} \int_{t_{i}}^{t_{i+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta} d\left[ \varepsilon(s_{1}) - \Pi_{i} \varepsilon(s_{1}) \right] ds_{2} \right| \\ &= \beta \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_{j}}^{t_{j+1}} \int_{t_{i}}^{t_{i+1}} \left[ \varepsilon(s_{1}) - \Pi_{i} \varepsilon(s_{1}) \right] (2t_{n+1} - s_{1} - s_{2})^{-\beta - 1} ds_{1} ds_{2} \right| \\ &\leq \beta \tilde{\mathbb{E}} \left| \sum_{i,j=0}^{n} \frac{\Delta \varepsilon_{j+1}}{\Delta t} \int_{t_{j}}^{t_{j+1}} \int_{t_{i}}^{t_{i+1}} c_{i} \Delta t^{2} (2t_{n+1} - s_{1} - s_{2})^{-\beta - 1} ds_{1} ds_{2} \right| \\ &\leq \beta \tilde{\mathbb{E}} C_{5} \Delta t \left| \sum_{j=0}^{n} \Delta \varepsilon_{j+1} \int_{t_{j}}^{t_{j+1}} \int_{0}^{t_{n+1}} (2t_{n+1} - s_{1} - s_{2})^{-\beta - 1} ds_{1} ds_{2} \right| \\ &= \tilde{\mathbb{E}} C_{5} \Delta t \left| \sum_{j=0}^{n} \Delta \varepsilon_{j+1} \int_{t_{j}}^{t_{j+1}} \int_{0}^{t_{j+1}} \left[ (t_{n+1} - s_{2})^{-\beta} - (2t_{n+1} - s_{2})^{-\beta} \right] ds_{2} \right|, \end{split}$$

where  $C_5 = \max_{0 \le i \le n} c_i$ . Then, it follows from Lemma B.4.1 that

$$\begin{split} I_1 + I_2 &\leq \frac{n \mathbb{E}C_1 C_3 C_4 \Delta t^{3-\beta}}{2\Gamma(1-\beta)} + \frac{\mathbb{E}C_1 C_5 \Delta t^{2-\beta}}{2\Gamma(1-\beta)} \left| \sum_{j=0}^n \Delta \varepsilon_{j+1} \right| \\ &= \frac{\mathbb{E}C_1 C_3 C_4 T \Delta t^{2-\beta}}{2\Gamma(1-\beta)} + \frac{\mathbb{E}C_1 C_5 \Delta t^{2-\beta}}{2\Gamma(1-\beta)} |\varepsilon_{n+1} - \varepsilon_0| \\ &\leq \frac{\mathbb{E}C_1 (C_3 C_4 T + 2C_2 C_5)}{2\Gamma(1-\beta)} \Delta t^{2-\beta}. \end{split}$$

	_	_	٦.

#### **APPENDIX C**

#### **DERIVATIONS IN CHAPTER 6**

# C.1 Proof of Proposition 1

*Proof.* Similar to the derivation of the tangent elasto-plastic modulus in classical plasticity [192], we start by taking the time derivative of the yield function to enforce the persistency condition:

$$\begin{split} \dot{f}(\sigma,\alpha) &= \frac{d}{dt} \Big\{ |\sigma(t)| - \left[ \sigma^Y + \mathbb{K}_0^C \mathcal{D}_t^{\beta K} \alpha(t) + H \alpha(t) \right] \Big\} \\ &= \operatorname{sign}(\sigma) \dot{\sigma}(t) - \left[ \mathbb{K} \frac{d}{dt} {}_0^C \mathcal{D}_t^{\beta K} \alpha(t) + H \dot{\alpha}(t) \right]. \end{split}$$

Using the SB stress-strain relationship (6.5), we obtain:

$$\dot{f}(\sigma,\alpha) = \operatorname{sign}(\sigma) \mathbb{E}\left[\frac{d}{dt} {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \varepsilon(t) - \frac{d}{dt} {}_{0}^{C} \mathcal{D}_{t}^{\beta E} \varepsilon^{\nu p}(t)\right] - \left[\mathbb{K}\frac{d}{dt} {}_{0}^{C} \mathcal{D}_{t}^{\beta K} \alpha(t) + H\dot{\alpha}(t)\right].$$
(C.1)

Employing definition (6.2) for the Caputo derivative, performing integration by parts and employing the Leibniz integral rule, we obtain:

$$\frac{d}{dt} {}_{0}^{C} \mathcal{D}_{t}^{\beta} u(t) = \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \int_{0}^{t} \frac{\dot{u}(s)}{(t-s)^{\beta}} ds \quad (\text{from(6.2)})$$

$$= \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \left[ \dot{u}(s) \frac{(t-s)^{1-\beta}}{1-\beta} \Big|_{t}^{0} + \int_{0}^{t} \frac{(t-s)^{1-\beta} \ddot{u}(s)}{1-\beta} ds \right]$$

$$= \frac{\dot{u}(0)t^{-\beta}}{\Gamma(1-\beta)} + \frac{1}{\Gamma(1-\beta)} \int_{0}^{t} \frac{\ddot{u}(s)}{(t-s)^{\beta}} ds$$

$$= \frac{\dot{u}(0)t^{-\beta}}{\Gamma(1-\beta)} + {}_{0}^{C} \mathcal{D}_{t}^{\beta} \dot{u}(t) \quad (C.2)$$

Substituting (C.2) into (C.1), setting  $\dot{\gamma}(0) = 0$ , and therefore  $\dot{\alpha}(0) = 0$  (from (6.20)) and  $\dot{\varepsilon}^{\nu p}(0) = 0$  (from (6.19)), we obtain:

$$\dot{f}(\sigma,\alpha) = \operatorname{sign}(\sigma) \mathbb{E}\left[\frac{\dot{\varepsilon}(0)t^{-\beta_E}}{\Gamma(1-\beta_E)} + {}_0^C \mathcal{D}_t^{\beta_E} \dot{\varepsilon}(t) - {}_0^C \mathcal{D}_t^{\beta_E} \dot{\varepsilon}^{vp}(t)\right] - \mathbb{K}_0^C \mathcal{D}_t^{\beta_K} \dot{\alpha}(t) - H\dot{\alpha}(t). \quad (C.3)$$

Finally, substituting (6.20) and (6.19) into (C.3), and enforcing the persistency condition  $\dot{f}(\sigma, \alpha) = 0$ , we obtain:

$$\mathbb{E}_{0}^{C}\mathcal{D}_{t}^{\beta_{E}}\dot{\gamma}(t) + \mathbb{K}_{0}^{C}\mathcal{D}_{t}^{\beta_{K}}\dot{\gamma}(t) + H\dot{\gamma}(t) = \operatorname{sign}(\sigma)\mathbb{E}\left[\frac{\dot{\varepsilon}(0)t^{-\beta_{E}}}{\Gamma(1-\beta_{E})} + {}_{0}^{C}\mathcal{D}_{t}^{\beta_{E}}\dot{\varepsilon}(t)\right].$$
(C.4)

# C.2 Discretization Terms for Fractional Viscoelastic Models

Scott-Blair:

$$C_1^{SB} = \frac{\mathbb{E}}{\Delta t^{\beta_1} \Gamma(2 - \beta_1)}.$$

Fractional Kelvin-Voigt:

$$C_1^{KV} = \frac{\mathbb{E}_1}{\Delta t^{\beta_1} \Gamma(2-\beta_1)}, \quad C_2^{KV} = \frac{\mathbb{E}_2}{\Delta t^{\beta_2} \Gamma(2-\beta_2)}.$$

Fractional Maxwell:

$$C_1^M = \frac{\mathbb{E}_2}{\Delta t^{\beta_2} \Gamma(2-\beta_2)}, \quad C_2^M = \frac{\mathbb{E}_2/\mathbb{E}_1}{\Delta t^{\beta_2-\beta_1} \Gamma(2-\beta_2+\beta_1)}.$$

Fractional Kelvin-Zener:

$$C_1^{KZ} = \frac{\mathbb{E}_2}{\Delta t^{\beta_2} \Gamma(2 - \beta_2)}, \quad C_2^{KZ} = \frac{\mathbb{E}_3}{\Delta t^{\beta_3} \Gamma(2 - \beta_3)}$$
$$C_3^{KZ} = \frac{\mathbb{E}_2 \mathbb{E}_3 / \mathbb{E}_1}{\Delta t^{\beta_2 + \beta_3 - \beta_1} \Gamma(2 - \beta_1 - \beta_3 + \beta_2)}, \quad C_4^{KZ} = \frac{\mathbb{E}_2 / \mathbb{E}_1}{\Delta t^{\beta_2 - \beta_1} \Gamma(2 - \beta_2 + \beta_1)}$$

Fractional Poynting-Thomson:

$$\begin{aligned} C_1^{PT} &= \frac{\mathbb{E}_1}{\Delta t^{\beta_1} \Gamma(2-\beta_1)}, \quad C_2^{PT} &= \frac{\mathbb{E}_2}{\Delta t^{\beta_2} \Gamma(2-\beta_2)} \\ C_3^{PT} &= \frac{\mathbb{E}_1/\mathbb{E}_3}{\Delta t^{\beta_1-\beta_3} \Gamma(2-\beta_1+\beta_3)}, \quad C_4^{PT} &= \frac{\mathbb{E}_2/\mathbb{E}_3}{\Delta t^{\beta_2-\beta_3} \Gamma(2-\beta_2+\beta_3)} \end{aligned}$$

Fractional Quasi Linear Visco-Elastic:

$$C_1^{QLV} = \frac{EAB}{\Delta t^{\beta} \Gamma(2-\beta)}.$$

#### **APPENDIX D**

### **DERIVATIONS IN CHAPTER 7**

## D.1 Derivation of Governing Equation Using Extended Hamilton's Principle

## **Equation of Motion**

We recast the integral (7.20) as  $\delta W = \int_0^L \int_A \sigma \,\delta\varepsilon \,dA \,ds$  for the considered cantilever beam, in which the variation of strain is  $\delta\varepsilon = -\eta \,\delta \frac{\partial\psi}{\partial s}$ , using (7.10). Therefore, by assuming the constitutive equation (7.19), the variation of total work is expressed as

$$\delta w = \int_{0}^{L} \int_{A} \left( -\eta E_{\infty} \frac{\partial \psi}{\partial s} - \eta E_{\alpha} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) (-\eta \delta \frac{\partial \psi}{\partial s}) dA ds$$
$$= \int_{0}^{L} \left( E_{\infty} \left( \int_{A} \eta^{2} dA \right) \frac{\partial \psi}{\partial s} + E_{\alpha} \left( \int_{A} \eta^{2} dA \right) \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) \delta \frac{\partial \psi}{\partial s} ds$$
$$= \int_{0}^{L} \left( E_{\infty} I \frac{\partial \psi}{\partial s} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) \delta \frac{\partial \psi}{\partial s} ds$$
(D.1)

where  $I = \int_{A} \eta^2 dA$ . By approximation (7.9), we write the variation of curvature as

$$\delta \frac{\partial \psi}{\partial s} = (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \,\delta \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} \frac{\partial v}{\partial s} \,\delta \frac{\partial v}{\partial s}. \tag{D.2}$$

Therefore, the variation of total energy becomes

$$\delta w = \int_{0}^{L} \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \delta \frac{\partial^{2} v}{\partial s^{2}} ds$$
$$+ \int_{0}^{L} \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) \frac{\partial^{2} v}{\partial s^{2}} \frac{\partial v}{\partial s} \delta \frac{\partial v}{\partial s} ds \qquad (D.3)$$

By expanding the terms and integrating by parts, we have

$$\begin{split} \delta w &= \int_{0}^{L} \frac{\partial^{2}}{\partial s^{2}} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right) \delta v \, ds \\ &- \int_{0}^{L} \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) \frac{\partial^{2} v}{\partial s^{2}} \frac{\partial v}{\partial s} \delta v \, ds \\ &+ \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \delta \frac{\partial v}{\partial s} \bigg|_{0}^{L} \\ &- \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right) \delta v \bigg|_{0}^{L} \\ &+ \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right) \delta v \bigg|_{0}^{L} \end{aligned} \tag{D.4}$$

The prescribed geometry boundary conditions at the base of the beam, s = 0, allow the variation of deflection and its first derivative to be zero at s = 0, i.e.  $\delta v(0, t) = \delta \frac{\partial v}{\partial s}(0, t) = 0$ . Therefore,

$$\begin{split} \delta w &= \int_{0}^{L} \frac{\partial^{2}}{\partial s^{2}} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right) \delta v \, ds \\ &- \int_{0}^{L} \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) \frac{\partial^{2} v}{\partial s^{2}} \frac{\partial v}{\partial s} \right) \delta v \, ds \\ &+ \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right|_{s=L} \delta \frac{\partial v}{\partial s} (L, t) \\ &- \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right) \right|_{s=L} \delta v(L, t) \\ &+ \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] \right) \frac{\partial^{2} v}{\partial s^{2}} \frac{\partial v}{\partial s} \right|_{s=L} \delta v(L, t)$$
(D.5)

Let  $\rho$  be mass per unit volume of the beam, M and J be the mass and rotatory inertia of the lumped mass at the tip of beam. By considering the displacement and velocity of the beam given in (7.2)

and (7.3), respectively, the kinetic energy is obtained as

$$T = \frac{1}{2} \int_{0}^{L} \int_{A} \varrho \left(\frac{\partial \mathbf{r}}{\partial t}\right)^{2} dA \, ds + \frac{1}{2} M \left( \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right)^{2} \right) \Big|_{s=L} + \frac{1}{2} J \left(\frac{\partial \psi}{\partial t}\right)^{2} \Big|_{s=L},$$

$$= \frac{1}{2} \int_{0}^{L} \int_{A} \varrho \left\{ \left(\frac{\partial u}{\partial t} - \eta \frac{\partial \psi}{\partial t} \cos(\psi)\right)^{2} + \left(\frac{\partial v}{\partial t} + \dot{v}_{b} - \eta \frac{\partial \psi}{\partial t} \sin(\psi)\right)^{2} \right\} dA \, ds$$

$$+ \frac{1}{2} M \left( \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right)^{2} \right) \Big|_{s=L} + \frac{1}{2} J \left(\frac{\partial \psi}{\partial t}\right)^{2} \Big|_{s=L},$$

$$= \frac{1}{2} \int_{0}^{L} \int_{A} \varrho \left\{ \left(\frac{\partial u}{\partial t}\right)^{2} - 2\eta \frac{\partial u}{\partial t} \frac{\partial \psi}{\partial t} \cos(\psi) + \eta^{2} \left(\frac{\partial \psi}{\partial t}\right)^{2} \cos^{2}(\psi) + \left(\frac{\partial v}{\partial t}\right)^{2} + \dot{v}_{b}^{2} + 2\frac{\partial v}{\partial t} \dot{v}_{b} - 2\eta \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right) \frac{\partial \psi}{\partial t} \sin(\psi) + \eta^{2} \left(\frac{\partial \psi}{\partial t}\right)^{2} \sin^{2}(\psi) \right\} dA \, ds$$

$$+ \frac{1}{2} M \left( \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right)^{2} \right) \Big|_{s=L} + \frac{1}{2} J \left(\frac{\partial \psi}{\partial t}\right)^{2} \Big|_{s=L},$$

$$= \frac{1}{2} \int_{0}^{L} \int_{A} \varrho \left\{ \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right)^{2} + \dot{v}_{b}^{2} + 2\frac{\partial v}{\partial t} \dot{v}_{b} - 2\eta \frac{\partial u}{\partial t} \frac{\partial \psi}{\partial t} \cos(\psi) + \eta^{2} \left(\frac{\partial \psi}{\partial t}\right)^{2} \Big|_{s=L},$$

$$= \frac{1}{2} \int_{0}^{L} \int_{A} \varrho \left\{ \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t}\right)^{2} + \dot{v}_{b}^{2} + 2\frac{\partial v}{\partial t} \dot{v}_{b} - 2\eta \frac{\partial u}{\partial t} \frac{\partial \psi}{\partial t} \cos(\psi) + \eta^{2} \left(\frac{\partial \psi}{\partial t}\right)^{2} \Big|_{s=L}.$$

$$D(h)$$

$$= 2\eta \left(\frac{\partial v}{\partial t} + \dot{v}_{b}\right) \frac{\partial \psi}{\partial t} \sin(\psi) \right\} dA \, ds + \frac{1}{2} M \left( \left(\frac{\partial u}{\partial t}\right)^{2} + \left(\frac{\partial v}{\partial t}\right)^{2} \right) \Big|_{s=L}.$$

Let

$$\rho = \int_{A} \varrho dA, \quad \mathcal{J}_{1} = \int_{A} \varrho \eta dA, \quad \mathcal{J}_{2} = \int_{A} \varrho \eta^{2} dA.$$

 $\rho$  is the mass per unit length of the beam,  $\mathcal{J}_1$  is the first moment of inertia and is zero because the reference point of coordinate system attached to the cross section coincides with the mass centroid, and  $\mathcal{J}_2$  is the second moment of inertia, which is very small for slender beam and can be ignored [281]. Assuming that the velocity along the length of the beam,  $\dot{u}$ , is relatively small compared to the lateral velocity  $\dot{v} + \dot{v}_b$ , the kinetic energy of the beam can be reduced to

$$T = \frac{1}{2} \rho \int_0^L \left(\frac{\partial v}{\partial t} + \dot{v_b}\right)^2 ds + \frac{1}{2} M \left(\frac{\partial v}{\partial t} + \dot{v_b}\right)^2 \Big|_{s=L} + \frac{1}{2} J \left(\frac{\partial \psi}{\partial t}\right)^2 \Big|_{s=L}, \tag{D.7}$$

where its variation can be taken as

$$\delta T = \rho \int_0^L \left(\frac{\partial v}{\partial t} + \dot{v_b}\right) \delta \frac{\partial v}{\partial t} \, ds + M \left(\frac{\partial v}{\partial t} + \dot{v_b}\right) \delta \frac{\partial v}{\partial t}\Big|_{s=L} + J \frac{\partial \psi}{\partial t} \delta \frac{\partial \psi}{\partial t}\Big|_{s=L},\tag{D.8}$$

in which  $\frac{\partial \psi}{\partial t}$  is given in (7.8) and  $\delta \frac{\partial \psi}{\partial t}$  can be obtained as

$$\delta \frac{\partial \psi}{\partial t} \simeq (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \delta \frac{\partial^2 v}{\partial t \partial s} + \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial t \partial s} \delta \frac{\partial v}{\partial s}.$$

Therefore,

$$\delta T \simeq \rho \int_{0}^{L} (\frac{\partial v}{\partial t} + \dot{v_{b}}) \delta \frac{\partial v}{\partial t} ds + M(\frac{\partial v}{\partial t} + \dot{v_{b}}) \delta \frac{\partial v}{\partial t} \Big|_{s=L} + J \left( \frac{\partial^{2} v}{\partial t \partial s} (1 + (\frac{\partial v}{\partial s})^{2}) \delta \frac{\partial^{2} v}{\partial t \partial s} + \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial t \partial s})^{2} \delta \frac{\partial v}{\partial s} \right) \Big|_{s=L}.$$
(D.9)

The time integration of  $\delta T$  takes the following form through integration by parts

$$\begin{split} \int_{t_{1}}^{t_{2}} \delta T \, dt &= \int_{t_{1}}^{t_{2}} \left\{ \rho \int_{0}^{L} \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \, ds + M \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \Big|_{s=L} \right. \\ &+ J \left( \frac{\partial^{2} v}{\partial t \partial s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) \delta \frac{\partial^{2} v}{\partial t \partial s} + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t \partial s} \right)^{2} \delta \frac{\partial v}{\partial s} \right) \Big|_{s=L} \right\} dt \\ &= \int_{t_{1}}^{t_{2}} \rho \int_{0}^{L} \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \, ds \, dt + M \int_{t_{1}}^{t_{2}} \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \Big|_{s=L} \, dt \\ &+ J \int_{t_{1}}^{t_{2}} \left( \frac{\partial^{2} v}{\partial t \delta s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) \delta \frac{\partial^{2} v}{\partial t \partial s} + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t \partial s} \right)^{2} \delta \frac{\partial v}{\partial s} \right) \Big|_{s=L} \, dt \\ &= \rho \int_{0}^{L} \int_{t_{1}}^{t_{2}} \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \, dt \, ds + M \int_{t_{1}}^{t_{2}} \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta \frac{\partial v}{\partial t} \, dt \Big|_{s=L} \\ &+ J \int_{t_{1}}^{t_{2}} \left( \frac{\partial^{2} v}{\partial t \delta s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) \delta \frac{\partial^{2} v}{\partial t \partial s} + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t \partial s} \right)^{2} \delta \frac{\partial v}{\partial s} \right) \, dt \Big|_{s=L} \end{split} \tag{D.10} \\ &= \rho \int_{0}^{L} \left[ \left( \frac{\partial v}{\partial t} + \dot{v}_{b} \right) \delta v \Big|_{t_{1}}^{t_{2}} - \int_{t_{1}}^{t_{2}} \left( \frac{\partial^{2} v}{\partial t^{2}} + \dot{v}_{b} \right) \delta v dt \Big|_{s=L} + J \frac{\partial v}{\partial t \partial s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) \delta \frac{\partial v}{\partial s} \, dt \Big|_{s=L} \Big|_{t_{1}}^{t_{2}} \\ &- M \int_{t_{1}}^{t_{2}} \left( \frac{\partial^{2} v}{\partial t^{2}} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) + \frac{\partial v}{\partial t} \left( \frac{\partial^{2} v}{\partial t^{2}} \right) \delta v dt \Big|_{s=L} \Big|_{t_{1}}^{t_{2}} \\ &- J \int_{t_{1}}^{t_{2}} \left( \frac{\partial^{3} v}{\partial t^{2}} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t^{2}} \right)^{2} \right) \delta \frac{\partial v}{\partial s} \, dt \Big|_{s=L} \\ &= - \int_{t_{1}}^{t_{2}} \left\{ \rho \int_{0}^{L} \left( \frac{\partial^{2} v}{\partial t^{2}} + \dot{v}_{b} \right) \delta v ds + M \left( \frac{\partial^{2} v}{\partial t^{2}} + \dot{v}_{b} \right) \delta v \Big|_{s=L} \\ &+ J \left( \frac{\partial^{3} v}{\partial t^{2} \partial s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t^{2} \partial s} \right)^{2} \right) \delta \frac{\partial v}{\partial s} \Big|_{s=L} \\ &+ J \left( \frac{\partial^{3} v}{\partial t^{2} \partial s} \left( 1 + \left( \frac{\partial v}{\partial s} \right)^{2} \right) + \frac{\partial v}{\partial s} \left( \frac{\partial^{2} v}{\partial t^{2} \partial s} \right)^{2} \right) \delta \frac{\partial v}{\partial s} \Big|_{s=L} \\ \end{aligned}$$

where we consider that  $\delta v = \delta \frac{\partial v}{\partial s} = 0$  at  $t = t_1$  and  $t = t_2$ . Therefore, the extended Hamilton's principle takes the form

$$\begin{split} \int_{t_1}^{t_2} \left\{ \int_0^L \left[ -\rho(\frac{\partial^2 v}{\partial t^2} + v_b) - \frac{\partial^2}{\partial s^2} \left( \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right) + E_{\alpha} I \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \\ + \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right) + \frac{\partial^2 v}{\partial s^2} \frac{\partial v}{\partial s} \right) \right] \delta v \, ds \\ - M(\frac{\partial^2 v}{\partial t^2} + v_b) \Big|_{s=L} \delta v(L, t) - J \left( \frac{\partial^3 v}{\partial t^2 \partial s} (1 + (\frac{\partial v}{\partial s})^2) + \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial t \partial s})^2 \right) \Big|_{s=L} \delta \frac{\partial v}{\partial s} (L, t) \\ - \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) + E_{\alpha} I \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) (1 \\ & + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \Big|_{s=L} \delta \frac{\partial v}{\partial s} (L, t) \\ + \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) + E_{\alpha} I \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) (1 \\ & + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \Big|_{s=L} \delta v(L, t) \\ + \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) + E_{\alpha} I \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) (1 \\ & + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \Big|_{s=L} \delta v(L, t) - \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) + E_{\alpha} I \frac{R_L}{\partial s} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) \frac{\partial^2 v}{\partial s^2} \frac{\partial v}{\partial s} \Big|_{s=L} \delta v(L, t) \Big|_{s=L} \delta v(L, t) + \frac{1}{2} (\frac{\partial v}{\partial s})^2 \right) \right|_{s=L} \delta v(L, t) = \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right|_{s=L} \delta v(L, t) - \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right|_{s=L} \delta v(L, t) + \frac{1}{2} (\frac{\partial v}{\partial s})^2 \right|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) = \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right|_{s=L} \delta v(L, t) \left|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) \right|_{s=L} \delta v(L, t) \right|_{$$

Invoking the arbitrariness of virtual displacement  $\delta v$ , we obtain the strong form of the equation of motion as:

$$\rho \frac{\partial^2 v}{\partial t^2} + E_{\infty} I \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2)^2 \right) + E_{\alpha} I \frac{\partial^2}{\partial s^2} \left( (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) - E_{\alpha} I \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] \right) = -\rho \, \vec{v_b},$$
(D.12)

which is subject to the following natural boundary conditions:

$$\begin{split} J\left(\frac{\partial^{3}v}{\partial t^{2}\partial s}(1+(\frac{\partial v}{\partial s})^{2})+\frac{\partial v}{\partial s}(\frac{\partial^{2}v}{\partial t\delta s})^{2}\right)+E_{\infty}I\frac{\partial^{2}v}{\partial s^{2}}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})^{2}\\ +E_{\alpha}I(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})\stackrel{RL}{_{0}}\mathcal{D}_{t}^{\alpha}\left[\frac{\partial^{2}v}{\partial s^{2}}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})\right]\Big|_{s=L}=0, M(\frac{\partial^{2}v}{\partial t^{2}}+\vec{v_{b}})\\ -\frac{\partial}{\partial s}\left(E_{\infty}I\frac{\partial^{2}v}{\partial s^{2}}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})^{2}+E_{\alpha}I(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})\stackrel{RL}{_{0}}\mathcal{D}_{t}^{\alpha}\left[\frac{\partial^{2}v}{\partial s^{2}}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})\right]\right)\\ +\left(E_{\infty}I\frac{\partial v}{\partial s}(\frac{\partial^{2}v}{\partial s^{2}})^{2}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})+E_{\alpha}I\frac{\partial v}{\partial s}\frac{\partial^{2}v}{\partial s^{2}}\stackrel{RL}{_{0}}\mathcal{D}_{t}^{\alpha}\left[\frac{\partial^{2}v}{\partial s^{2}}(1+\frac{1}{2}(\frac{\partial v}{\partial s})^{2})\right]\right)\Big|_{s=L}\\ =0. \end{split}$$

Following a similar approach as in (7.9) in deriving the beam curvature, we obtain the approximations below, where we only consider up to third order terms and remove the higher order terms (HOTs).

$$\frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2)^2 = \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + \text{HOTs}$$

$$(1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] = \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} + \text{HOTs}$$

$$\frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) = \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + \text{HOTs}$$

$$\frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] = \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} + \text{HOTs}$$

Therefore, the strong form can be approximated up to the third order and the problem then reads as: find  $v \in V$  such that

$$m \frac{\partial^2 v}{\partial t^2} + \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 \right) - \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 \right) + E_r \frac{\partial^2}{\partial s^2} \left( {}^{RL}_0 \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} (\frac{\partial v}{\partial s})^2 {}^{RL}_0 \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right)$$
(D.14)  
$$- E_r \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} {}^{RL}_0 \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) = -m \ddot{v}_b,$$

By rearranging

$$m\frac{\partial^{2}v}{\partial t^{2}} + \frac{\partial^{2}}{\partial s^{2}} \left( \frac{\partial^{2}v}{\partial s^{2}} + \frac{\partial^{2}v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2}v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2}v}{\partial s^{2}} \right) - \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} (\frac{\partial^{2}v}{\partial s^{2}})^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2}v}{\partial s^{2}} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2}v}{\partial s^{2}} \right) = -m \ddot{v_{b}},$$
(D.15)

subject to the following boundary conditions:

$$\begin{aligned} v\Big|_{s=0} &= \frac{\partial v}{\partial s}\Big|_{s=0} \\ &= 0, \\ \frac{Jm}{\rho} \left(\frac{\partial^3 v}{\partial t^2 \partial s} (1 + (\frac{\partial v}{\partial s})^2) + \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial t \partial s})^2\right) \left(\frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[\frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2)\right] \\ &+ \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2}\right)\Big|_{s=L} \\ &= 0, \\ \frac{Mm}{\rho} (\frac{\partial^2 v}{\partial t^2} + \ddot{v}_b) - \frac{\partial}{\partial s} \left(\frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[\frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2)\right] + \frac{E_r}{2} (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2}\right) \\ &+ \left(\frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} R_L \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2}\right)\Big|_{s=L} \\ &= 0, \end{aligned} \tag{D.16}$$

where  $m = \frac{\rho}{E_{\infty} I}$  and  $E_r = \frac{E_{\alpha}}{E_{\infty}}$ .

## Nondimensionalization

Let the following dimensionless variables:

$$s^{*} = \frac{s}{L}, \quad v^{*} = \frac{v}{L}, \quad t^{*} = t \left(\frac{1}{mL^{4}}\right)^{1/2}, \quad E_{r}^{*} = E_{r} \left(\frac{1}{mL^{4}}\right)^{\alpha/2}, \quad J^{*} = \frac{J}{\rho L^{3}}, \quad M^{*} = \frac{M}{\rho L}, \quad v_{b}^{*} = \frac{v_{b}}{L}.$$
(D.17)

We obtain the following dimensionless equation by substituting the above dimensionless variables.

$$\begin{split} & m \frac{L}{mL^4} \frac{\partial^2 v^*}{\partial t^{*2}} + \frac{1}{L^2} \frac{\partial^2}{\partial s^{*2}} \Bigg| \frac{L}{L^2} \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{L}{L^2} \frac{\partial^2 v^*}{\partial s^{*2}} (\frac{L}{L} \frac{\partial v^*}{\partial s^*})^2 \\ & + \frac{E_r^* (mL^4)^{\alpha/2}}{2} \frac{1}{(mL^4)^{\alpha/2}} \frac{L}{L^2} (\frac{L}{L})^2 \frac{R_L}{0} \mathcal{D}_{t^*}^{\alpha} \frac{\partial^2 v^*}{\partial s^{*2}} (\frac{\partial v^*}{\partial s^*})^2 \\ & + E_r^* (mL^4)^{\alpha/2} \frac{1}{(mL^4)^{\alpha/2}} \frac{L}{L^2} \frac{R_L}{0} \mathcal{D}_{t^*}^{\alpha} \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{1}{2} E_r^* (mL^4)^{\alpha/2} (\frac{L}{L} \frac{\partial v^*}{\partial s^*})^2 \frac{1}{(mL^4)^{\alpha/2}} \frac{L}{L^2} \frac{R_L}{0} \mathcal{D}_{t^*}^{\alpha} \frac{\partial^2 v^*}{\partial s^{*2}} \\ & - \frac{1}{L} \frac{\partial}{\partial s^*} \Bigg[ \frac{L}{L} \frac{\partial v^*}{\partial s^*} (\frac{L}{L^2} \frac{\partial^2 v^*}{\partial s^{*2}})^2 + E_r^* (mL^4)^{\alpha/2} \frac{L}{L} \frac{\partial v^*}{\partial s^*} \frac{L}{L^2} \frac{\partial^2 v^*}{\partial s^{*2}} \frac{1}{(mL^4)^{\alpha/2}} \frac{L}{L^2} \frac{R_L}{0} \mathcal{D}_{t^*}^{\alpha} \frac{\partial^2 v^*}{\partial s^{*2}} \Bigg] \\ & = -m \frac{L}{mL^4} \frac{\partial^2 v_b^*}{\partial t^{*2}}, \end{split}$$
(D.18)

which can be simplified to

$$\frac{\partial^{2}v^{*}}{\partial t^{*2}} + \frac{\partial^{2}}{\partial s^{*2}} \left[ \frac{\partial^{2}v^{*}}{\partial s^{*2}} + \frac{\partial^{2}v^{*}}{\partial s^{*2}} (\frac{\partial v^{*}}{\partial s^{*}})^{2} + \frac{E_{r}^{*}}{2} \frac{R_{L}}{0} \mathcal{D}_{t^{*}}^{\alpha} \frac{\partial^{2}v^{*}}{\partial s^{*2}} (\frac{\partial v^{*}}{\partial s^{*}})^{2} \right] \\
+ E_{r}^{*} \frac{R_{L}}{0} \mathcal{D}_{t^{*}}^{\alpha} \frac{\partial^{2}v^{*}}{\partial s^{*2}} + \frac{1}{2} E_{r}^{*} (\frac{\partial v^{*}}{\partial s^{*}})^{2} \frac{R_{L}}{0} \mathcal{D}_{t^{*}}^{\alpha} \frac{\partial^{2}v^{*}}{\partial s^{*2}} \right] \\
- \frac{\partial}{\partial s^{*}} \left[ \frac{\partial v^{*}}{\partial s^{*}} (\frac{\partial^{2}v^{*}}{\partial s^{*2}})^{2} + E_{r}^{*} \frac{\partial v^{*}}{\partial s^{*}} \frac{\partial^{2}v^{*}}{\partial s^{*2}} \frac{R_{L}}{0} \mathcal{D}_{t^{*}}^{\alpha} \frac{\partial^{2}v^{*}}{\partial s^{*2}} \right] = -\frac{\partial^{2}v_{b}^{*}}{\partial t^{*2}},$$
(D.19)

The dimensionless boundary conditions are also obtained by substituting dimensionless vari-

ables in (D.16). We can show similarly that they preserve their structure as:

$$\begin{split} v^* \Big|_{s^*=0} &= \frac{\partial v^*}{\partial s^*} \Big|_{s^*=0} \\ &= 0, \\ \frac{J^* \rho L^3 m}{\rho} \frac{1}{m L^4} \left[ \frac{\partial^3 v^*}{\partial t^* \partial^2 s^*} \left( 1 + \left( \frac{\partial v^*}{\partial s^*} \right)^2 \right) + \frac{\partial v^*}{\partial s^*} \left( \frac{\partial^2 v^*}{\partial t^* \partial s^*} \right)^2 \right] + \frac{1}{L} \left[ \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{\partial^2 v^*}{\partial s^{*2}} \left( \frac{\partial v^*}{\partial s^*} \right)^2 + E_r^* \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{1}{2} E_r^* \left( \frac{\partial v^*}{\partial s^*} \right)^2 \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \right] \Big|_{s^*=1} \\ &= 0, \\ \frac{M^* \rho Lm}{\rho} \frac{L}{m L^4} \left( \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{\partial^2 v_b^*}{\partial s^{*2}} \right) \\ &- \frac{1}{L^2} \frac{\partial v^*}{\partial s^*} \left[ \frac{\partial^2 v^*}{\partial s^{*2}} + \frac{\partial^2 v^*}{\partial s^{*2}} \left( \frac{\partial v^*}{\partial s^*} \right)^2 + \frac{E_r^*}{2} \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \left( \frac{\partial v^*}{\partial s^{*2}} \right)^2 + E_r^* \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \left( \frac{\partial v^*}{\partial s^{*2}} \right)^2 + E_r^* \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \right] \\ &+ \frac{1}{2} E_r^* \left( \frac{\partial v^*}{\partial s^*} \right)^2 \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \right] + \frac{1}{L^2} \left[ \frac{\partial v^*}{\partial s^*} \left( \frac{\partial^2 v^*}{\partial s^{*2}} \right)^2 + E_r^* \frac{\partial v^*}{\partial s^*} \frac{\partial^2 v^*}{\partial s^{*2}} \frac{R_L}{0} \mathcal{D}_{t^*}^\alpha \frac{\partial^2 v^*}{\partial s^{*2}} \right] \right|_{s^*=1} \\ &= 0, \end{split}$$

Therefore, the dimensionless equation of motion becomes (after dropping \* for the sake of simplicity)

$$\frac{\partial^{2}v}{\partial t^{2}} + \frac{\partial^{2}}{\partial s^{2}} \left( \frac{\partial^{2}v}{\partial s^{2}} + \frac{\partial^{2}v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2}v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2}v}{\partial s^{2}} \right) - \frac{\partial}{\partial s} \left( \frac{\partial v}{\partial s} (\frac{\partial^{2}v}{\partial s^{2}})^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2}v}{\partial s^{2}} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2}v}{\partial s^{2}} \right) = -\vec{v}_{b},$$
(D.20)

which is subject to the following dimensionless boundary conditions

$$\begin{aligned} v \Big|_{s=0} &= \frac{\partial v}{\partial s} \Big|_{s=0} \\ &= 0, \\ J \left( \frac{\partial^3 v}{\partial t^2 \partial s} (1 + (\frac{\partial v}{\partial s})^2) + \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s \partial t})^2 \right) \\ &+ \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \Big|_{s=1} \\ &= 0, \\ M (\frac{\partial^2 v}{\partial t^2} + \dot{v}_b) - \frac{\partial}{\partial s} \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r (\frac{\partial v}{\partial s})^2 \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \\ &+ \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{R_L}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \Big|_{s=1} \\ &= 0. \end{aligned} \tag{D.21}$$

# **D.2** Single Mode Decomposition

In order to demonstrate that the single mode decomposition satisfies the weak form solution and boundary conditions, we consider the case of no lumped mass at the tip, *i.e.*, M = J = 0, and check if the proposed approximate solution solves the weak form and corresponding boundary conditions. First we substitute the boundary conditions in the weak formulation and then we use single-mode approximation to recover equation (7.30). Therefore, start integrating Equation (7.24) by parts as follows:

$$\begin{split} &\int_{0}^{1} \frac{\partial^{2} v}{\partial t^{2}} \tilde{v} ds + \frac{\partial}{\partial s} \left( \frac{\partial^{2} v}{\partial s^{2}} + \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \tilde{v} \Big|_{0}^{1} \\ &- \left( \frac{\partial^{2} v}{\partial s^{2}} + \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \frac{\partial \tilde{v}}{\partial s} \Big|_{0}^{1} \\ &+ \int_{0}^{1} \left( \frac{\partial^{2} v}{\partial s^{2}} + \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \frac{\partial^{2} \tilde{v}}{\partial s^{2}} ds \\ &- \left( \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial s^{2}})^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2} v}{\partial s^{2}} R_{L}^{\alpha} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \tilde{v} \Big|_{0}^{1} + \int_{0}^{1} \left( \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial s^{2}} )^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2} v}{\partial s^{2}} \right) \frac{\partial \tilde{v}}{\partial s} ds = f(t) \\ & (D.22) \end{split}$$

When M = J = 0 the boundary conditions in equation (7.22) are given by:

$$\begin{aligned} v \Big|_{s=0} &= \frac{\partial v}{\partial s} \Big|_{s=0} = 0, \\ \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r \left( \frac{\partial v}{\partial s} \right)^2 \frac{RL}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial^2 s} \right) \Big|_{s=1} = 0, \\ &- \frac{\partial v}{\partial s} \left( \frac{\partial^2 v}{\partial s^2} + \frac{\partial^2 v}{\partial s^2} (\frac{\partial v}{\partial s})^2 + E_r \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^2) \right] + \frac{1}{2} E_r \left( \frac{\partial v}{\partial s} \right)^2 \frac{RL}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \\ &+ \left( \frac{\partial v}{\partial s} (\frac{\partial^2 v}{\partial s^2})^2 + E_r \frac{\partial v}{\partial s} \frac{\partial^2 v}{\partial s^2} \frac{RL}{0} \mathcal{D}_t^{\alpha} \frac{\partial^2 v}{\partial s^2} \right) \Big|_{s=1} = 0, \end{aligned}$$
(D.23)

By substituting (D.23) in (D.22) we obtain:

$$\int_{0}^{1} \frac{\partial^{2} v}{\partial t^{2}} \tilde{v} \, ds$$

$$+ \int_{0}^{1} \left( \frac{\partial^{2} v}{\partial s^{2}} + \frac{\partial^{2} v}{\partial s^{2}} (\frac{\partial v}{\partial s})^{2} + E_{r} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} (1 + \frac{1}{2} (\frac{\partial v}{\partial s})^{2}) \right] + \frac{1}{2} E_{r} (\frac{\partial v}{\partial s})^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \, ds$$

$$+ \int_{0}^{1} \left( \frac{\partial v}{\partial s} (\frac{\partial^{2} v}{\partial s^{2}})^{2} + E_{r} \frac{\partial v}{\partial s} \frac{\partial^{2} v}{\partial s^{2}} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial^{2} v}{\partial s^{2}} \right) \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \tilde{v}' \, ds = f(t),$$

$$(D.24)$$

The modal discretization utilized in (7.27) can be simplified as  $v(s, t) = q(t)\phi(s)$ , where we choose  $\phi(0) = \phi'(0) = 0$ , and  $\phi''(0) = \phi'''(0) = 0$ . Furthermore, setting  $\tilde{v} = \phi(s)$ , (D.24) is given by:

$$\ddot{q} \int_{0}^{1} \phi \phi ds + \int_{0}^{1} \left( q \phi'' + q^{3} \phi'' \phi'^{2} \right) \phi'' ds + \int_{0}^{1} E_{r} \phi'' \frac{RL}{0} \mathcal{D}_{t}^{\alpha} q \phi'' ds + \int_{0}^{1} \frac{1}{2} E_{r} \phi''(\phi')^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} q^{3} \phi'' ds + \int_{0}^{1} \frac{1}{2} E_{r} \phi'^{2} \phi'' q^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} q \phi'' ds + \int_{0}^{1} \left( \phi' \phi''^{2} q^{3} + E_{r} \phi' \phi'' \phi'' q^{2} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} q \right) \phi' ds = f(t), \quad (D.25)$$

considering (7.31) for the case without a lumped mass, we have,

$$\mathcal{M} = \int_{0}^{1} \phi^{2} ds, \quad \mathcal{K}_{l} = C_{l} = \int_{0}^{1} \phi''^{2} ds, \quad \mathcal{K}_{nl} = C_{nl} = \int_{0}^{1} \phi'^{2} \phi''^{2} ds, \quad \mathcal{M}_{b} = \int_{0}^{1} \phi ds.$$
(D.26)

Substituting the above relationships into (D.25), we obtain (7.30):

$$\mathcal{M}\ddot{q} + \mathcal{K}_l q + E_r C_l \, {}^{RL}_0 \mathcal{D}_t^{\alpha} q + 2\mathcal{K}_{nl} q^3 + \frac{E_r C_{nl}}{2} \left( {}^{RL}_0 \mathcal{D}_t^{\alpha} q^3 + 3 \, q^2 \, {}^{RL}_0 \mathcal{D}_t^{\alpha} q \right) = -\mathcal{M}_b \, \ddot{v_b}. \tag{D.27}$$

## **D.3** Deriving the Linearized Equation of Motion

Since our problem considers geometrical nonlinearities, we let the following kinematic linearizations under the assumption small motions, respective, for the rotation angle (7.7), angular velocity (7.8), and curvature (7.9):

$$\psi \simeq \frac{\partial v}{\partial s}, \qquad \frac{\partial \psi}{\partial t} \simeq \frac{\partial^2 v}{\partial t \partial s}, \qquad \frac{\partial \psi}{\partial s} \simeq \frac{\partial^2 v}{\partial s^2}, \tag{D.28}$$

With their corresponding variations given by:

$$\delta\psi \simeq \delta \frac{\partial v}{\partial s}, \qquad \delta \frac{\partial \psi}{\partial t} \simeq \delta \frac{\partial^2 v}{\partial t \partial s}, \qquad \delta \frac{\partial \psi}{\partial s} \simeq \delta \frac{\partial^2 v}{\partial s^2}$$
(D.29)

Similar to D.1, the variation of total work is expressed as:

$$\delta w = \int_{0}^{L} \int_{A} \left( -\eta E_{\infty} \frac{\partial \psi}{\partial s} - \eta E_{\alpha} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) (-\eta \delta \frac{\partial \psi}{\partial s}) dA ds$$
$$= \int_{0}^{L} \left( E_{\infty} \left( \int_{A} \eta^{2} dA \right) \frac{\partial \psi}{\partial s} + E_{\alpha} \left( \int_{A} \eta^{2} dA \right) \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) \delta \frac{\partial \psi}{\partial s} ds$$
$$= \int_{0}^{L} \left( E_{\infty} I \frac{\partial \psi}{\partial s} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \frac{\partial \psi}{\partial s} \right) \delta \frac{\partial \psi}{\partial s} ds. \tag{D.30}$$

Employing approximation (D.29) for the variation of curvature, the variation of total energy becomes:

$$\delta w = \int_0^L \left( E_\infty I \frac{\partial^2 v}{\partial s^2} + E_\alpha I \frac{R_L}{0} \mathcal{D}_t^\alpha \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \delta \frac{\partial^2 v}{\partial s^2} \, ds. \tag{D.31}$$

Expanding the terms and integrating by parts, we have

$$\delta w = \int_{0}^{L} \frac{\partial^{2}}{\partial s^{2}} \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \delta v \, ds + \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \delta \frac{\partial v}{\partial s} \Big|_{0}^{L} - \frac{\partial}{\partial s} \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \delta v \Big|_{0}^{L}$$
(D.32)

Employing the boundary conditions  $\delta v(0, t) = \delta \frac{\partial v}{\partial s}(0, t) = 0$  into (D.32), we obtain:

$$\delta w = \int_{0}^{L} \frac{\partial^{2}}{\partial s^{2}} \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \delta v ds + \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \bigg|_{s=L} \delta \frac{\partial v}{\partial s} (L, t)$$

$$- \frac{\partial}{\partial s} \left( \left( E_{\infty} I \frac{\partial^{2} v}{\partial s^{2}} + E_{\alpha} I \frac{R_{L}}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \right) \bigg|_{s=L} \delta v(L, t). \tag{D.33}$$

From D.1, the kinetic energy of the beam is given to:

$$T = \frac{1}{2} \rho \int_0^L \left(\frac{\partial v}{\partial t} + \dot{v_b}\right)^2 ds + \frac{1}{2} M \left(\frac{\partial v}{\partial t} + \dot{v_b}\right)^2 \Big|_{s=L} + \frac{1}{2} J \left(\frac{\partial \psi}{\partial t}\right)^2 \Big|_{s=L},$$
 (D.34)

where its variation can be taken as

$$\delta T = \rho \int_0^L \left(\frac{\partial v}{\partial t} + \dot{v_b}\right) \delta \frac{\partial v}{\partial t} \, ds + M \left(\frac{\partial v}{\partial t} + \dot{v_b}\right) \delta \frac{\partial v}{\partial t} \Big|_{s=L} + J \frac{\partial \psi}{\partial t} \delta \frac{\partial \psi}{\partial t} \Big|_{s=L},\tag{D.35}$$

Employing the approximations (D.28) and (D.29), to the above equation, we obtain:

$$\delta T \simeq \rho \int_0^L (\frac{\partial v}{\partial t} + \dot{v_b}) \delta \frac{\partial v}{\partial t} ds + M (\frac{\partial v}{\partial t} + \dot{v_b}) \delta \frac{\partial v}{\partial t} \Big|_{s=L} + J \frac{\partial^2 v}{\partial t \partial s} \delta \frac{\partial^2 v}{\partial t \partial s} \Big|_{s=L}.$$
 (D.36)

The time integration of  $\delta T$  takes the following form through integration by parts

$$\begin{split} \int_{t_1}^{t_2} \delta T \, dt &= \int_{t_1}^{t_2} \left\{ \rho \int_0^L \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \, ds + M \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \Big|_{s=L} + J \left( \frac{\partial^2 v}{\partial t \partial s} \right) \delta \frac{\partial^2 v}{\partial t \partial s} \Big|_{s=L} \right\} dt \\ &= \int_{t_1}^{t_2} \rho \int_0^L \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \, ds \, dt \\ &+ M \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \Big|_{s=L} \, dt + J \int_{t_1}^{t_2} \left( \frac{\partial^2 v}{\partial t \partial s} \right) \delta \frac{\partial^2 v}{\partial t} \, ds \, dt \\ &= \rho \int_0^L \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \, dt \, ds + M \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \, dt \, ds + M \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta \frac{\partial v}{\partial t} \, dt \, ds + M \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta v \Big|_{s=L} \\ &+ J \int_{t_1}^{t_2} \left( \frac{\partial^2 v}{\partial t \partial s} \right) \delta \frac{\partial^2 v}{\partial t \partial s} \, dt \, ds + M \int_{t_1}^{t_2} \left( \frac{\partial v}{\partial t} + v_b \right) \delta v \Big|_{s=L} \\ &= \rho \int_0^L \left[ \left( \frac{\partial v}{\partial t} + v_b \right) \delta v \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \left( \frac{\partial^2 v}{\partial t^2} + v_b^* \right) \delta v dt \right] \, ds + M \left( \frac{\partial v}{\partial t} + v_b \right) \delta v \Big|_{s=L} \right|_{t_1}^{t_2} \\ &- M \int_{t_1}^{t_2} \left( \frac{\partial^2 v}{\partial t^2} + v_b^* \right) \delta v dt \Big|_{s=L} + J \left( \frac{\partial^2 v}{\partial t^2} \right) \delta \frac{\partial v}{\partial s} \Big|_{s=L} \right|_{t_1}^{t_2} - J \int_{t_1}^{t_2} \left( \frac{\partial^3 v}{\partial t^2 \partial s} \right) \delta \frac{\partial v}{\partial s} \, dt \Big|_{s=L} \\ &= - \int_{t_1}^{t_2} \left\{ \rho \int_0^L \left( \frac{\partial^2 v}{\partial t^2} + v_b^* \right) \delta v ds + M \left( \frac{\partial^2 v}{\partial t^2} + v_b^* \right) \delta v \Big|_{s=L} + J \left( \frac{\partial^3 v}{\partial t^2 \partial s} \right) \delta \frac{\partial v}{\partial s} \Big|_{s=L} \right\} dt, \end{aligned}$$
(D.37)

where we consider that  $\delta v = \delta \frac{\partial v}{\partial s} = 0$  at  $t = t_1$  and  $t = t_2$ . Therefore, the extended Hamilton's

principle takes the form

$$\int_{t_1}^{t_2} \left\{ \int_0^L \left[ -\rho(\frac{\partial^2 v}{\partial t^2} + \dot{v_b}) - \frac{\partial^2}{\partial s^2} \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \right] \delta v \, ds \\ - \left[ M(\frac{\partial^2 v}{\partial t^2} + \dot{v_b}) - \frac{\partial}{\partial s} \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \right] \delta v \Big|_{s=L}$$

$$- \left[ J \left( \frac{\partial^3 v}{\partial t^2 \partial s} \right) - \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \right] \delta \frac{\partial v}{\partial s} \Big|_{s=L}$$

$$- \left[ J \left( \frac{\partial^3 v}{\partial t^2 \partial s} \right) - \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \right] \delta \frac{\partial v}{\partial s} \Big|_{s=L} \right\} dt = 0.$$

Invoking the arbitrariness of virtual displacement  $\delta v$ , we obtain the strong form of the equation of motion as:

$$\rho \frac{\partial^2 v}{\partial t^2} + E_{\infty} I \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} \right) + E_{\alpha} I \frac{\partial^2}{\partial s^2} \left( {}^{RL}_{0} \mathcal{D}^{\alpha}_t \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) = -\rho \ddot{v}_b \tag{D.39}$$

which is subject to the following natural boundary conditions:

$$\begin{cases} J \frac{\partial^3 v}{\partial t^2 \partial s} - E_{\infty} I \frac{\partial^2 v}{\partial s^2} - E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \end{cases} \bigg|_{s=L} = 0, \\ \begin{cases} M \left( \frac{\partial^2 v}{\partial t^2} + \ddot{v}_b \right) - \frac{\partial}{\partial s} \left( E_{\infty} I \frac{\partial^2 v}{\partial s^2} + E_{\alpha} I \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \end{cases} \bigg|_{s=L} = 0. \end{cases}$$
(D.40)

Therefore, the strong form reads as: find  $v \in V$  such that

$$m \frac{\partial^2 v}{\partial t^2} + \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} + E_r \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) = -m \ddot{v}_b, \tag{D.41}$$

subject to the following boundary conditions:

$$\begin{aligned} v \Big|_{s=0} &= \frac{\partial v}{\partial s} \Big|_{s=0} = 0, \end{aligned}$$
(D.42) 
$$\begin{aligned} &\frac{Jm}{\rho} \frac{\partial^3 v}{\partial t^2 \partial s} - \left( \frac{\partial^2 v}{\partial s^2} + E_r \, \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \Big|_{s=L} &= 0, \end{aligned}$$
$$\begin{aligned} &\frac{Mm}{\rho} \left( \frac{\partial^2 v}{\partial t^2} + \ddot{v}_b \right) - \frac{\partial}{\partial s} \left( \frac{\partial^2 v}{\partial s^2} + E_r \, \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \Big|_{s=L} &= 0, \end{aligned}$$

where  $m = \frac{\rho}{E_{\infty} I}$  and  $E_r = \frac{E_{\alpha}}{E_{\infty}}$ .

#### Nondimensionalization of Linearized Equation of Motion

Employing the dimensionless variables defined by (D.17) in a similar fashion as D.1, and dropping the superscript \* for simplicity, our dimensionless linearized equation of motion becomes:

$$\frac{\partial^2 v}{\partial t^2} + \frac{\partial^2}{\partial s^2} \left( \frac{\partial^2 v}{\partial s^2} + E_r \frac{RL}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) = -\ddot{v}_b, \tag{D.43}$$

which is subject to the following dimensionless boundary conditions

$$\begin{aligned} v \Big|_{s=0} &= \frac{\partial v}{\partial s} \Big|_{s=0} = 0, \\ J \frac{\partial^3 v}{\partial t^2 \partial s} - \left( \frac{\partial^2 v}{\partial s^2} + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \Big|_{s=1} = 0, \\ M \left( \frac{\partial^2 v}{\partial t^2} + \ddot{v}_b \right) - \frac{\partial}{\partial s} \left( \frac{\partial^2 v}{\partial s^2} + E_r \frac{R_L}{0} \mathcal{D}_t^{\alpha} \left[ \frac{\partial^2 v}{\partial s^2} \right] \right) \Big|_{s=1} = 0, \end{aligned}$$
(D.44)

To obtain the corresponding weak form, we multiply both sides of (D.43) by proper test functions  $\tilde{v}(s) \in \tilde{V}$  and integrate the result over  $\Omega_s = [0, 1]$ . Therefore:

$$\int_{0}^{1} \frac{\partial^{2} v}{\partial t^{2}} \tilde{v} \, ds + \int_{0}^{1} \frac{\partial^{2}}{\partial s^{2}} \left( \frac{\partial^{2} v}{\partial s^{2}} + E_{r} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \right) \tilde{v} \, ds = -\int_{0}^{1} \frac{\partial^{2} v_{b}}{\partial t^{2}} \tilde{v} \, ds. \tag{D.45}$$

Integrating be above expression by parts and employing the corresponding boundary conditions (D.44) with M = J = 0, we obtain:

$$\int_{0}^{1} \frac{\partial^{2} v}{\partial t^{2}} \tilde{v} \, ds + \int_{0}^{1} \frac{\partial^{2} v}{\partial s^{2}} \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \, ds + E_{r} \int_{0}^{1} \frac{RL}{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v}{\partial s^{2}} \right] \frac{\partial^{2} \tilde{v}}{\partial s^{2}} \, ds = -\int_{0}^{1} \frac{\partial^{2} v_{b}}{\partial t^{2}} \tilde{v} \, ds. \tag{D.46}$$

Using (7.27) and (7.28), the problem (D.46) reads: find  $v_N \in V_N$  such that

$$\int_{0}^{1} \frac{\partial^{2} v_{N}}{\partial t^{2}} \tilde{v}_{N} \, ds + \int_{0}^{1} \frac{\partial^{2} v_{N}}{\partial s^{2}} \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} \, ds + E_{r} \int_{0}^{1} {}^{RL}_{0} \mathcal{D}_{t}^{\alpha} \left[ \frac{\partial^{2} v_{N}}{\partial s^{2}} \right] \frac{\partial^{2} \tilde{v}_{N}}{\partial s^{2}} \, ds, = -\int_{0}^{1} \frac{\partial^{2} v_{b}}{\partial t^{2}} \tilde{v} \, ds.$$
(D.47)

for all  $\tilde{v}_N \in \tilde{V}_N$ . Substituting the single-mode approximation in (D.47) in a similar fashion as Section 7.2.6, we obtain the following unimodal governing equation of motion:

$$\mathcal{M}\ddot{q} + \mathcal{K}_l q + E_r C_l \frac{RL}{0} \mathcal{D}_t^{\alpha} q = -\mathcal{M}_b \ddot{v}_b, \qquad (D.48)$$

where the coefficients  $\mathcal{M}$ ,  $\mathcal{K}_l$ ,  $C_l$  and  $\mathcal{M}_b$  are given by (D.26). Finally, multiplying both sides of (D.48) by  $1/\mathcal{M}$ , we obtain:

$$\ddot{q} + E_r c_l \frac{RL}{0} \mathcal{D}_t^{\alpha} q + k_l q = -m_b \ddot{v}_b, \qquad (D.49)$$

with the coefficients  $c_l = \frac{C_l}{M}$ ,  $k_l = \frac{K_l}{M}$  and  $m_n = \frac{M_b}{M}$ . We note that although we previously assumed M = J = 0 for the boundary conditions, we push the effects of the lumped mass with M = J = 1 through the choice of our spatial eigenfunctions  $\phi(s)$  (see D.4).

## **D.4 Eigenvalue Problem of Linear Model**

The assumed modes  $\phi_i(s)$  in discretization (7.27) are obtained by solving the corresponding eigenvalue problem of free vibration of undamped linear counterparts to our model. Thus, the dimensionless linearized undamped equation of motion takes the form

$$\frac{\partial^2}{\partial t^2}v(s,t) + \frac{\partial^4}{\partial s^4}v(s,t) = 0.$$
(D.50)

subject to linearized boundary conditions:

$$v(0,t) = 0, \qquad \qquad \frac{\partial^2 v}{\partial s^2}(1,t) = -J \ddot{v}'(1,t),$$
  
$$v'(0,t) = 0, \qquad \qquad v'''(1,t) = M \ddot{v}(1,t), \qquad (D.51)$$

where  $(\dot{}) = \frac{d}{dt}$  and  $(\dot{})' = \frac{d}{ds}$ . We derive the corresponding eigenvalue problem by applying the separation of variables, i.e. v(x, t) = X(s)T(t) to (D.50). Therefore,

$$\ddot{T}(t)X(s) + T(t)X'''(s) = 0, \qquad \frac{\ddot{T}(t)}{T(t)} + \frac{X'''(s)}{X(s)} = 0, \qquad \frac{\ddot{T}(t)}{T(t)} = -\frac{X'''(s)}{X(s)} = \lambda, \qquad (D.52)$$

which gives the following equations

$$\ddot{T}(t) + \omega^2 T(t) = 0,$$
 (D.53)

$$X''''(s) - \beta^4 X(s) = 0, \tag{D.54}$$

where  $\beta^4 = \omega^2$  and the boundary conditions are

$$X(0) = 0, X''(1) = J \omega^2 X'(1),$$
  

$$X'(0) = 0, X'''(1) = -M \omega^2 X(1).$$

the solution to (D.54) is of the form  $X(s) = A \sin(\beta s) + B \cos(\beta s) + C \sinh(\beta s) + D \cosh(\beta s)$ , where C = -A and D = -B, using the boundary conditions at s = 0. Therefore,

$$X(s) = A \left( \sin(\beta s) - \sinh(\beta s) \right) + B \left( \cos(\beta s) - \cosh(\beta s) \right).$$

Applying the first bondary condition at s = 1, i.e.  $X''(1) = J \omega^2 X'(1)$  gives

$$B = -\frac{\sin(\beta) + \sinh(\beta) + J\beta^3(\cos(\beta) - \cosh(\beta))}{\cos(\beta) + \cosh(\beta) - J\beta^3(\sin(\beta) - \sinh(\beta))}A,$$

that results in

$$X(s) = A \left[ (\sin(\beta s) - \sinh(\beta s)) - \frac{\sin(\beta) + \sinh(\beta) + J\beta^3(\cos(\beta) - \cosh(\beta))}{\cos(\beta) + \cosh(\beta) - J\beta^3(\sin(\beta) - \sinh(\beta))} (\cos(\beta s) - \cosh(\beta s)) \right].$$

Finally, using the second boundary condition at s = 1 gives the following transcendental equation for the case where M = J = 1:

$$-\left(1+\beta^{4}+\cos(\beta)\cosh(\beta)\right)+\beta\left(\sin(\beta)\cosh(\beta)-\cos(\beta)\sinh(\beta)\right)+\beta^{3}\left(\sin(\beta)\cosh(\beta)-\sinh(\beta)\cosh(\beta)\right)$$
$$+\beta^{4}\left(\sin(\beta)\sinh(\beta)+\cos(\beta)\cosh(\beta)\right)=0.$$
(D.55)

The first eigenvalue is computed as  $\beta_1^2 = \omega_1 = 1.38569$ , which results to the following first normalized eigenfunction, given in Fig. D.1 (left).

$$\phi(s) = X_1(s) = 5.50054 \sin(\beta_1 s) - 0.215842 \cos(\beta_1 s) - 5.50054 \sinh(\beta_1 s) + 0.215842 \cosh(\beta_1 s),$$
(D.56)

with  $\beta_1^2 = 1.38569$ . We note that (D.55) reduces to  $1 + \cos(\beta) \cosh(\beta) = 0$  for the case that there is no lumped mass at the tip of beam; this in fact gives the natural frequencies of a linear cantilever beam. In this case, the first eigenvalue is computed as  $\beta_1^2 = \omega_1 = 3.51602$ , which results to the following first normalized eigenfunction, given in Fig. D.1 (right).

$$\phi(s) = X_1(s) = 0.734096 \sin(\beta_1 s) - \cos(\beta_1 s) - 0.734096 \sinh(\beta_1 s) + \cosh(\beta_1 s), \quad \beta_1^2 = 3.51602.$$
(D.57)



Figure D.1: Top: The first eigenfunctions,  $X_1(s)$ , of the undamped linear counterpart of our model. It is used as the spatial functions in the single mode approximation. Bottom: The first eigenfunctions,  $X_1(s)$ , of the undamped linear counterpart of our model with no lumped mass at the tip. It is used as the spatial functions in the single mode approximation.

#### **APPENDIX E**

#### **DERIVATIONS IN CHAPTER 8**

#### **E.1 Discretization Coefficients for Fractional Derivatives**

We present the  $\alpha$ - and  $\Delta t$ - dependent coefficients for the local (8.16) and history (8.17) approximations for the RL fractional derivative, which are given by [5]:

$$\begin{cases} d_0^{(1)} = -\frac{\alpha \Delta t^{\alpha}}{\Gamma(2+\alpha)}, \quad d_1^{(1)} = \frac{\Delta t^{\alpha}}{\Gamma(2+\alpha)}, \qquad p = 1, \\ \\ d_0^{(2)} = -\frac{\alpha \Delta t^{\alpha}}{2\Gamma(3+\alpha)}, \quad d_1^{(2)} = \frac{\alpha(3+\alpha)\Delta t^{\alpha}}{\Gamma(3+\alpha)}, \quad d_2^{(2)} = \frac{(4+\alpha)\Delta t^{\alpha}}{2\Gamma(3+\alpha)}, \quad p = 2. \end{cases}$$
(E.1)

$$b_{j}^{(1)} = \frac{\Delta t^{\alpha}}{2\Gamma(\alpha)} \left[ a_{j}^{(\alpha+2)} - (2j-1) a_{j}^{(\alpha+1)} + j (j-1) a_{j}^{(\alpha)} \right],$$
(E.2)

$$b_{j}^{(2)} = -\frac{\Delta t^{\alpha}}{\Gamma(\alpha)} \left[ a_{j}^{(\alpha+2)} - 2ja_{j}^{(\alpha+1)} + (j+1)(j-1)a_{j}^{(\alpha)} \right],$$
(E.3)

$$b_{j}^{(3)} = \frac{\Delta t^{\alpha}}{2\Gamma(\alpha)} \left[ a_{j}^{(\alpha+2)} - (2j+1) a_{j}^{(\alpha+1)} + j (j+1) a_{j}^{(\alpha)} \right],$$
(E.4)

$$a_j^{(\alpha)} = \frac{1}{\alpha} \left[ (j+1)^{\alpha} - j^{\alpha} \right].$$
(E.5)

#### Singularity-Capturing Formulation for a Single Correction Term and **E.2 Time-Step**

Let the time domain  $\tilde{\Omega} = [0, \Delta t]$ , and let  $E : \mathbb{R} \to \mathbb{R}^+$  be the following quadratic error function over  $\sigma$ :

$$E(\boldsymbol{\sigma}) = ||u^{data}(t) - u^{N}(t;\boldsymbol{\sigma})||_{L^{2}(\tilde{\Omega})}^{2},$$

where we assume  $u^{data}(t)$  to be known, and  $u^{N}(t; \sigma)$  represents the numerical approximation of  $u^{data}(t)$ , with  $\sigma \in \mathbb{R}$  to be determined, such that  $E(\sigma)$  is minimized. Therefore, let the case for M = 1 correction term and for the first time-step  $t_1 = \Delta t$ . We obtain the following cost function:

$$E(\boldsymbol{\sigma}) = \left(u_1^{data} - u_1^N(\boldsymbol{\sigma})\right)^2 = \left(\Delta t^{\boldsymbol{\sigma}^*} - u_1^N(\boldsymbol{\sigma})\right)^2,$$
(E.6)

where  $u_1^N(\sigma)$  denotes the numerical solution for the FDE (8.6) at  $t = \Delta t$ , obtained through (8.13) and (8.27) in the following fashion:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}u^{N}(t)|_{t=\Delta t} + W_{1,1}\left(u^{N}_{1} - u_{0}\right) = \sum_{j=1}^{S} \frac{\Gamma(1 + \sigma^{*}_{j})}{\Gamma(1 + \sigma^{*}_{j} - \alpha)} \Delta t^{\sigma^{*}_{j} - \alpha}.$$
(E.7)

Recalling (8.11), we obtain the initial correction weight  $W_{1,1}$  by the following equation:

$${}^{RL}_{0}\mathcal{D}^{\alpha}_{t}\left(t^{\sigma_{1}}\right)|_{t=\Delta t}+W_{1,1}\left(t^{\sigma}_{1}\right)=\frac{\Gamma(1+\sigma_{1})}{\Gamma(1+\sigma_{1}-\alpha)}t^{\sigma_{1}-\alpha}_{1},$$

Recalling (8.16) with p = 1:

$$d_1^{(1)} \Delta t^{\sigma_1} + \Delta t^{\sigma_1} W_{1,1} = \frac{\Gamma(1+\sigma_1)}{\Gamma(1+\sigma_1-\alpha)} \Delta t^{\sigma_1-\alpha},$$

therefore, we obtain the closed form for the correction weight:

$$W_{1,1} = \frac{\Gamma(1+\sigma_1)}{\Gamma(1+\sigma_1-\alpha)} \Delta t^{-\alpha} - d_1^{(1)},$$
 (E.8)

Substituting (E.8) into (E.7), rewriting the RL derivative in its discretized form at  $t = \Delta t$ , and assuming homogeneous initial conditions  $u_0 = 0$ , we obtain:

$$d_1^{(1)}u_1^N + \left(\frac{\Gamma(1+\sigma_1)}{\Gamma(1+\sigma_1-\alpha)}\Delta t^{-\alpha} - d_1^{(1)}\right)u_1^N = f_1^{data},$$

hence,

$$u_1^N = \Delta t^{\alpha} \frac{\Gamma(1+\sigma_1-\alpha)}{\Gamma(1+\sigma_1)} f_1^{data}.$$
(E.9)

Substituting (E.9) into (E.6), we obtain, for  $t = \Delta t$ :

$$E(\sigma_1) = \left(u_1^{data} - \Delta t^{\alpha} \frac{\Gamma(1 + \sigma_1 - \alpha)}{\Gamma(1 + \sigma_1)} f_1^{data}\right)^2.$$
(E.10)

We assume that the above equation has a root at  $\sigma_1 = \sigma^*$ , that is,  $E(\sigma^*) = 0$ . Therefore, given an initial guess  $\sigma_1^{(0)}$ , we can apply a Newton scheme to iteratively obtain  $\sigma_1^{k+1}$  in the following fashion:

$$\sigma_1^{k+1} = \sigma_1^k - \frac{E(\sigma_1)}{\frac{\partial E(\sigma_1)}{\partial \sigma_1}} \Big|_{\sigma_1 = \sigma_1^k}, \tag{E.11}$$

where  $\frac{\partial E(\sigma_1)}{\partial \sigma_1}$  can be obtained analytically, and is given by:

$$\frac{\partial E(\sigma_1)}{\partial \sigma_1} = -2\psi^* \Delta t^\alpha \frac{\Gamma(1+\sigma_1-\alpha)}{\Gamma(1+\sigma_1)} \left( u_1^{data} - \Delta t^\alpha \frac{\Gamma(1+\sigma_1-\alpha)}{\Gamma(1+\sigma_1)} \right), \tag{E.12}$$

with  $\psi^* = \psi_0(1 + \sigma_1 - \alpha) - \psi_0(1 + \sigma_1)$ , where  $\psi_0(z)$  denotes the Polygamma function. We observe that the computational cost of the above procedure per iteration k is minimal, since there is no history computation when evaluating the corresponding time-fractional derivatives of  $u_1^N$ .

#### **APPENDIX F**

## **DERIVATIONS IN CHAPTER 9**

# F.1 Discretization Coefficients for the History Load Term

We present the coefficients  $\gamma_{k,j}^{(p)}$   $(0 \le j \le k, 0 \le k \le N, p = 0, 1)$  defined in (9.16):

$$\begin{split} \gamma_{0,0}^{(0)} &= 0, \quad \gamma_{0,0}^{(1)} = 0, \quad \gamma_{1,0}^{(1)} = \frac{\mathcal{A}_{1,1} - \mathcal{A}_{1,0}}{h}, \\ \gamma_{1,1}^{(1)} &= \frac{\mathcal{A}_{1,0} - \mathcal{A}_{1,1}}{h}, \quad \gamma_{2,0}^{(1)} = \frac{-2\mathcal{A}_{2,0} + \mathcal{A}_{2,1} - \mathcal{A}_{2,2}}{2h} + \frac{\mathcal{B}_{2,1} - \mathcal{B}_{2,2}}{(2 - \alpha)h^2}, \\ \gamma_{2,1}^{(1)} &= \frac{\mathcal{A}_{2,0} - \mathcal{A}_{2,1} + 2\mathcal{A}_{2,2}}{h} - \frac{2\mathcal{B}_{2,1} - 2\mathcal{B}_{2,2}}{(2 - \alpha)h^2}, \quad \gamma_{2,2}^{(1)} = \frac{\mathcal{A}_{2,1} - 3\mathcal{A}_{2,2}}{2h} + \frac{\mathcal{B}_{2,1} - \mathcal{B}_{2,2}}{(2 - \alpha)h^2}, \end{split}$$

for  $k \ge 1$ ,

$$\gamma_{k,j}^{(0)} = \begin{cases} \frac{\mathcal{A}_{k,1} - \mathcal{A}_{k,0}}{h}, & j = 0, \\ \frac{\mathcal{A}_{k,j-1} - 2\mathcal{A}_{k,j} + \mathcal{A}_{k,j+1}}{h}, & 1 \le j \le k - 1, \\ \frac{\mathcal{A}_{k,k-1} - \mathcal{A}_{k,k}}{h}, & j = k, \end{cases}$$

and, for  $k \ge 3$ ,

$$\gamma_{k,j}^{(1)} = \begin{cases} \frac{-2\mathcal{A}_{k,0} + \mathcal{A}_{k,1} - \mathcal{A}_{k,2}}{2h} + \frac{\mathcal{B}_{k,1} - \mathcal{B}_{k,2}}{(2-\alpha)h^2}, & j = 0, \\ \frac{2\mathcal{A}_{k,0} - 2\mathcal{A}_{k,1} + 3\mathcal{A}_{k,2} - \mathcal{A}_{k,3}}{2h} + \frac{-2\mathcal{B}_{k,1} + 3\mathcal{B}_{k,2} - \mathcal{B}_{k,3}}{(2-\alpha)h^2}, & j = 1, \\ \frac{\mathcal{A}_{k,j-1} - 3\mathcal{A}_{k,j} + 3\mathcal{A}_{k,j+1} - \mathcal{A}_{k,j+2}}{2h} + \frac{\mathcal{B}_{k,j-1} - 3\mathcal{B}_{k,j} + 3\mathcal{B}_{k,j+1} - \mathcal{B}_{k,j+2}}{(2-\alpha)h^2}, & 2 \le j \le k-2, \\ \frac{\mathcal{A}_{k,k-2} - 3\mathcal{A}_{k,k-1} + 4\mathcal{A}_{k,k}}{2h} + \frac{\mathcal{B}_{k,k-2} - 3\mathcal{B}_{k,k-1} + 2\mathcal{B}_{k,k}}{(2-\alpha)h^2}, & j = k-1, \\ \frac{\mathcal{A}_{k,k-1} - 3\mathcal{A}_{k,k}}{2h} + \frac{\mathcal{B}_{k,k-1} - \mathcal{B}_{k,k}}{(2-\alpha)h^2}, & j = k. \end{cases}$$

# F.2 Proofs

#### F.2.1 Proof of lemma 9.2.1

Before proof of Lemma 9.2.1, we need some preparatory results by introducing the notations:

$$a_{l}^{(\alpha)} = (l + \theta + 1)^{1-\alpha} - (l + \theta)^{1-\alpha}, \quad l \ge 0,$$
(F.1)

$$b_l^{(\alpha)} = \frac{(l+\theta+1)^{2-\alpha} - (l+\theta)^{2-\alpha}}{2-\alpha} - \frac{(l+\theta+1)^{1-\alpha} + (l+\theta)^{1-\alpha}}{2}, \quad l \ge 0,$$
(F.2)

and

$$c_{l}^{(\alpha)} = \begin{cases} a_{0}^{(\alpha)} + b_{0}^{(\alpha)}, & l = 0, \\ a_{l}^{(\alpha)} + b_{l}^{(\alpha)} - b_{l-1}^{(\alpha)}, & 1 \le l \le k - 2, \\ a_{l}^{(\alpha)} - b_{l-1}^{(\alpha)}, & l = k - 1. \end{cases}$$
(F.3)

where  $\theta \in [0, 1]$ . The following lemma states the properties of the above defined notations.

**Lemma F.2.1.** For any  $\alpha$  (0 <  $\alpha \leq 1$ ) and  $\{a_l^{(\alpha)}\}, \{b_l^{(\alpha)}\}\$  and  $\{c_l^{(\alpha)}\}\$  defined in (F.1)-(F.3), respectively, it holds that

• 
$$a_0^{(\alpha)} > a_1^{(\alpha)} > a_2^{(\alpha)} > \dots > a_l^{(\alpha)} > 0 \text{ as } l \to \infty, \ a_0^{(\alpha)} \le v_0;$$
  
•  $b_0^{(\alpha)} > b_1^{(\alpha)} > b_2^{(\alpha)} > \dots > b_l^{(\alpha)} > 0 \text{ as } l \to \infty;$   
•  $c_2^{(\alpha)} > c_3^{(\alpha)} > c_4^{(\alpha)} > \dots > c_{k-1}^{(\alpha)} > 0, \ \left| c_l^{(\alpha)} \right| \le v_0 \ (l = 0 \text{ or } 1), \ c_2^{(\alpha)} \le v_0,$ 

where  $v_0 > 0$  is a constant.

*Proof.* From the definition of  $a_l^{(\alpha)}$ , we can verify that  $a_0^{(\alpha)} = (\theta + 1)^{1-\alpha} - \theta^{1-\alpha}$  can be bounded by a constant  $v_1 > 0$  and

$$a_l^{(\alpha)} = (1 - \alpha) \int_l^{l+1} (x + \theta)^{-\alpha} dx, \quad l = 0, 1, 2, \dots,$$

where  $(x + \theta)^{-\alpha} > 0$  is a monotone decreasing function. Then it is no difficult to verify that

$$a_0^{(\alpha)} > a_1^{(\alpha)} > a_2^{(\alpha)} > \dots > a_l^{(\alpha)} > 0.$$

For the second conclusion and the first part of the third conclusion, the proofs are similar to that for Lemma 2.1 and Lemma 2.2 in [30]. Besides, in view of the definition (F.3) of  $c_1^{(\alpha)}$ , we have that

$$\begin{split} \left| c_0^{(\alpha)} \right| &= \left| \frac{(\theta+1)^{1-\alpha} - 3\theta^{1-\alpha}}{2} + \frac{(\theta+1)^{2-\alpha} - \theta^{2-\alpha}}{2-\alpha} \right| \\ &= \left| \frac{(\theta+1)^{1-\alpha} - 3\theta^{1-\alpha}}{2} + \frac{(2-\alpha)(\theta+\xi)^{1-\alpha}}{2-\alpha} \right| \le \frac{3\left[ (\theta+1)^{1-\alpha} + \theta^{1-\alpha} \right]}{2} \end{split}$$

where  $\xi \in (0, 1)$  and the mean value theorem has been used. It means  $|c_0^{(\alpha)}|$  can be bounded by a constant  $v_2 > 0$ . Similarly, we can get there exists a constant  $v_3 > 0$ , such that

$$\left| c_{1}^{(\alpha)} \right| \leq \frac{3(\theta+2)^{1-\alpha} + 4(\theta+1)^{1-\alpha} + \theta^{1-\alpha}}{2} \leq v_{3}$$

For  $c_2^{(\alpha)}$ , it follows  $\begin{aligned} c_2^{(\alpha)} &= \frac{(\theta+3)^{1-\alpha} - 2(\theta+2)^{1-\alpha} + (\theta+1)^{1-\alpha}}{2} + \frac{(\theta+3)^{2-\alpha} - 2(\theta+2)^{2-\alpha} + (\theta+1)^{2-\alpha}}{2-\alpha} \\ &= \frac{(\theta+3)^{1-\alpha} - 2(\theta+2)^{1-\alpha} + (\theta+1)^{1-\alpha}}{2} + \frac{(2-\alpha)(\theta+\eta_2)^{1-\alpha} - (2-\alpha)(\theta+\eta_1)^{1-\alpha}}{2-\alpha} \\ &\leq \frac{3(\theta+3)^{1-\alpha} - 2(\theta+2)^{1-\alpha} - (\theta+1)^{1-\alpha}}{2} \leq v_4, \end{aligned}$ 

where  $\eta_1 \in (1, 2), \eta_2 \in (2, 3)$  and  $v_4 > 0$  is a constant. Hence, by setting  $v_0 = \max_{1 \le l \le 4} v_l$  and summarizing the above results, all this completes the proof.

Next, we present the proof for Lemma 9.2.1.

*Proof.* Firstly, we consider the situation of p = 0. From (9.16), when j = 0, we have that

$$\begin{split} \gamma_{k,0}^{(0)} &= \frac{\mathcal{A}_{k,1} - \mathcal{A}_{k,0}}{h} = \frac{1}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \left[ (v - t_1)^{1 - \alpha} - (v - t_0)^{1 - \alpha} \right] dv \\ &= \frac{(t_{k+\tilde{\theta}} - t_1)^{1 - \alpha} - (t_{k+\tilde{\theta}} - t_0)^{1 - \alpha}}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv = -\frac{a_{k-1}^{(\alpha)}}{\alpha} < 0, \end{split}$$

where  $t_{k+\tilde{\theta}} = (k+\tilde{\theta})h$ ,  $\tilde{\theta} \in [0, 1]$  and the first mean value theorem for integrals has been used. For j = 1, 2, ..., k - 1, one has

$$\begin{split} \gamma_{k,j}^{(0)} &= \frac{\mathcal{A}_{k,j-1} - 2\mathcal{A}_{k,j} + \mathcal{A}_{k,j+1}}{h} \\ &= \frac{1}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \left[ (v - t_{j-1})^{1 - \alpha} - 2(v - t_j)^{1 - \alpha} + (v - t_{j+1})^{1 - \alpha} \right] dv \\ &= \frac{(t_{k+\tilde{\theta}} - t_{j-1})^{1 - \alpha} - 2(t_{k+\tilde{\theta}} - t_j)^{1 - \alpha} + (t_{k+\tilde{\theta}} - t_{j+1})^{1 - \alpha}}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv \\ &= \frac{a_{k-j}^{(\alpha)} - a_{k-j-1}^{(\alpha)}}{\alpha} < 0. \end{split}$$

For j = k, it holds that

$$\begin{split} \gamma_{k,k}^{(0)} &= \frac{\mathcal{A}_{k,k-1} - \mathcal{A}_{k,k}}{h} = \frac{1}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \left[ (v - t_{k-1})^{1 - \alpha} - (v - t_k)^{1 - \alpha} \right] dv \\ &= \frac{(t_{k+\tilde{\theta}} - t_{k-1})^{1 - \alpha} - (t_{k+\tilde{\theta}} - t_k)^{1 - \alpha}}{h} \int_{t_k}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv = \frac{a_0^{(\alpha)}}{\alpha} > 0, \end{split}$$

and  $\gamma_{k,k}^{(0)} = \frac{a_0^{(\alpha)}}{\alpha} \le \frac{v_0}{\alpha}$ , where Lemma F.2.1 has been used. Similarly, for  $\gamma_{k,j}^{(1)}$ , by using the first mean value theorem for integrals, we obtain

$$\gamma_{k,j}^{(1)} = \begin{cases} -\frac{c_{k-1}^{(\alpha)}}{\alpha}, & j = 0, \\ \frac{-c_{k-j-1}^{(\alpha)} + c_{k-j}^{(\alpha)}}{\alpha}, & 1 \le j \le k-1, \\ \frac{c_{0}^{(\alpha)}}{\alpha}, & j = k. \end{cases}$$

This, together with Lemma F.2.1, imply that  $\gamma_{k,j}^{(1)} < 0 \ (0 \le j \le k - 3)$  and

$$\begin{aligned} \left| \gamma_{k,k-2}^{(1)} \right| &= \left| \frac{-c_1^{(\alpha)} + c_2^{(\alpha)}}{\alpha} \right| \le \frac{2\nu_0}{\alpha}, \\ \left| \gamma_{k,k-1}^{(1)} \right| &= \left| \frac{-c_0^{(\alpha)} + c_1^{(\alpha)}}{\alpha} \right| \le \frac{2\nu_0}{\alpha}, \quad \left| \gamma_{k,k}^{(1)} \right| = \left| \frac{c_0^{(\alpha)}}{\alpha} \right| \le \frac{\nu_0}{\alpha}. \end{aligned}$$
Suppose that u(t) = 1 for  $t \in [0, T]$ , it follows from (9.16) that

$$\mathcal{H}^{k}(t_{k+1}) = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(0)} = \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \gamma_{k,j}^{(1)} = 0,$$

so we get  $\sum_{j=0}^{k} \gamma_{k,j}^{(0)} = 0$  and  $\sum_{j=0}^{k} \gamma_{k,j}^{(1)} = 0$ . Hence the lemma is proven.

## F.2.2 Proof of lemma 9.2.2

*Proof.* It follows from (9.11) that

$$\begin{split} & \left| t_{k} I_{t}^{\alpha} u(t) \right|_{t=t_{k+1}} - h^{\alpha} \sum_{j=0}^{p} \beta_{j}^{(p)} u(t_{k+1-j}) \right| \\ &= \frac{1}{\Gamma(\alpha)} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \left[ u(v) - \sum_{j=0}^{p} u(t_{k+1-j}) \prod_{i=0, i \neq j}^{p} \frac{v - t_{k+1-i}}{t_{k+1-j} - t_{k+1-i}} \right] dv \right| \\ &\leq \frac{1}{\Gamma(\alpha)} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} u^{(p+1)}(\varsigma) \prod_{i=0}^{p} (v - t_{k+1-i}) dv \right| \\ &\leq \frac{h^{p+1} |u^{(p+1)}(\varsigma)|}{\Gamma(\alpha)} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv \right| \leq v_{5} h^{\alpha + p+1} t_{k+1}^{\sigma - p - 1}, \end{split}$$

where  $\varsigma \in (t_k, t_{k+1})$  and  $v_5 > 0$  is a constant independent of *h*. This completes the proof.

## F.2.3 Proof of lemma 9.2.3

*Proof.* By (9.12), we have for k = 2, 3, ..., N - 1,  $N \ge 3$  (the cases for k = 0, 1 are easy to check, so we omit these case here) that

$$\begin{split} & \left| \mathcal{H}^{k}(t_{k+1}) - \mathcal{H}^{k}_{0}(t_{k+1}) \right| \\ = & \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \left| \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \sum_{j=0}^{k-1} \int_{t_{j}}^{t_{j+1}} \frac{u'(s) - (\Pi_{1,j}u(s))'}{(v-s)^{\alpha}} ds dv \right| \\ \leq & \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \left| \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \int_{0}^{t_{1}} \frac{u'(s) - (\Pi_{1,0}u(s))'}{(v-s)^{\alpha}} ds dv \right| \\ & + \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \left| \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \sum_{j=1}^{\hat{k}-1} \int_{t_{j}}^{t_{j+1}} \frac{u'(s) - (\Pi_{1,j}u(s))'}{(v-s)^{\alpha}} ds dv \right| \\ & + \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \left| \int_{t_{k}}^{t_{k+1}} \frac{1}{(t_{k+1}-v)^{1-\alpha}} \sum_{j=\hat{k}}^{k-1} \int_{t_{j}}^{t_{j+1}} \frac{u'(s) - (\Pi_{1,j}u(s))'}{(v-s)^{\alpha}} ds dv \right| \\ \vdots = & \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \left( I_{1} + I_{2} + I_{3} \right), \end{split}$$

where  $\hat{k} \in (1, k)$ . For  $I_1$ , by using the integration by parts, one gets that

$$\begin{split} I_{1} &= \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha} d\left[ u(s) - \Pi_{1,0} u(s) \right] dv \right| \\ &= \alpha \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha - 1} \left[ u(s) - \frac{s - t_{1}}{-t_{1}} u(0) - \frac{s}{t_{1}} u(t_{1}) \right] ds dv \right| \\ &= \alpha \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha - 1} \left[ \frac{s - t_{1}}{-t_{1}} \int_{0}^{s} u'(\tau) d\tau - \frac{s}{t_{1}} \int_{s}^{t_{1}} u'(\tau) d\tau \right] ds dv \right| \\ &= \alpha \sigma \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha - 1} \left[ \frac{s - t_{1}}{-t_{1}} \int_{0}^{s} \tau^{\sigma - 1} d\tau - \frac{s}{t_{1}} \int_{s}^{t_{1}} \tau^{\sigma - 1} d\tau \right] ds dv \right| \\ &\leq \alpha \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha - 1} s^{\sigma} ds dv \right| \\ &+ \alpha \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \int_{0}^{t_{1}} (v - s)^{-\alpha - 1} (t_{1}^{\sigma} - s^{\sigma}) ds dv \right| \\ &\leq 3\alpha t_{1}^{\sigma + 1} (t_{k} - t_{1})^{-\alpha - 1} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv \right| = 3h^{\sigma + \alpha + 1} t_{k-1}^{-\alpha - 1}. \end{split}$$

On the other hand, for  $I_2$ , by using the mean value theorem and the Euler-Maclaurin formula, we arrive at

$$\begin{split} &I_{2} = \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=1}^{\hat{k} - 1} \int_{t_{j}}^{t_{j+1}} \frac{2s - t_{j} - t_{j+1}}{2(v - s)^{\alpha}} u''(\xi_{j}) ds dv \right| \\ &\leq \sigma(\sigma - 1)h \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=1}^{\hat{k} - 1} t_{j}^{\sigma - 2} \int_{t_{j}}^{t_{j+1}} (v - s)^{-\alpha} ds dv \right| \\ &= \frac{\sigma(\sigma - 1)h}{1 - \alpha} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=1}^{\hat{k} - 1} t_{j}^{\sigma - 2} \left[ (v - t_{j})^{1 - \alpha} - (v - t_{j+1})^{1 - \alpha} \right] dv \right| \\ &\leq \sigma(\sigma - 1)h \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=1}^{\hat{k} - 1} t_{j}^{\sigma - 2} (v - t_{j+1})^{-\alpha} dv \right| \\ &\leq \sigma(\sigma - 1)h \sum_{j=1}^{\hat{k} - 1} t_{j}^{\sigma - 2} (t_{k} - t_{j+1})^{-\alpha} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv \right| \\ &\leq \frac{\sigma(\sigma - 1)}{\alpha} h^{\alpha + 1} t_{k}^{\sigma - \alpha - 1}, \end{split}$$

where  $\xi_j \in (t_j, t_{j+1})$   $(j = 1, 2, \dots, \hat{k} - 1)$ . Next, it holds that

$$\begin{split} I_{3} &= \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=\hat{k}}^{k-1} \int_{t_{j}}^{t_{j+1}} \frac{2s - t_{j} - t_{j+1}}{2(v - s)^{\alpha}} u''(\xi_{j}) ds dv \right| \\ &\leq \sigma(\sigma - 1)h \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \sum_{j=\hat{k}}^{k-1} t_{j}^{\sigma - 2} \int_{t_{j}}^{t_{j+1}} (v - s)^{-\alpha} ds dv \right| \\ &= \frac{\sigma(\sigma - 1)t_{\hat{k}}^{\sigma - 2}h}{1 - \alpha} \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} \left[ (v - t_{\hat{k}})^{1 - \alpha} - (v - t_{k})^{1 - \alpha} \right] dv \right| \\ &= \frac{\sigma(\sigma - 1)t_{\hat{k}}^{\sigma - 2}h}{1 - \alpha} \left[ (t_{k+\hat{\theta}} - t_{\hat{k}})^{1 - \alpha} - (t_{k+\hat{\theta}} - t_{k})^{1 - \alpha} \right] \left| \int_{t_{k}}^{t_{k+1}} (t_{k+1} - v)^{\alpha - 1} dv \right| \\ &\leq \frac{\sigma(\sigma - 1)t_{\hat{k}}^{\sigma - 2}h^{1 + \alpha}}{\alpha(1 - \alpha)} \left[ (t_{k+\hat{\theta}} - t_{\hat{k}})^{1 - \alpha} - (t_{k+\hat{\theta}} - t_{k})^{1 - \alpha} \right] \\ &\leq \frac{\sigma(\sigma - 1)t_{\hat{k}}^{\sigma - 2}h^{1 + \alpha}}{\alpha(1 - \alpha)} \left[ (t_{k+\hat{\theta}} - t_{\hat{k}})^{1 - \alpha} - (t_{k+\hat{\theta}} - t_{k})^{1 - \alpha} \right] \\ &\leq \frac{\sigma(\sigma - 1)T}{\alpha(1 - \alpha)} \left[ \frac{1}{(k - \hat{k} + \hat{\theta})^{\alpha}} - \frac{1}{\hat{\theta}^{\alpha}} \right] ht_{\hat{k}}^{\sigma - 2}, \end{split}$$

where  $\hat{\theta} \in [0, 1], \xi_j \in (t_j, t_{j+1})$   $(j = \hat{k}, \hat{k} + 1, \dots, k - 1)$ . Then for a suitable  $\hat{k}$ , there exists a constant  $v_6 > 0$  independent of *h* such that

$$\begin{split} \left| \mathcal{H}^{k}(t_{k+1}) - \mathcal{H}^{k}_{0}(t_{k+1}) \right| &\leq \frac{1}{\Gamma(\alpha)\Gamma(1-\alpha)} \Biggl\{ 3h^{\sigma+\alpha+1}t_{k-1}^{-\alpha-1} + \frac{\sigma(\sigma-1)}{\alpha}h^{\alpha+1}t_{k}^{\sigma-\alpha-1} + \frac{\sigma(\sigma-1)T}{\alpha(1-\alpha)} \left[ \frac{1}{(k-\hat{k}+\hat{\theta})^{\alpha}} - \frac{1}{\hat{\theta}^{\alpha}} \right] ht_{\hat{k}}^{\sigma-2} \Biggr\} \\ &\leq v_{6} \left( h^{\sigma+\alpha+1}t_{k+1}^{-\alpha-1} + h^{\alpha+1}t_{k+1}^{\sigma-\alpha-1} + h \right). \end{split}$$

Similarly, we can get there exists a constant  $v_7 > 0$  independent of h such that

$$\left|\mathcal{H}^k(t_{k+1})-\mathcal{H}^k_1(t_{k+1})\right| \leq v_7 \left(h^{\sigma+\alpha+1}t_{k+1}^{-\alpha-1}+h^{\alpha+2}t_{k+1}^{\sigma-\alpha-2}+h^2\right).$$

Therefore, when setting  $C_3 = \max \{v_7, v_8\}$ , the lemma is proved.

# F.2.4 Proof of lemma 9.2.5

*Proof.* From Lemma 9.2.2 we know that

$$\frac{h^{\alpha}t_{k}^{\sigma_{r}}}{\Gamma(\alpha+1)}{}_{2}F_{1}\left(-\sigma_{r},1;\alpha+1;-\frac{1}{k}\right) - h^{\alpha}\sum_{j=0}^{p}\beta_{j}^{(p)}t_{k+1-j}^{\sigma_{r}} = O(h^{\alpha+p+1}t_{k+1}^{\sigma_{r}-p-1}),$$

which is equivalent to

$$\frac{k^{\sigma_r}}{\Gamma(\alpha+1)} {}_2F_1\left(-\sigma_r,1;\alpha+1;-\frac{1}{k}\right) - \sum_{j=0}^p \beta_j^{(p)}(k+1-j)^{\sigma_r} = O((k+1)^{\sigma_r-p-1}).$$

Hence, by (9.22), we have

$$\sum_{j=1}^{m_{u}} W_{k,j}^{(\alpha,\sigma,p)} j^{\sigma_{r}} = O((k+1)^{\sigma_{r}-p-1}), \quad r = 1, 2, \dots, m_{u}$$

Similarly, by using Lemma 9.2.2 and 9.2.3, we can obtain

$$\begin{split} \sum_{j=1}^{m_f} W_{k,j}^{(\alpha,\delta,p)} j^{\delta_r} &= O((k+1)^{\delta_r - p - 1}), \quad r = 1, 2, \dots, m_f, \\ \sum_{j=1}^{\tilde{m}_u} \tilde{W}_{k,j}^{(\alpha,\sigma,p)} j^{\sigma_r} &= O((k+1)^{-\alpha - 1}) + O((k+1)^{\sigma_r - p - 1}), \quad r = 1, 2, \dots, \tilde{m}_u. \end{split}$$

Moreover, for  $W_{k,j}^{(\delta,p)}$  in (9.42), we can get that

$$\sum_{j=1}^{\tilde{m}_{f}} W_{k,j}^{(\delta,0)} j^{\delta_{r}} = (k+1)^{\delta_{r}} - k^{\delta_{r}} = O((k+1)^{\delta_{r-1}}), \quad r = 1, 2, \dots, \tilde{m}_{f},$$

$$\sum_{j=1}^{\tilde{m}_{f}} W_{k,j}^{(\delta,1)} j^{\delta_{r}} = (k+1)^{\delta_{r}} - 2k^{\delta_{r}} + (k-1)^{\delta_{r}} = O((k+1)^{\delta_{r-2}}), \quad r = 1, 2, \dots, \tilde{m}_{f},$$
ends the proof.

which ends the proof.

### F.2.5 Proof of theorem 9.2.6

*Proof.* Let  $e_{k+1} = u(t_{k+1}) - u_{k+1}$ . When p = 0, subtracting (9.46) from (9.47) and using the Lipschitz condition (9.32) yield

$$\begin{split} \|e_{k+1}\|_{\infty} \leq \|e_{k}\|_{\infty} + |\lambda|h^{\alpha} \left(\beta_{0}^{(0)}\|e_{k+1}\|_{\infty} + \sum_{j=1}^{m_{u}} \left|W_{k,j}^{(\alpha,\sigma,0)}\right| \|e_{j}\|_{\infty}\right) \\ &+ \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \left|\gamma_{k,j}^{(0)}\right| \|e_{j}\|_{\infty} + \sum_{j=1}^{\tilde{m}_{u}} \left|\widetilde{W}_{k,j}^{(\alpha,\sigma,0)}\right| \|e_{j}\|_{\infty} \\ &+ L\beta_{0}^{(0)}h^{\alpha} \left(\|e_{k}\|_{\infty} + \sum_{j=1}^{\tilde{m}_{f}} \left|W_{k,j}^{(\delta,0)}\right| \|e_{j}\|_{\infty}\right) + Lh^{\alpha} \sum_{j=1}^{m_{f}} \left|W_{k,j}^{(\alpha,\delta,0)}\right| \|e_{j}\|_{\infty} + R_{k+1} \\ \leq |\lambda|\beta_{0}^{(0)}h^{\alpha}\|e_{k+1}\|_{\infty} + \|e_{k}\|_{\infty} + L\beta_{0}^{(0)}h^{\alpha}\|e_{k}\|_{\infty} + \sum_{j=1}^{M} \tilde{W}_{k,j}\|e_{j}\|_{\infty} \\ &+ \frac{1}{\Gamma(\alpha)\Gamma(2-\alpha)} \sum_{j=0}^{k} \left|\gamma_{k,j}^{(0)}\right| \|e_{j}\|_{\infty} + R_{k+1}, \end{split}$$
(F.4)

where

$$\tilde{W}_{k,j} = \left|\lambda\right|h^{\alpha} \left|W_{k,j}^{(\alpha,\sigma,0)}\right| + Lh^{\alpha} \left|W_{k,j}^{(\alpha,\delta,0)}\right| + \left|\tilde{W}_{k,j}^{(\alpha,\sigma,0)}\right| + L\beta_0^{(0)}h^{\alpha} \left|W_{k,j}^{(\delta,0)}\right|$$

and

$$R_{k+1} = R_{k+1}^{u} + R_{k+1}^{f} + \tilde{R}_{k+1}^{u} + h^{\alpha} \beta_{0}^{(p)} \tilde{R}_{k+1}^{f} \le v_{9} h_{0}^{q},$$

with  $q_0 = \min\left\{1, \sigma_{\tilde{m}_u+1}, \sigma_{m_u+1} + \alpha, \delta_{m_f+1} + \alpha, \delta_{\tilde{m}_f+1} + \alpha\right\}$  and  $v_9 > 0$  is a constant independent of *h*. It follows from Lemma 9.2.5 there exists a constant  $v_{10} > 0$  such that

$$\tilde{W}_{k,j} \le v_{10}$$
, when  $\sigma_{\tilde{m}_u} \le 1$ ,  $\sigma_{m_u}, \delta_{m_f}, \delta_{\tilde{m}_f} \le \alpha + 1$ .

We rewrite (F.4) as

$$\begin{split} (1 - |\lambda|\beta_0^{(0)}h^{\alpha}) \|e_{k+1}\|_{\infty} \leq & (1 + L\beta_0^{(0)}h^{\alpha}) \|e_k\|_{\infty} + \sum_{j=1}^M \tilde{W}_{k,j} \|e_j\|_{\infty} \\ & + \frac{1}{\Gamma(\alpha)\Gamma(2 - \alpha)} \sum_{j=0}^k \left|\gamma_{k,j}^{(0)}\right| \|e_j\|_{\infty} + R_{k+1}. \end{split}$$

Since by using Lemma 9.2.1 we have

$$\sum_{j=0}^{k} \left| \gamma_{k,j}^{(0)} \right| = 2\gamma_{k,k}^{(0)} \le 2C_1.$$

Then, when  $|\lambda|\beta_0^{(0)}h^{\alpha} < 1$ , we can obtain that

$$\begin{split} \|e_{k+1}\|_{\infty} \leq & \frac{1}{1 - |\lambda|\beta_{0}^{(0)}h^{\alpha}} \exp\left[1 + L\beta_{0}^{(0)}h^{\alpha} + \frac{2C_{1}}{\Gamma(\alpha)\Gamma(2 - \alpha)}\right] \left(\sum_{j=1}^{M} \tilde{W}_{k,j} \|e_{j}\|_{\infty} + R_{k+1}\right) \\ \leq & v_{11}\left(\sum_{j=1}^{M} \tilde{W}_{k,j} \|e_{j}\|_{\infty} + R_{k+1}\right) \leq v_{11}\left(v_{9}\sum_{j=1}^{M} \|e_{j}\|_{\infty} + v_{10}h^{q_{0}}\right), \end{split}$$

where the discrete Gronwall inequality in [334] has been used. For p = 1, we can also obtain that

$$\|e_{k+1}\|_{\infty} \leq v_{12} \left( \sum_{j=1}^{M} \|e_j\|_{\infty} + h^{q_1} \right),$$

with  $q_1 = \min \{2, \sigma_{\tilde{m}_u+1} + 1, \sigma_{m_u+1} + \alpha + 1, \delta_{m_f+1} + \alpha + 1, \delta_{\tilde{m}_f+1} + \alpha + 1\}$  and  $v_{12}$  is a positive constant independent of *h*. Therefore, this completes the proof.

BIBLIOGRAPHY

#### BIBLIOGRAPHY

- [1] J.L. Suzuki, M. Zayernouri, M.L. Bittencourt, and G.E. Karniadakis. Fractional-order uniaxial visco-elasto-plastic models for structural analysis. <u>Computer Methods in Applied</u> Mechanics and Engineering, 308:443–467, 2016.
- [2] D. Hull and D.J. Bacon. Introduction to Dislocations. Butterworth-Heinemann, 2011.
- [3] R.B. Sills, W.P. Kuykendall, A. Aghaei, and W. Cai. <u>Fundamentals of Dislocation Dynamics</u> Simulations. Springer, 2016.
- [4] V. Bulatov and W. Cai. <u>Computer Simulations of Dislocations</u>. Oxford University Press, 2006.
- [5] F. Zeng, I. Turner, and K. Burrage. A stable fast time-stepping method for fractional integral and derivative operators. J. Sci. Comput., 2018.
- [6] G.H. McKinley and A. Jaishankar. Critical gels, scott blair and the fractional calculus of soft squishy materials. Presentation, 2013.
- [7] R. Metzler and J. Klafter. The random walk's guide to anomalous diffusion: a fractional dynamics approach. Physics Reports, 339(1):1 77, 2000.
- [8] F.C. Meral, T.J. Royston, and R. Magin. Fractional calculus in viscoelasticity: An experimental study. Commun. Nonlinear Sci. Numer. Simul., 15:939–945, 2010.
- [9] R. Magin and T.J. Royston. Fractional-order elastic models of cartilage: A multi-scale approach. Commun. Nonlinear Sci. Numer. Simul., 15:657–664, 2010.
- [10] D. Craiem, F.J. Rojo, J.M. Atienza, R.L. Armentano, and G.V. Guinea. Fractional-order viscoelasticity applied to describe uniaxial stress relaxation of human arteries. <u>Phys. Med.</u> <u>Biol</u>, 53(17):4543, 2008.
- [11] B. Suki, A.L. Barabasi, and K.R. Lutchen. Lung tissue viscoelasticity: a mathematical framework and its molecular basis. Journal of Applied Physiology, 76(6):2749–2759, 1994.
- [12] V.D. Djordjević, J. Jarić, B. Fabry, J.J. Fredberg, and Dimitrije Stamenović. Fractional derivatives embody essential features of cell rheological behavior. <u>Ann. Biomed. Eng.</u>, 31(6):692–699, 2003.
- [13] S. Nicolle, P. Vezin, and J.-F. Palierne. A strain-hardening bi-power law for the nonlinear behaviour of biological soft tissues. Journal of Biomechanics, 43(5):927 932, 2010.
- [14] M. Puig-de Morales-Marinkovic, K.T. Turner, J.P. Butler, J.J. Fredberg, and S. Suresh. Viscoelasticity of the human red blood cell. <u>American Journal of Physiology - Cell Physiology</u>, 293(2):C597–C605, 2007.

- [15] H.H. Winter and M. Mours. Rheology of polymers near liquid-solid transitions. <u>Advances</u> in polymer science, 134:165–234, 1997.
- [16] R. J. Ketz, R. K. Prud'homme, and W. W. Graessley. Rheology of concentrated microgel solutions. Rheologica Acta, 27(5):531–539, 1988.
- [17] H.A. Baghdadi, H. Sardinha, and S.R. Bhatia. Rheology and gelation kinetics in laponite dispersions containing poly(ethylene oxide). <u>Journal of Polymer Science Part B: Polymer</u> Physics, 43(2):233–240, 2005.
- P. Sollich. Rheological constitutive equation for a model of soft glassy materials. <u>Phys. Rev.</u> E, 58(1):738–759, 1998.
- [19] K.D. Nnetu, M. Knorr, S. Pawlizak, T. Fuhs, and J.A. Käs. Slow and anomalous dynamics of an mcf-10a epithelial cell monolayer. Soft Matter, 39, 2013.
- [20] J.D. Pajerowski, K.N. Dahl, F.L. Zhong, P.J. Sammak, and D.E. Discher. Physical plasticity of the nucleus in stem cell differentiation. Proc. Natl. Acad. Sci. USA, 40, 2007.
- [21] N. Bonadkar, R. Gerum, M. Kuhn, M. Sporer, A. Lippert, W. Schneider, K.E. Aifantis, and B. Fabry. Mechanical plasticity of cells. Nat. Mater., 15:1090 – 1094, 2016.
- [22] I.Y. Wong, M.L. Gardel, D.R. Reichman, E.R. Weeks, M.T. Valentine, A.R. Bausch, and D.A. Weitz. Anomalous diffusion probes microstructure dynamics of entangled f-actin networks. Physical Review Letters, 92, 2004.
- [23] M. Kapnistos, M. Lang, D. Vlassopoulos, D. Pyckhout-Hintzen, D. Richter, D. Cho, T. Chang, and M. Rubinstein. Unexpected power-law stress relaxation of entangled ring polymers. Nature Materials, 7:997–1002, 2008.
- [24] A. Jaishankar and G.H. McKinley. Power-law rheology in the bulk and at the interface: quasi-properties and fractional constitutive equations. Proc R Soc A 469: 20120284, 2013.
- [25] D. Stamenović, N. Rosenblatt, M. Montoya-Zavala, B.D. Matthews, S. Hu, B. Suki, N. Wang, and D.E. Ingber. Rheological behavior of living cells is timescale-dependent. <u>Biophys J.</u>, 93(8):L39–L41, 2007.
- [26] T. Richeton, J. Weiss, and F. Louchet. Breakdown of avalanche critical behaviour in polycrystalline plasticity. Nat. Mater., 4:465 – 469, 2005.
- [27] M.-Carmen Miguel, A. Vespignani, S. Zapperi, J. Weiss, and J-R. Grasso. Intermittent dislocation flow in viscoplastic deformation. Nature, 410:667–671, 2001.
- [28] A. Marchenko, D. Fichou, D. Bonamy, and D. Bouchaud. Time resolved observation of fracture events in mica crystal using scanning tunneling microscope. <u>Applied Physics</u> Letters, 89, 2006.
- [29] D. Bonamy, S. Santucci, and Ponson. L. Crackling dynamics in material failure as the signature of a self-organized dynamic phase transition. Physical Review Letters, 101, 2008.

- [30] G-h. Gao, Z-z. Sun, and H-w Zhang. A new fractional numerical differentiation formula to approximate the caputo fractional derivative and its applications. J. Comp. Phys., 259:33–50, 2014.
- [31] I Podlubny. Fractional Differential Equations. San Diego, CA, USA: Academic Press, 1999.
- [32] F. Mainardi and G. Spada. Creep, relaxation and viscosity properties for basic fractional models in rheology. arXiv:1110.3400v1, 2011.
- [33] Igor Podlubny. Fractional differential equations: an introduction to fractional derivatives, fractional differential equations, to methods of their solution and some of their applications. Elsevier, 1998.
- [34] H. Schiessel and A. Blumen. Hierarchical analogues to fractional relaxation equations. J. Phys. A: Math. Gen., 26:5057–5069, 1993.
- [35] A. Lion. On the thermodynamics of fractional damping elements. <u>Continuum Mech.</u> Thermodyn., 9:83 – 96, 1997.
- [36] H. Schiessel. Generalized viscoelastic models: their fractional equations with solutions. J. Phys. A: Math. Gen., 28:6567–6584, 1995.
- [37] R.L. Bagley and P.J. Torvik. A theoretical basis for the application of fractional calculus to viscoelasticity. Journal of rheology, 27:201–210, 1983.
- [38] Walter G Glöckle and Theo F Nonnenmacher. Fox function representation of non-debye relaxation processes. Journal of Statistical Physics, 71(3):741–757, 1993.
- [39] Thomas G Mason. Estimating the viscoelastic moduli of complex fluids using the generalized stokes–einstein equation. Rheologica acta, 39(4):371–378, 2000.
- [40] S. Mashayekhi, Y. Hussaini, and W. Oates. A physical interpretation of fractional viscoelasticity based on the fractal structure of media: Theory and experimental validation. J. Mech. Phys. Solids, 128:137–150, 2019.
- [41] GW Scott Blair, BC Veinoglou, and JE Caffyn. Limitations of the newtonian time scale in relation to non-equilibrium rheological states and a theory of quasi-properties. <u>Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences</u>, 189(1016):69– 87, 1947.
- [42] M. Naghibolhosseini. Estimation of outer-middle ear transmission using DPOAEs and fractional-order modeling of human middle ear. PhD thesis, City University of New York, NY., 2015.
- [43] M. Naghibolhosseini and G.R. Long. Fractional-order modelling and simulation of human ear. Int. J. Comput. Math., 95(6-7):1257–1273, 2018.
- [44] J. Chen and L. Li. Parallelizing the conjugate gradient algorithm for multilevel Toeplitz systems. Procedia Comput. Sci., 18:571–580, 2013.

- [45] TJ Faber, A Jaishankar, and GH McKinley. Describing the firmness, springiness and rubberiness of food gels using fractional calculus. Part I: Theoretical framework. Food Hydrocolloids, 62:311–324, 2017.
- [46] R. Xiao, H. Sun, and W. Chen. A finite deformation fractional viscoplastic model for the glass transition behavior of amorphous polymers. Int. J. Nonlin. Mech., 93:7–14, 2017.
- [47] Wojciech Sumelka. Application of fractional continuum mechanics to rate independent plasticity. Acta Mechanica, 225(11):3247–3264, 2014.
- [48] W Sumelka. Fractional viscoplasticity. Mech. Res. Commun., 56:31–36, 2014.
- [49] Y. Sun and W Sumelka. Fractional viscoplastic model for soils under compression. <u>Acta</u> Mech., 230(9):3365–3377, 2019.
- [50] HongGuang Sun, Yong Zhang, Dumitru Baleanu, Wen Chen, and YangQuan Chen. A new collection of real world applications of fractional calculus in science and engineering. Communications in Nonlinear Science and Numerical Simulation, 64:213–231, 2018.
- [51] Michele Caputo and Mauro Fabrizio. Damage and fatigue described by a fractional derivative model. Journal of Computational Physics, 293:400–408, 2015.
- [52] M. Fabrizio. Fractional rheological models for thermomechanical systems. dissipation and free energies. Fract. Calc. Appl. Anal., 17(1):206 – 223, 2013.
- [53] G. Alfano and M. Musto. Thermodynamic derivation and damage evolution for a fractional cohesive zone model. J. Eng. Mech., 143(7), 2017.
- [54] W Sumelka, B Łuczak, T Gajewski, and GZ Voyiadjis. Modelling of aaa in the framework of time-fractional damage hyperelasticity. <u>International Journal of Solids and Structures</u>, 206:30–42, 2020.
- [55] Angela Beltempo, Massimiliano Zingales, Oreste S Bursi, and Luca Deseri. A fractionalorder model for aging materials: An application to concrete. <u>International Journal of Solids</u> and Structures, 138:13–23, 2018.
- [56] Ruifan Meng, Deshun Yin, and Corina S Drapaca. Variable-order fractional description of compression deformation of amorphous glassy polymers. <u>Computational Mechanics</u>, 64(1):163–171, 2019.
- [57] S. Patnaik and F. Semperlotti. Variable-order fracture mechanics and its application to dynamic fracture. NPJ Comput. Mater., 7(27), 2021.
- [58] Sansit Patnaik, John P Hollkamp, and Fabio Semperlotti. Applications of variable-order fractional operators: a review. <u>Proceedings of the Royal Society A</u>, 476(2234):20190498, 2020.
- [59] W. Ding, S. Patnaik, S. Sidhardh, and F. Semperlotti. Applications of distributed-order fractional operators: A review. Entropy, 23:110, 2021.

- [60] Arttu Lehtinen, Fredric Granberg, Lasse Laurson, Kai Nordlund, and Mikko J. Alava. Multiscale modeling of dislocation-precipitate interactions in fe: From molecular dynamics to discrete dislocations. Phys. Rev. E, 93(1):013309, 2016.
- [61] S. Plimpton. Fast parallel algorithms for short-range molecular dynamics. J. Comp. Phys., 117:1–19, 1995.
- [62] A. Arsenlis, W. Cai, M. Tang, M. Rhee, T. Oppelstrup, G. Hommes, T.G. Pierce, and V.V. Bulatov. Enabling strain hardening simulations with dislocation dynamics. <u>Modeling and</u> Simulation in Materials Science and Engineering, 15(6), 2007.
- [63] Eduardo A Barros de Moraes, Jorge L Suzuki, and Mohsen Zayernouri. Atomistic-tomeso multi-scale data-driven graph surrogate modeling of dislocation glide. <u>Computational</u> Materials Science, 197:110569, 2021.
- [64] W Sumelka. Fractional viscoplasticity. In <u>37th Solid Mechanics Conference, Warsaw, Poland</u>, pages 102–103, 2012.
- [65] W Sumelka. Fractional viscoplasticity: an introduction. In <u>Workshop 2012 Dynamic</u> Behavior of Materials and Safety of Structures, Poznan, Poland, pages 1–2, 2012.
- [66] W Sumelka. Fractional viscoplasticity. <u>Mechanics Research Communications</u>, 56:31 36, 2014.
- [67] C. Zhang, Z. Zhu, S. Zhu, D. He, D. Zhu, J. Liu, and S. Meng. Nonlinear creep damage constitutive model of concrete based on fractional calculus theory. <u>Materials</u>, 12:1 – 14, 2014.
- [68] J. Kang, F. Zhou, C. Liu, and Y. Liu. A fractional non-linear creep model for coal considering damage effect and experimental validation. Int. J. Nonlin. Mech., 76:20–28, 2015.
- [69] M. Caputo and M. Fabrizio. Damage and fatigue described by a fractional derivative model. J. Comp. Phys., 293:400 – 408, 2015.
- [70] H. Tang, D. Wang, R. Huang, X. Pei, and W. Chen. A new rock creep model based on variable-order fractional derivatives and continuum damage mechanics. <u>B. Eng. Geol.</u> Environ., 77:375–383, 2018.
- [71] O. Giraldo-Londoño, G.H. Paulino, and W.G. Buttlar. Fractional calculus derivation of a rate-dependent PPR-based cohesive fracture model: theory, implementation, and numerical results. Int. J. Fract., 216:1–29, 2019.
- [72] M. Fabrizio. Fractional rheological models for thermomechanical systems. dissipation and free energies. <u>Fract. Calc. Appl. Anal.</u>, 17(1):206 – 223, 2014.
- [73] L. Deseri, M. DiPaola, and M. Zingales. Free energy and states of fractional-order hereditariness. Int. J. Solids Struct., 51:3156 – 3167, 2014.
- [74] K. Adolfsson, M. Enelund, and P. Olsson. On the fractional order model of viscoelasticity. Mech. Time-Depend. Mat., 9(1):15–34, 2005.

- [75] Jorge Suzuki, Yongtao Zhou, Marta D'Elia, and Mohsen Zayernouri. A thermodynamically consistent fractional visco-elasto-plastic model with memory-dependent damage for anomalous materials. <u>Computer Methods in Applied Mechanics and Engineering</u>, 373:113494, 2021.
- [76] P. Łabędzki, R. Pawlikowski, and A. Radowicz. Transverse vibration of a cantilever beam under base excitation using fractional rheological model. In <u>AIP Conference Proceedings</u>, volume 2029, page 020034. AIP Publishing, 2018.
- [77] R. Ansari, M. Faraji Oskouie, and R. Gholami. Size-dependent geometrically nonlinear free vibration analysis of fractional viscoelastic nanobeams based on the nonlocal elasticity theory. Physica E: Low-dimensional Systems and Nanostructures, 75:266 – 271, 2016.
- [78] M. Faraji Oskouie, R. Ansari, and F. Sadeghi. Nonlinear vibration analysis of fractional viscoelastic euler—bernoulli nanobeams based on the surface stress theory. <u>Acta Mechanica</u> Solida Sinica, 30(4):416–424, 2017.
- [79] G.J. Eyebe, G. Betchewe, A. Mohamadou, and T.C. Kofane. Nonlinear vibration of a nonlocal nanobeam resting on fractional-order viscoelastic pasternak foundations. <u>Fractal</u> and Fractional, 2(21), 2017.
- [80] Roman Lewandowski and Przemysław Wielentejczyk. Nonlinear vibration of viscoelastic beams described using fractional order derivatives. Journal of Sound and Vibration, 399:228– 243, 2017.
- [81] H. Brunner and T. Tang. Polynomial spline collocation methods for the nonlinear basset equation. Computers Math. Applic., 18:449–457, 1989.
- [82] R. Garrappa. Trapezoidal methods for fractional differential equations: Theoretical and computational aspects. Math.Comput.Simulation, 110:96–112, 2015.
- [83] S.B. Yuste and Q.-M. Joaquín. A finite difference method with non-uniform timesteps for fractional diffusion equations. Comput. Phys. Commun., 183:2594–2600, 2012.
- [84] Y.-N. Zhang, Z.-Z. Sun, and H.-L. Liao. Finite difference methods for the time fractional diffusion equation on non-uniform meshes. J. Comput. Phys., 265:195–210, 2014.
- [85] M. Stynes, E. O'Riordan, and J.L. Gracia. Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. <u>SIAM J. Numer. Anal.</u>, 55(2):1057– 1079, 2017.
- [86] C. Lubich. Discretized fractional calculus. SIAM J. Math. Anal., 17:704–719, 1986.
- [87] F. Zeng, Z. Zhang, and G.E. Karniadakis. Second-order numerical methods for multi-term fractional differential equations: smooth and non-smooth solutions. <u>Comput. Methods Appl.</u> Mech. Eng., 327:478–502, 2017.
- [88] Ch Lubich. On the stability of linear multistep methods for Volterra convolution equations. IMA J. Numer. Anal., 3(4):439–465, 1983.

- [89] Tao Tang. A finite difference scheme for partial integro-differential equations with a weakly singular kernel. Appl. Numer. Math., 11(4):309–319, 1993.
- [90] Kai Diethelm. An algorithm for the numerical solution of differential equations of fractional order. Electron. Trans. Numer. Anal., 5(1):1–6, 1997.
- [91] Yumin Lin and Chuanju Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. J. Comp. Phys., 225(2):1533–1552, 2007.
- [92] Fanhai Zeng, Changpin Li, Fawang Liu, and Ian Turner. Numerical algorithms for timefractional subdiffusion equation with second-order accuracy. <u>SIAM J. Sci. Comput.</u>, 37(1):A55–A78, 2015.
- [93] Z. Li, Z. Liang, and Y. Yan. High-order numerical methods for solving time fractional partial differential equations. J. Sci. Comput., 71:785–803, 2017.
- [94] Kai Diethelm, Neville J Ford, and Alan D Freed. Detailed error analysis for a fractional Adams method. Numer. Algorithms, 36(1):31–52, 2004.
- [95] M. Zayernouri, W. Cao, Z. Zhang, and G. E. Karniadakis. Spectral and discontinuous spectral element methods for fractional delay equations. <u>SIAM J. Sci. Comput.</u>, 36(6):B904–B929, 2014.
- [96] M. Zayernouri and G. E. Karniadakis. Exponentially accurate spectral and spectral element methods for fractional ODEs. J. Comp. Phys., 257:460–480, 2014.
- [97] M. Zayernouri and G. E. Karniadakis. Fractional spectral collocation methods for linear and nonlinear variable order FPDEs. J. Comp. Phys. (Special issue on FPDEs: Theory, Numerics, and Applications), 293:312–338, 2015.
- [98] E. Kharazmi, M. Zayernouri, and G. E. Karniadakis. A Petrov–Galerkin spectral element method for fractional elliptic problems. <u>Comput. Methods Appl. Mech. Eng.</u>, 324:512–536, 2017.
- [99] M. Samiee, M. Zayernouri, and M. M. Meerschaert. A unified spectral method for FPDEs with two-sided derivatives; part I: A fast solver. J. Comp. Phys., 385:225–243, 2019.
- [100] M. Samiee, M. Zayernouri, and M. M. Meerschaert. A unified spectral method for FPDEs with two-sided derivatives; part II: Stability, and error analysis. J. Comp. Phys., 385:244–261, 2019.
- [101] E. Kharazmi and M. Zayernouri. Fractional sensitivity equation method: Applications to fractional model construction. J. Sci. Comput., 80:110–140, 2019.
- [102] A. Lischke, M. Zayernouri, and G.E. Karniadakis. A petrov–galerkin spectral method of linear complexity for fractional multiterm odes on the half line. <u>SIAM J. Sci. Comput.</u>, 39(3):A922–A946, 2017.
- [103] C. Lubich and A. Schädle. Fast convoluion for nonreflecting boundary conditions. <u>SIAM J.</u> <u>Sci. Comput.</u>, 24:161–182, 2002.

- [104] A. Schädle, M. López-Fernández, and C. Lubich. Fast and oblivious convolution quadrature. SIAM J. Sci. Comput., 28(2):421–438, 2006.
- [105] Y. Yu, P. Perdikaris, and G.E. Karniadakis. Fractional modeling of viscoelasticity in 3d cerebral arteries and aneurysms. J. Comp. Phys., 323:219–242, 2016.
- [106] Fanhai Zeng, Ian Turner, and Kevin Burrage. A stable fast time-stepping method for fractional integral and derivative operators. J. Sci. Comput., 77(1):283–307, 2018.
- [107] Daniel Baffet and Jan S. Hesthaven. High-order accurate adaptive kernel compression timestepping schemes for fractional differential equations. <u>Journal of Scientific Computing</u>, 72(3):1169–1195, 2017.
- [108] K. Diethelm and N. J. Ford. Analysis of fractional differential equations. J. Math. Anal. Appl., 265(2):229–248, 2002.
- [109] Luciano Galeone and Roberto Garrappa. On multistep methods for differential equations of fractional order. Mediterr. J. Math., 3:565–580, 2006.
- [110] Luciano Galeone and Roberto Garrappa. Explicit methods for fractional differential equations and their stability properties. J. Comput. Appl. Math., 228(2):548–560, 2009.
- [111] Roberto Garrappa. On linear stability of predictor-corrector algorithms for fractional differential equations. Int. J. Comput. Math., 87(10):2281–2290, 2010.
- [112] M. Zayernouri and A. Matzavinos. Fractional Adams-Bashforth/Moulton methods: An application to the fractional Keller-Segel chemotaxis system. J. Comp. Phys., 317:1–14, 2016.
- [113] W. Cao, F. Zeng, Z. Zhongqiang, and G.E. Karniadakis. Implicit-explicit difference schemes for nonlinear fractional differential equations with nonsmooth solutions. <u>SIAM J. Sci.</u> Comput., 38:A3070–A3093, 2016.
- [114] Fanhai Zeng, Ian Turner, Kevin Burrage, and George Em Karniadakis. A new class of semi-implicit methods with linear complexity for nonlinear fractional differential equations. SIAM J. Sci. Comput., 40(5):A2986–A3011, 2018.
- [115] Anindya Ghoshal, Muthuvel Murugan, Michael J. Walock, Luis Bravo, Jeffrey J. Swab, Clara Hofmeister-Mock, Samuel G. Hirsch, Robert J. Dowding, M. Pepi, Andy Nieto, Larry Fehrenbacher, Kelvin Wong, Acree Technologies, Victor Grubsky, Matthew T. Webster, Nishan Jain, Alison B. Flatau, Andrew Wright, and Jian Luo. Advanced high temperature propulsion materials research project: An update. 2019.
- [116] Ed Habtour, Daniel P Cole, Jaret C Riddick, Volker Weiss, Mark Robeson, Raman Sridharan, and Abhijit Dasgupta. Detection of fatigue damage precursor using a nonlinear vibration approach. Structural Control and Health Monitoring, 23(12):1442–1463, 2016.
- [117] J. Chang, W. Cai, V. Bulatov, and S. Yip. Dislocation motion in bcc metals by molecular dynamics. <u>Materials Science and Engineering</u>: A, 309-310:160–163, 2001.

- [118] F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W.A. Curtin. Screw dislocation structure and mobility in body centered cubic fe predicted by a gaussian approximation potential. <u>npj</u> Computational Materials, 4, 2018.
- [119] S.J. Zhou, D.L. Preston, P.S. Lomdahl, and D.M. Beazley. Large-scale molecular dynamics simulations of dislocation intersection in copper. Science, 279(5356):1525–1527, 1998.
- [120] A. Lehtinen, L. Laurson, F. Granberg, K. Nordlund, and M.J. Alava. Effects of precipitates and dislocation loops on the yield stress of irradiated iron. <u>Scientific Reports</u>, 8(1):6914, 2018.
- [121] V. Bulatov, L. Hsiung, M. Tang, A. Arsenlis, M. Bartelt, W. Cai, J. Florando, M. Hiratani, M. Rhee, G. Hommes, T. Pierce, and T. Diaz de la Rubia. Dislocation multi-junctions and strain hardening. Nature, 440:1174–1178, 2006.
- [122] KOE Henriksson, C Björkas, and Kai Nordlund. Atomistic simulations of stainless steels: a many-body potential for the fe-cr-c system. <u>Journal of Physics: Condensed Matter</u>, 25(44):445401, 2013.
- [123] Cheng Chen, Fanchao Meng, and Jun Song. Core structures analyses of (a+ c)-edge dislocations in wurtzite gan through atomistic simulations and peierls-nabarro model. <u>Journal of</u> <u>Applied Physics</u>, 117(19):194301, 2015.
- [124] P.M. Larsen, S. Schmidt, and J. Schiøtz. Robust structural identification via polyhedral template matching. Modelling Simul. Mater. Sci. Eng., 24(5), 2016.
- [125] A. Stukowski. Visualization and analysis of atomistic simulation data with ovito-the open visualization tool. Modelling Simul. Mater. Sci. Eng., 18:015012, 2007.
- [126] V. Imbeni, J.J. Kruzic, G.W. Marshall, and R.O. Ritchie. The dentin-enamel junction and the fracture of human teeth. Nat. Mater., 4:229–232, 2005.
- [127] F. Amblard, A.C. Maggs, B. Yurke, A.N. Pargellis, and S. Leibler. Subdiffusion and anomalous local viscoelasticity in actin networks. Phys. Rev. Letters, 77(21), 1996.
- [128] A. Jaishankar and G.H. McKinley. A fractional K-BKZ constitutive formulation for describing the nonlinear rheology of multiscale complex fluids. J. Rheol., 58, 2014.
- [129] Mehdi Samiee, Ali Akhavan-Safaei, and Mohsen Zayernouri. A fractional subgrid-scale model for turbulent flows: Theoretical formulation and a priori study. <u>Physics of Fluids</u>, 32(5):055102, 2020.
- [130] Mehdi Samiee, Ali Akhavan-Safaei, and Mohsen Zayernouri. Tempered Fractional LES Modeling. arXiv preprint arXiv:2103.01481, 2021.
- [131] Ali Akhavan-Safaei, Mehdi Samiee, and Mohsen Zayernouri. Data-driven fractional subgridscale modeling for scalar turbulence: A nonlocal LES approach. <u>Journal of Computational</u> Physics, 446:110571, 2021.

- [132] Ali Akhavan-Safaei and Mohsen Zayernouri. A Parallel Integrated Computational-Statistical Platform for Turbulent Transport Phenomena. arXiv preprint arXiv:2012.04838, 2020.
- [133] Ali Akhavan-Safaei, S Hadi Seyedi, and Mohsen Zayernouri. Anomalous features in internal cylinder flow instabilities subject to uncertain rotational effects. <u>Physics of Fluids</u>, 32(9):094107, 2020.
- [134] MS Ansari, Anil Gulia, Aneesh Srivastava, and Rakesh Kapoor. Risk factors for progression to end-stage renal disease in children with posterior urethral valves. <u>Journal of pediatric</u> urology, 6(3):261–264, 2010.
- [135] P Lopez Pereira, MJ Martinez Urrutia, L Espinosa, R Lobato, M Navarro, and E Jaureguizar. Bladder dysfunction as a prognostic factor in patients with posterior urethral valves. <u>BJU</u> international, 90(3):308–311, 2002.
- [136] Sotirios Korossis, Fiona Bolland, Jenny Southgate, Eileen Ingham, and John Fisher. Regional biomechanical and histological characterisation of the passive porcine urinary bladder: Implications for augmentation and tissue engineering strategies. <u>Biomaterials</u>, 30(2):266–275, 2009.
- [137] Enrique Morales-Orcajo, Tobias Siebert, and Markus Böl. Location-dependent correlation between tissue structure and the mechanical behaviour of the urinary bladder. <u>Acta</u> Biomaterialia, 75:263–278, 2018.
- [138] Joseph Chen, Beth A Drzewiecki, W David Merryman, and John C Pope IV. Murine bladder wall biomechanics following partial bladder obstruction. <u>Journal of biomechanics</u>, 46(15):2752–2755, 2013.
- [139] Thomas W Gilbert, Silvia Wognum, Erinn M Joyce, Donald O Freytes, Michael S Sacks, and Stephen F Badylak. Collagen fiber alignment and biaxial mechanical behavior of porcine urinary bladder derived extracellular matrix. Biomaterials, 29(36):4775–4782, 2008.
- [140] Fangzhou Cheng, Lori A Birder, F Aura Kullmann, Jack Hornsby, Paul N Watton, Simon Watkins, Mark Thompson, and Anne M Robertson. Layer-dependent role of collagen recruitment during loading of the rat bladder wall. <u>Biomechanics and modeling in mechanobiology</u>, 17(2):403–417, 2018.
- [141] Ron van Mastrigt, BLRA Coolsaet, and WA Van Duyl. Passive properties of the urinary bladder in the collection phase. <u>Medical and Biological Engineering and Computing</u>, 16(5):471–482, 1978.
- [142] A.N. Natali, A.L. Audenino, W. Artibani, C.G. Fontanella, E.L. Carniel, and E.M. Zanetti. Bladder tissue biomechanical behavior: Experimental tests and constitutive formulation. Journal of Biomechanics, 48(12):3088–3096, 2015.
- [143] Silvia Wognum, David E Schmidt, and Michael S Sacks. On the mechanical role of de novo synthesized elastin in the urinary bladder wall. 2009.

- [144] Anna S Nagle, Adam P Klausner, Jary Varghese, Rachel J Bernardo, Andrew F Colhoun, Robert W Barbee, Laura R Carucci, and John E Speich. Quantification of bladder wall biomechanics during urodynamics: A methodologic investigation using ultrasound. Journal of biomechanics, 61:232–241, 2017.
- [145] I Korkmaz and B Rogg. A simple fluid-mechanical model for the prediction of the stress– strain relation of the male urinary bladder. Journal of biomechanics, 40(3):663–668, 2007.
- [146] Margot S Damaser and Steven L Lehman. The effect of urinary bladder shape on its mechanics during filling. Journal of biomechanics, 28(6):725–732, 1995.
- [147] R Van Mastrigt and DJ Griffiths. Contractility of the urinary bladder. <u>Urologia internationalis</u>, 34(6):410–420, 1979.
- [148] Ron Van Mastrigt. Mechanical properties of (urinary bladder) smooth muscle. Journal of Muscle Research & Cell Motility, 23(1):53–57, 2002.
- [149] Claude H Regnier, Herbert Kolsky, Peter D Richardson, Gamal M Ghoniem, and Jacques G Susset. The elastic behavior of the urinary bladder for large deformations. <u>Journal of</u> biomechanics, 16(11):915–922, 1983.
- [150] Margot S Damaser and Steven L Lehman. Two mathematical models explain the variation in cystometrograms of obstructed urinary bladders. <u>Journal of biomechanics</u>, 29(12):1615– 1619, 1996.
- [151] Hiroki Watanabe, KIKUO AKIYAMA, TAKESI SAITO, and FUMIYA OKI. A finite deformation theory of intravesical pressure and mural stress of the urinary bladder. <u>The</u> Tohoku journal of experimental medicine, 135(3):301–307, 1981.
- [152] Firdaweke G Habteyes, S Omid Komari, Anna S Nagle, Adam P Klausner, Rebecca L Heise, Paul H Ratz, and John E Speich. Modeling the influence of acute changes in bladder elasticity on pressure and wall tension during filling. Journal of the mechanical behavior of biomedical materials, 71:192–200, 2017.
- [153] BLRA Coolsaet, WA Van Duyl, Ron Van Mastrigt, and A Van der Zwart. Step-wise cystometry of urinary bladder new dynamic procedure to investigate viscoelastic behavior. Urology, 2(3):255–257, 1973.
- [154] WA Van Duyl. A model for both the passive and active properties of urinary bladder tissue related to bladder function. Neurourology and Urodynamics, 4(4):275–283, 1985.
- [155] BLRA Coolsaet, WA Van Duyl, R Van Mastrigt, and A Van Der Zwart. Visco-eiastic properties of the bladder wall. <u>Urologia internationalis</u>, 30(1):16–26, 1975.
- [156] R Van Mastrigt, BLRA Coolsaet, and WA Van Duyl. First results of stepwise straining of the human urinary bladder and human bladder strips. Invest Urol, 19(1):58–61, 1981.
- [157] JJ Glerum, Ron Van Mastrigt, and AJ Van Koeveringe. Mechanical properties of mammalian single smooth muscle cells iii. passive properties of pig detrusor and human a terme uterus cells. Journal of Muscle Research & Cell Motility, 11(5):453–462, 1990.

- [158] Ron van Mastrigt and JC Nagtegaal. Dependence of the viscoelastic response of the urinary bladder wall on strain rate. <u>Medical and Biological Engineering and Computing</u>, 19(3):291– 296, 1981.
- [159] ROBERT S Alexander. Viscoplasticity of smooth muscle of urinary bladder. <u>American</u> Journal of Physiology-Legacy Content, 224(3):618–622, 1973.
- [160] JG Susset and CH Regnier. Viscoelastic properties of bladder strips: standardization of a technique. Investigative urology, 18(8):445–450, 1981.
- [161] Atsuo Kondo and Jacques G Susset. Physical properties of the urinary detrusor muscle: a mechanical model based upon the analysis of stress relaxation curve. Journal of biomechanics, 6(2):141–151, 1973.
- [162] ROBERT S Alexander. Mechanical properties of urinary bladder. <u>American Journal of</u> Physiology-Legacy Content, 220(5):1413–1421, 1971.
- [163] JOSE G Venegas. Viscoelastic properties of the contracting detrusor. i. theoretical basis. American Journal of Physiology-Cell Physiology, 261(2):C355–C363, 1991.
- [164] JOSE G Venegas, JOHN P Woll, STEVEN B Woolfson, EARNEST G Cravalho, NEIL Resnick, and SUBBARAO V Yalla. Viscoelastic properties of the contracting detrusor. ii. experimental approach. <u>American Journal of Physiology-Cell Physiology</u>, 261(2):C364– C375, 1991.
- [165] Jiro Nagatomi, D Claire Gloeckner, Michael B Chancellor, William C Degroat, and Michael S Sacks. Changes in the biaxial viscoelastic response of the urinary bladder following spinal cord injury. Annals of biomedical engineering, 32(10):1409–1419, 2004.
- [166] Jiro Nagatomi, Kevin K Toosi, Michael B Chancellor, and Michael S Sacks. Contribution of the extracellular matrix to the viscoelastic behavior of the urinary bladder wall. <u>Biomechanics</u> and modeling in mechanobiology, 7(5):395–404, 2008.
- [167] Tyler G Tuttle, Duncan Morhardt, Andrea Poli, John M Park, Ellen M Arruda, and Sara Roccabianca. Investigation of fiber-driven mechanical behavior of human and porcine bladder tissue tested under identical conditions. Journal of Biomechanical Engineering, 2021.
- [168] Yuan-cheng Fung. <u>Biomechanics: mechanical properties of living tissues</u>. Springer Science & Business Media, 2013.
- [169] Todd C Doehring, Alan D Freed, Evelyn O Carew, and Ivan Vesely. Fractional order viscoelasticity of the aortic valve cusp: an alternative to quasilinear viscoelasticity. 2005.
- [170] Yehia M Haddad. Viscoelasticity of engineering materials. <u>Chapman & Hall, 2-6 Boundary</u> Row, London, SE 1 8 HN, UK, 1995. 378, 1995.
- [171] F. Mainardi. Fractional calculus and waves in linear viscoelasticity. Imperial College Press, 2010.

- [172] G.W.S Blair, B.C. Veinoglou, and B. Caffyn. Limitations of the Newtonian time scale in relation to non-equilibrium rheological states and a theory of quasi-properties. <u>Proc. R. Soc.</u> Lond. A, 189(1016):69–87, 1947.
- [173] Julian Vincent. Structural biomaterials. Princeton University Press, 2012.
- [174] Alessandra Bonfanti, Jonathan Louis Kaplan, Guillaume Charras, and Alexandre J Kabla. Fractional viscoelastic models for power-law materials. Soft Matter, 2020.
- [175] J.L. Suzuki, M. Naghibolhosseini, and M. Zayernouri. A class of fractional return-mapping algorithms for linear and nonlinear fractional visco-elasto-plastic models. <u>(in preparation)</u>, 2021.
- [176] Y. Lin and C. Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. Journal of Computational Physics, 225(2):1533–1552, 2007.
- [177] Jorge L. Suzuki and Mohsen Zayernouri. A self-singularity-capturing scheme for fractional differential equations. <u>International Journal of Computer Mathematics</u>, 98(5):933–960, 2021.
- [178] James Kennedy and Russell Eberhart. Particle swarm optimization. In Proceedings of ICNN'95-international conference on neural networks, volume 4, pages 1942–1948. IEEE, 1995.
- [179] Paris Perdikaris and George Em Karniadakis. Fractional-order viscoelasticity in onedimensional blood flow models. Annals of biomedical engineering, 42(5):1012–1023, 2014.
- [180] Yue Yu, Paris Perdikaris, and George Em Karniadakis. Fractional modeling of viscoelasticity in 3d cerebral arteries and aneurysms. Journal of computational physics, 323:219–242, 2016.
- [181] Miklos Z Kiss, Tomy Varghese, and Timothy J Hall. Viscoelastic characterization of in vitro canine tissue. Physics in Medicine & Biology, 49(18):4207, 2004.
- [182] Adela Capilnasiu, Lynne Bilston, Ralph Sinkus, and David Nordsletten. Nonlinear viscoelastic constitutive model for bovine liver tissue. <u>Biomechanics and modeling in</u> mechanobiology, pages 1–22, 2020.
- [183] G.B. Davis, M. Kohandel, S. Sivaloganathan, and G. Tenti. The constitutive properties of the brain paraenchyma: Part 2. fractional derivative approach. <u>Medical Engineering & Physics</u>, 28(5):455–459, 2006.
- [184] Maryam Naghibolhosseini and Glenis R. Long. Fractional-order modelling and simulation of human ear. International Journal of Computer Mathematics, 95(6-7):1257–1273, 2018.
- [185] Maryam Sami Jokandan, Fatemeh Ajalloueian, Magnus Edinger, Peter Reimer Stubbe, Stefania Baldursdottir, and Ioannis S. Chronakis. Bladder wall biomechanics: A comprehensive study on fresh porcine urinary bladder. Journal of the Mechanical Behavior of Biomedical Materials, 79:92–103, 2018.

- [186] B. J. West, M. Bologna, and P. Grigolini. <u>Physics of Fractal Operators</u>. New York, NY: Springer Verlag., 2003.
- [187] M. Naghibolhosseini. <u>Estimation of outer-middle ear transmission using DPOAEs and fractional-order modeling of human middle ear</u>. PhD thesis, City University of New York, NY., 2015.
- [188] M Ichise, Y Nagayanagi, and T Kojima. An analog simulation of non-integer order transfer functions for analysis of electrode processes. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 33(2):253–265, 1971.
- [189] David A Benson, Stephen W Wheatcraft, and Mark M Meerschaert. Application of a fractional advection-dispersion equation. <u>Water Resources Research</u>, 36(6):1403–1412, 2000.
- [190] Rainer Klages, Günter Radons, and Igor M Sokolov. <u>Anomalous Transport: Foundations</u> and Applications. Wiley-VCH, 2008.
- [191] J. Bonet and R.D. Wood. <u>Nonlinear continuum mechanics for finite element analysis</u>. Cambridge, 2nd edition, 2008.
- [192] J.C. Simo and T.J.R. Hughes. Computational inelasticity. Springer, 1998.
- [193] Piotr Perzyna. The constitutive equations for rate sensitive plastic materials. Technical report, DTIC Document, 1962.
- [194] W Sumelka. Application of fractional continuum mechanics to rate independent plasticity. Acta Mechanica, 225(11):3247 – 3264, 2014.
- [195] JM Sanz-Serna. A numerical method for a partial integro-differential equation. <u>SIAM</u> Journal on Numerical Analysis, 25(2):319–327, 1988.
- [196] N Sugimoto. Burgers equation with a fractional derivative; hereditary effects on nonlinear acoustic waves. J. Fluid Mech., 225(4):631–653, 1991.
- [197] Rudolf Gorenflo, Francesco Mainardi, Daniele Moretti, and Paolo Paradisi. Time fractional diffusion: a discrete random walk approach. Nonlinear Dyn., 29(1-4):129–143, 2002.
- [198] TAM Langlands and BI Henry. The accuracy and stability of an implicit solution method for the fractional diffusion equation. Journal of Computational Physics, 205(2):719–736, 2005.
- [199] Zhi-zhong Sun and Xiaonan Wu. A fully discrete difference scheme for a diffusion-wave system. Appl. Numer. Math., 56(2):193–209, 2006.
- [200] M. Zayernouri, M. Ainsworth, and G. E. Karniadakis. A unified Petrov–Galerkin spectral method for fractional PDEs. Comput. Methods Appl. Mech. Eng., 283:1545–1569, 2015.
- [201] M. Zayernouri and T. Matzavinos. Fractional Adams-Bashforth/Moulton methods: An application to the fractional Keller-Segel chemotaxis system. Journal of Computational Physics (In Press), 2016.

- [202] Zhuo-Jia Fu, Wen Chen, and Hai-Tian Yang. Boundary particle method for laplace transformed time fractional diffusion equations. <u>Journal of Computational Physics</u>, 235:52 – 66, 2013.
- [203] Guofei Pang, Wen Chen, and Zhuojia Fu. Space-fractional advection–dispersion equations by the kansa method. Journal of Computational Physics, 293:280 296, 2015.
- [204] Wen Chen and Guofei Pang. A new definition of fractional laplacian with application to modeling three-dimensional nonlocal heat conduction. <u>Journal of Computational Physics</u>, 309:350 – 367, 2016.
- [205] M.L. Bittencourt. <u>Computational Solid Mechanics: Variational Formulation and High Order</u> Approximation. CRC Press, 2014.
- [206] Peter Wriggers. Nonlinear Finite Element Methods. Springer, 2008.
- [207] T.A Carniel, P.A Muõz Rojas, and M Vaz Jr. A viscoelastic viscoplastic constitutive model including mechanical degradation: Uniaxial transient finite element formulation at finite strains and application to space truss structures. <u>Applied Mathematical Modelling</u>, 39:1725– 1739, 2015.
- [208] D. Ingman and J. Suzdalnitsky. Iteration method for equation of viscoelastic motion with fractional differential operator of damping. <u>Computer Methods in Applied Mechanics and</u> Engineering, 190(37–38):5027 – 5036, 2001.
- [209] D. Ingman and J. Suzdalnitsky. Control of damping oscillations by fractional differential operator with time-dependent order. <u>Computer Methods in Applied Mechanics and</u> Engineering, 193(52):5585 – 5595, 2004.
- [210] Y.J. Shen, S.P. Yang, H.J Xing, and H.X. Ma. Primary resonance of duffing oscillator with two kinds of fractional-order derivatives. <u>International Journal of Non-Linear Mechanics</u>, 47:975–983, 2012.
- [211] J. Lemaitre and R. Desmorat. Engineering Damage Mechanics. Springer, 2005.
- [212] J.C. Simo. On a fully three-dimensional finite-strain viscoelastic damage model: Formulation and computational aspects. <u>Comp. Methods Appl. Mech. Eng.</u>, 60:153–173, 1987.
- [213] J. Lemaitre. A course on damage mechanics. Springer, 1996.
- [214] JL Boldrini, EA Barros de Moraes, LR Chiarelli, FG Fumes, and ML Bittencourt. A nonisothermal thermodynamically consistent phase field framework for structural damage and fatigue. Computer Methods in Applied Mechanics and Engineering, 312:395–427, 2016.
- [215] LR Chiarelli, FG Fumes, EA Barros de Moraes, GA Haveroth, José Luiz Boldrini, and Marco L Bittencourt. Comparison of high order finite element and discontinuous galerkin methods for phase field equations: Application to structural damage. <u>Computers &</u> Mathematics with Applications, 74(7):1542–1564, 2017.

- [216] Eduardo A Barros de Moraes, Mohsen Zayernouri, and Mark M Meerschaert. An integrated sensitivity-uncertainty quantification framework for stochastic phase-field modeling of material damage. <u>International Journal for Numerical Methods in Engineering</u>, 122(5):1352– 1377, 2021.
- [217] Geovane A Haveroth, Eduardo A Moraes, José L Boldrini, and Marco L Bittencourt. Comparison of semi and fully-implicit time integration schemes applied to a damage and fatigue phase field model. Latin American Journal of Solids and Structures, 15, 2018.
- [218] Eduardo A Barros de Moraes, Hadi Salehi, and Mohsen Zayernouri. Data-driven failure prediction in brittle materials: A phase field-based machine learning framework. Journal of Machine Learning for Modeling and Computing, 2(1), 2021.
- [219] S.G.W. Blair and F.M.V. Coppen. The estimation of firmness in soft materials. <u>Amer. J.</u> Psychol., 56:234–246, 1943.
- [220] S.P. Näsholm and S. Holm. On a fractional zener elastic wave equation. Fract. Calc. Appl. Anal., 16(1):26–60, 2013.
- [221] A. Giusti. On infinite order differential operators in fractional viscoelasticity. Fract. Calc. Appl. Anal., 20(4):854–867, 2017.
- [222] D. Dolićanin-Đekić. On a new class of constitutive equations for linear viscoelastic body. Fract. Calc. Appl. Anal., 20(2):521–536, 2017.
- [223] X. Hei, W. Chen, G. Pang, R. Xiao, and C. Zhang. A new visco-elasto-plastic model via time-space derivative. Mech. Time-Depend. Mater., 22:129–141, 2018.
- [224] Yongtao Zhou, Jorge L Suzuki, Chengjian Zhang, and Mohsen Zayernouri. Implicitexplicit time integration of nonlinear fractional differential equations. <u>Applied Numerical</u> Mathematics, 156:555–583, 2020.
- [225] M. Samiee, A. Akhavan-Safaei, and M. Zayernouri. A fractional subgrid-scale model for turbulent flows: Theoretical formulation and a priori study. <u>arXiv preprint arXiv:1909.09943</u>, 2019.
- [226] E. Kharazmi and M. Zayernouri. Operator-based uncertainty quantification of stochastic fractional pdes. ASME J. Verif. Valid. Uncert. (in press), 2018.
- [227] A. Burlon, F.P. Pinnola, and M. Zingales. A numerical assessment of the free energy function for fractional-order relaxation. In <u>ICFDA'14 - International Conference on Fractional</u> Differentiation and its Applications, Catania, Italy, 2014.
- [228] U.G.K. Wegst, H. Bai, E. Saiz, A.P. Tomsia, and R.O. Ritchie. Bioinspired structural materials. Nat. Mater., 14:23–36, 2015.
- [229] Q. Du, J. Yang, and Z. Zhou. Analysis of a nonlocal-in-time parabolic equation. Discrete & Continuous Dynamical Systems B, 22(2):339–368, 2017.

- [230] Q. Du, M. Gunzburger, R. B. Lehoucq, and K. Zhou. A nonlocal vector calculus, nonlocal volume–constrained problems, and nonlocal balance laws. <u>Mathematical Models and</u> Methods in Applied Sciences, 23(03):493–540, 2013.
- [231] Marta D'Elia and Max Gunzburger. The fractional laplacian operator on bounded domains as a special case of the nonlocal diffusion operator. <u>Computers & Mathematics with</u> Applications, 66:1245–1260, 2013.
- [232] A. Bejan. Advanced Engineering Thermodynamics, Fourth Edition. Wiley, 2016.
- [233] M.E. Gurtin, E. Fried, and L. Anand. <u>The mechanics and thermodynamics of continua</u>. Cambridge University Press, 2010.
- [234] E.A. de Souza Neto, D. Perić, and D.R.J. Owen. <u>Computational Methods for Plasticity:</u> Theory and Applications. John Wiley & Sons, 2008.
- [235] T.-S Cao, A. Gaillac, P. Montmitonnet, and P.-O. Bouchard. Identification methodology and comparison of phenomenological ductile damage models via hybrid numerical–experimental analysis of fracture experiments conducted on a zirconium alloy. <u>Int. J. Solids Struct.</u>, 50:3984–3999, 2013.
- [236] P.-O. Bouchard, L. Bourgeon, S. Fayolle, and K. Mocellin. An enhanced lemaitre model formulation for materials processing damage computation. <u>Int. J. Mater. Form.</u>, 4:299–315, 2011.
- [237] E. Roux and P.-O. Bouchard. On the interest of using full field measurements in ductile damage model calibration. Int. J. Solids Struct., 72:50–62, 2015.
- [238] L. Feng and V. Linetsky. Pricing options in jump-diffusion models: An extrapolation approach. Oper. Res., 56(2):304–325, 2008.
- [239] P. Sagaut and C. Cambon. Homogeneous Turbulence Dynamics. Springer, 2018.
- [240] A. Akhavan-Safaei, S.H. Seyedi, and M. Zayernouri. Anomalous features in internal cylinder flow instabilities subject to uncertain rotational effects. Physics of Fluids, 32:094107, 2020.
- [241] R. Christensen. Theory of viscoelasticity: an introduction. Elsevier, 2012.
- [242] R.C. Aster, B. Borchers, and C.H. Thurber. <u>Parameter estimation and inverse problems (third</u> edition). Elsevier, 2019.
- [243] R.L. Bagley. Power law and fractional calculus model of viscoelasticity. <u>AIAA journal</u>, 27(10):1412–1417, 1989.
- [244] P.G. Nutting. A new general law of deformation. Journal of the Franklin Institute, 191(5):679–685, 1921.
- [245] A. Gemant. A method of analyzing experimental results obtained from elasto-viscous bodies. Physics, 7(8):311–317, 1936.

- [246] R.L. Bagley and P.J. Torvik. A theoretical basis for the application of fractional calculus to viscoelasticity. Journal of Rheology, 27(3):201–210, 1983.
- [247] M. Naghibolhosseini and G.R. Long. Fractional-order modelling and simulation of human ear. International Journal of Computer Mathematics, 95(6-7):1257–1273, 2018.
- [248] M.V. Shitikova, Y.A. Rossikhin, and V. Kandu. Interaction of internal and external resonances during force driven vibrations of a nonlinear thin plate embedded into a fractional derivative medium. Procedia engineering, 199:832–837, 2017.
- [249] Y.A. Rossikhin and M.V. Shitikova. Applications of fractional calculus to dynamic problems of linear and nonlinear hereditary mechanics of solids. <u>Applied Mechanics Reviews</u>, 50(1):15–67, 1997.
- [250] M. Samiee, A. Akhavan-Safaei, and M. Zayernouri. A fractional subgrid-scale model for turbulent flows: Theoretical formulation and a priori study. <u>Physics of Fluids</u>, 32:055102, 2020.
- [251] C.F. Lorenzo and T.T. Hartley. Variable order and distributed order fractional operators. Nonlinear dynamics, 29(1-4):57–98, 2002.
- [252] T.M. Atanackovic, L. Oparnica, and S. Pilipović. Distributional framework for solving fractional differential equations. <u>Integral Transforms and Special Functions</u>, 20(3-4):215– 222, 2009.
- [253] M. Caputo. Distributed order differential equation modelling dielectric induction and diffusion. Fract. Calc. Appl. Anal., 4:421–442, 2001.
- [254] A.V. Chechkin, R. Gorenflo, and I.M. Sokolov. Retarding subdiffusion and accelerating superdiffusion governed by distributed-order fractional diffusion equations. <u>Physical Review</u> E, 66(4):046129, 2002.
- [255] A.V. Chechkin, V.Y. Gonchar, R. Gorenflo, N. Korabel, and I.M. Sokolov. Generalized fractional diffusion equations for accelerating subdiffusion and truncated lévy flights. <u>Physical</u> Review E, 78(2):021111, 2008.
- [256] Y. Li, H. Sheng, and Y.Q. Chen. On distributed order integrator/differentiator. <u>Signal</u> Processing, 91(5):1079–1084, 2011.
- [257] Y. Li and Y.Q. Chen. Lyapunov stability of fractional-order nonlinear systems: A distributedorder approach. In <u>ICFDA'14 International Conference on Fractional Differentiation and Its</u> Applications 2014, pages 1–6. IEEE, 2014.
- [258] J.S. Duan and D. Baleanu. Steady periodic response for a vibration system with distributed order derivatives to periodic excitation. <u>Journal of Vibration and Control</u>, 24(14):3124–3131, 2018.
- [259] R.L. Bagley and P.J. Torvik. On the existence of the order domain and the solution of distributed order equations-part i. <u>International Journal of Applied Mathematics</u>, 2(7):865– 882, 2000.

- [260] E. Kharazmi, M. Zayernouri, and G. E. Karniadakis. Petrov–Galerkin and spectral collocation methods for distributed order differential equations. <u>SIAM J. Sci. Comput.</u>, 39(3):A1003– A1037, 2017.
- [261] E. Kharazmi and M. Zayernouri. Fractional pseudo-spectral methods for distributed-order fractional PDEs. Int. J. Comput. Math., pages 1–22, 2018.
- [262] Wei Ding, Sansit Patnaik, Sai Sidhardh, and Fabio Semperlotti. Applications of distributedorder fractional operators: A review. Entropy, 23(1):110, 2021.
- [263] Geoffrey A Manley, Anthony W Gummer, Arthur N Popper, and Richard R Fay. Understanding the cochlea, volume 62. Springer, 2017.
- [264] M. Samiee, M. Zayernouri, and M.M. Meerschaert. A unified spectral method for fpdes with two-sided derivatives; part i: a fast solver. <u>Journal of Computational Physics</u>, 385:225–243, 2019.
- [265] M. Samiee, M. Zayernouri, and M.M. Meerschaert. A unified spectral method for fpdes with two-sided derivatives; part ii: Stability, and error analysis. <u>Journal of Computational</u> Physics, 385:244–261, 2019.
- [266] M. Samiee, E. Kharazmi, M. Zayernouri, and M. M. Meerschaert. Petrov-Galerkin method for fully distributed-order fractional partial differential equations. <u>arXiv preprint</u> arXiv:1805.08242, 2018.
- [267] C. Lubich. Discretized fractional calculus. <u>SIAM Journal on Mathematical Analysis</u>, 17(3):704–719, 1986.
- [268] M. Zayernouri, M. Ainsworth, and G.E. Karniadakis. Tempered fractional sturm–liouville eigenproblems. SIAM Journal on Scientific Computing, 37(4):A1777–A1800, 2015.
- [269] M. Zayernouri and A. Matzavinos. Fractional adams-bashforth/moulton methods: an application to the fractional keller-segel chemotaxis system. <u>Journal of Computational Physics</u>, 317:1–14, 2016.
- [270] F. Mainardi. Fractional calculus and waves in linear viscoelasticity: an introduction to mathematical models. World Scientific, 2010.
- [271] S. Rogosin and F. Mainardi. George william scott blair-the pioneer of factional calculus in rheology. arXiv preprint arXiv:1404.3295, 2014.
- [272] F. Mainardi and R. Gorenflo. Time-fractional derivatives in relaxation processes: a tutorial survey. arXiv preprint arXiv:0801.4914, 2008.
- [273] F. Mainardi and G. Spada. Creep, relaxation and viscosity properties for basic fractional models in rheology. The European Physical Journal Special Topics, 193(1):133–160, 2011.
- [274] L. Meirovitch. Fundamentals of vibrations. Waveland Press, 2010.

- [275] J. Bonet and R.D. Wood. <u>Nonlinear continuum mechanics for finite element analysis</u>. Cambridge university press, 1997.
- [276] A. Lion. On the thermodynamics of fractional damping elements. <u>Continuum Mechanics</u> and Thermodynamics, 9(2):83–96, 1997.
- [277] E. Tadmor. A review of numerical methods for nonlinear partial differential equations. Bulletin of the American Mathematical Society, 49(4):507–554, 2012.
- [278] L Azrar, R Benamar, and RG White. Semi-analytical approach to the non-linear dynamic response problem of s-s and c-c beams at large vibration amplitudes part i: general theory and application to the single mode approach to free and forced vibration analysis. Journal of sound and vibration, 224(2):183–207, 1999.
- [279] W-Y Tseng and John Dugundji. Nonlinear vibrations of a buckled beam under harmonic excitation. 1971.
- [280] Spyridon Loutridis, Evanthia Douka, and LJ Hadjileontiadis. Forced vibration behaviour and crack detection of cracked beams using instantaneous frequency. <u>Ndt & E International</u>, 38(5):411–419, 2005.
- [281] M.N. Hamdan and M.H.F. Dado. Large amplitude free vibrations of a uniform cantilever beam carrying an intermediate lumped mass and rotary inertia. <u>Journal of Sound and</u> Vibration, 206(2):151–168, 1997.
- [282] W Lestari and S Hanagud. Nonlinear vibration of buckled beams: some exact solutions. International Journal of Solids and Structures, 38(26-27):4741–4757, 2001.
- [283] Joe G Eisley. Nonlinear vibration of beams and rectangular plates. Zeitschrift für angewandte Mathematik und Physik ZAMP, 15(2):167–175, 1964.
- [284] CS Hsu. On the application of elliptic functions in non-linear forced oscillations. <u>Quarterly</u> of Applied Mathematics, 17(4):393–407, 1960.
- [285] SRR Pillai and B Nageswara Rao. On nonlinear free vibrations of simply supported uniform beams. Journal of sound and vibration, 159(3):527–531, 1992.
- [286] David A Evensen. Nonlinear vibrations of beams with various boundary conditions. <u>AIAA</u> journal, 6(2):370–372, 1968.
- [287] A. Svenkeson, B. Glaz, S. Stanton, and B.J. West. Spectral decomposition of nonlinear systems with memory. Physical Review E, 93(2):022211, 2016.
- [288] O. Shoshani, S.W. Shaw, and M.I. Dykman. Anomalous decay of nanomechanical modes going through nonlinear resonance. Scientific reports, 7(1):18091, 2017.
- [289] A.H. Nayfeh and D.T. Mook. Nonlinear oscillations. John Wiley & Sons, 2008.
- [290] Y. A Rossikhin and M.V. Shitikova. Application of fractional calculus for dynamic problems of solid mechanics: novel trends and recent results. <u>Applied Mechanics Reviews</u>, 63(1):010801, 2010.

- [291] S.G. Samko, A.A. Kilbas, and O.I. Marichev. <u>Fractional integrals and derivatives: theory</u> and applications. CRC, 1993.
- [292] JL Suzuki and PA Muñoz-Rojas. Transient analysis of geometrically non-linear trusses considering coupled plasticity and damage. In <u>Tenth World Congress on Computational</u> Mechanics, page 98, 2014.
- [293] P. Perdikaris and G.E. Karniadakis. Fractional-order viscoelasticity in one-dimensional blood flow models. Ann. Biomed. Eng., 42(5):1012–1023, 2014.
- [294] J.L. Suzuki. Aspects of fractional-order modeling and efficient bases to simulate complex materials using finite element methods. PhD thesis, University of Campinas, Brazil., 2017.
- [295] Yong Zhang, HongGuang Sun, Harold H. Stowell, Mohsen Zayernouri, and Samantha E. Hansen. A review of applications of fractional calculus in earth system dynamics. <u>Chaos</u>, Solitons & Fractals, 102:29–46, 2017.
- [296] Y. Liang, W. Chen, B.S. Akpa, T. Neuberger, A.G. Webb, and R.L. Magin. Using spectral and cumulative spectral entropy to classify anomalous diffusion in sephadex<sup>™</sup>gels. <u>Comput.</u> Math. Appl., 73:765–774, 2017.
- [297] C.F. Rodrigues, J.L. Suzuki, and M.L. Bittencourt. Construction of minimum energy highorder Helmholtz bases for structured elements. J. Comp. Phys., 306:269–290, 2016.
- [298] APC Dias, Jorge L Suzuki, GL Valente, and Marco L Bittencourt. Simulation of non-linear structural elastodynamic and impact problems using minimum energy and simultaneous diagonalization high-order bases. arXiv preprint arXiv:2104.13466, 2021.
- [299] J.L. Suzuki and M.L. Bittencourt. Application of the hp-FEM for Hyperelastic Problems with Isotropic Damage, pages 113–150. Springer International Publishing, 2016.
- [300] W. Chen and Y. Gu. An improved formulation of singular boundary method. <u>Adv. Appl.</u> Math. Mech., 4:543–558, 2012.
- [301] R. Hiptmair and A. Schädle. Non-reflecting boundary conditions for maxwell's equations. Computing, 71:265–292, 2003.
- [302] J-R. Li. A fast time stepping method for evaluating fractional integrals. <u>SIAM J. Sci.</u> Comput., 31(6):4696–4714, 2010.
- [303] T. Breiten, V. Simoncini, and M. Stoll. Low-rank solvers for fractional differential equations. Electron. Trans. Numer. Anal., 45:107–132, 1983.
- [304] D. Baffet and J.S. Hesthaven. A kernel compression scheme for fractional differential equations. SIAM J. Numer. Anal., 55(2):496–520, 2017.
- [305] H. Fu, M.K. Ng, and H. Wang. A divide-and-conquer fast finite difference method for space-time fractional partial differential equation. <u>Comput. Math. Appl.</u>, 73:1233–1242, 2017.

- [306] F. Zeng, Z. Zhang, and G.E. Karniadakis. A generalized spectral collocation method with tunable accuracy for variable-order fractional differential equations. <u>SIAM J. Sci. Comput.</u>, 37(6):A2710–A2732, 2015.
- [307] K. Diethelm, J.M. Ford, N.J. Ford, and M. Weilbeer. Pitfalls in fast numerical solvers for fractional differential equations. J. Comput. Appl. Math., 186:482–503, 2006.
- [308] S. Esmaeili, M. Shamsi, and Y. Luchko. Numerical solution of fractional differential equations with a collocation method based on müntz polynomials. <u>Comput. Math. Appl.</u>, 62(3):918–929, 2011.
- [309] D. Hou and C. Xu. A fractional spectral method with applications to some singular problems. Adv. Comput. Math., 43(5):911–944, 2017.
- [310] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo. <u>Theory and Applications of Fractional</u> <u>Differential Equations, Volume 204 (North-Holland Mathematics Studies)</u>. Elsevier Science Inc., New York, NY, USA, 2006.
- [311] S. G. Samko, A. A. Kilbas, and O. I. Marichev. <u>Fractional Integrals and Derivatives: Theory</u> and Applications. Gordon and Breach Science Publishers, Switzerland, 1993.
- [312] D. Delbosco and L. Rodino. Existence and uniqueness for a nonlinear fractional differential equation. J. Math. Anal. Appl., 204(2):609–625, 1996.
- [313] S. Boyd and L. Vandenberghe. Convex Optimization. Cambridge University Press, 2004.
- [314] J Barzilai and J.M. Borwein. Two-point step size gradient methods. <u>IMA J. Numer. Anal.</u>, 8:141–148, 1988.
- [315] Weisstein, E.W. Regularized Hypergeometric Function, 2003.
- [316] Yong Zhang, HongGuang Sun, Harold H Stowell, Mohsen Zayernouri, and Samantha E Hansen. A review of applications of fractional calculus in Earth system dynamics. <u>Chaos</u> Solitons Fractals, 102:29–46, 2017.
- [317] Yong Zhou and Li Peng. On the time-fractional Navier-Stokes equations. <u>Comput. Math.</u> Appl., 73(6):874–891, 2017.
- [318] Fangying Song, Chuanju Xu, and George Em Karniadakis. A fractional phase-field model for two-phase flows with tunable sharpness: Algorithms and simulations. <u>Comput. Methods</u> Appl. Mech. Engrg., 305:376–404, 2016.
- [319] Jorge L Suzuki, Ehsan Kharazmi, Pegah Varghaei, Maryam Naghibolhosseini, and Mohsen Zayernouri. Anomalous nonlinear dynamics behavior of fractional viscoelastic beams. Journal of Computational and Nonlinear Dynamics, 2021.
- [320] Hermann Brunner. The numerical solution of weakly singular Volterra integral equations by collocation on graded meshes. Math. Comp., 45(172):417–437, 1985.

- [321] Hermann Brunner. On the numerical solution of nonlinear Volterra-Fredholm integral equations by collocation methods. SIAM J. Numer. Anal., 27(4):987–1000, 1990.
- [322] Xin Lu, HongKui Pang, and HaiWei Sun. Fast approximate inversion of a block triangular Toeplitz matrix with applications to fractional sub-diffusion equations. <u>Numer. Linear</u> Algebra Appl., 22(5):866–882, 2015.
- [323] Yongtao Zhou, Chengjian Zhang, and L. Brugnano. Preconditioned quasi-compact boundary value methods for space-fractional diffusion equations. Numer. Algorithms, 2019.
- [324] Yongtao Zhou and Chengjian Zhang. One-leg methods for nonlinear stiff fractional differential equations with Caputo derivatives. Appl. Math. Comput., 348:594–608, 2019.
- [325] Yongtao Zhou, Chengjian Zhang, and Huiru Wang. Boundary value methods for Caputo fractional differential equations. J. Comput. Math. (in press), 2019.
- [326] Yongtao Zhou and Chengjian Zhang. Convergence and stability of block boundary value methods applied to nonlinear fractional differential equations with Caputo derivatives. <u>Appl.</u> Numer. Math., 135:367–380, 2019.
- [327] Igor Podlubny. Fractional Differential Equations. San Diego, CA, USA: Academic Press, 1999.
- [328] Weihua Deng. Short memory principle and a predictor-corrector approach for fractional differential equations. J. Comput. Appl. Math., 206(1):174–188, 2007.
- [329] Ch Lubich. A stability analysis of convolution quadraturea for Abel-Volterra integral equations. IMA J. Numer. Anal., 6(1):87–101, 1986.
- [330] Ravi P Agarwal, Maria Meehan, and Donal O'Regan. <u>Fixed Point Theory and Applications</u>. Cambridge University Press, 2001.
- [331] John William Pearson. <u>Computation of hypergeometric functions</u>. PhD thesis, University of Oxford, 2009.
- [332] Milton Abramowitz and Irene A Stegun. <u>Handbook of Mathematical Functions: with</u> Formulas, Graphs, and Mathematical Tables. Courier Corporation, 1965.
- [333] Walter Gautschi. Gauss quadrature approximations to hypergeometric and confluent hypergeometric functions. J. Comput. Appl. Math., 139(1):173–187, 2002.
- [334] John G Heywood and Rolf Rannacher. Finite-element approximation of the nonstationary Navier-Stokes problem. Part IV: Error analysis for second-order time discretization. <u>SIAM</u> J. Numer. Anal., 27(2):353–384, 1990.