Extending IMSRG to Nuclear Matter with Novel Insights on UCC and IMSRG

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FRIB

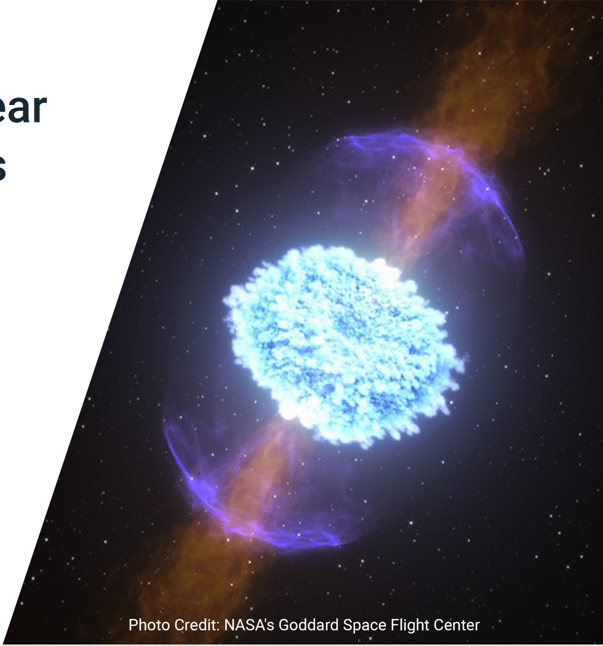
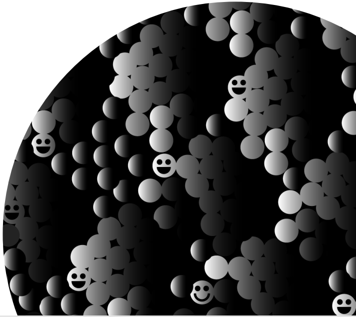


Photo Credit: NASA's Goddard Space Flight Center

Abbreviations

- ❏ NM - Nuclear matter
- ❏ EOS - Equation-of-state
- ❏ MBPT - Many-Body Perturbation Theory
- ❏ IMSRG - In-Medium Similarity Renormalization Group
- ❏ CC - Coupled-Cluster
- ❏ UCC - Unitary Coupled-Cluster
- ❏ χ-EFT - Chiral Effective Field Theory



The Nuclear Matter Equation-of-State

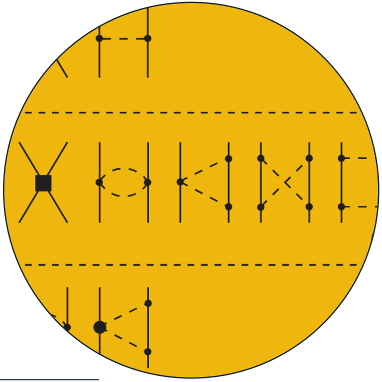
The NM-EOS is given by $E(\rho)/A$ where $E(\rho)$ is the total energy of a system containing $A \to \infty$ interacting nucleons confined in a $\mathcal{V} \to \infty$ volume at density ρ.

- ❏ It determines the stability and bulk properties of NM—e.g. response to gravitational compression.
  - ❖ Directly linked to astrophysical phenomena—e.g. neutron star physics
  - ❖ Indicative of possible new states of compressed matter

- ❏ Constrained NM-EOS allows the testing and improvement of nuclear force models
  - ❖ Deficiencies of χ-EFT in heavy nuclei linked to poor saturation (overbinding, radii too small)

Recent *Ab Initio* Developments

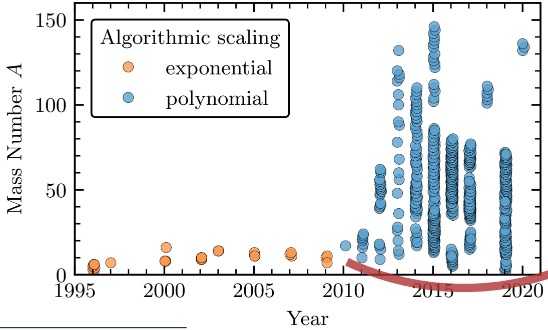
- ❏ χ-EFT—hierarchy of NN, 3N, ... interactions
  - ❖ Wide range available for many-body calculations



[1] C. Drischler et al., Annual Review of Nuclear and Particle Science **71**, 403 (2021).

Recent *Ab Initio* Developments

- MBPT, and non-perturbative methods CC, UCC, IMSRG—polynomial scaling[1,2,3]



Explosion due to RG softening

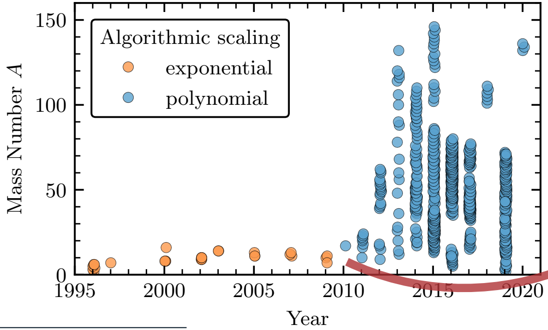
+ soft χ-EFT forces

[1] C. Drischler and S. K. Bogner, Few-Body Systems **62**, 10.1007/s00601-021-01677-2 (2021).
[2] H. Hergert, Frontiers in Physics **8**, 10.3389/fphy.2020.00379 (2020).
[3] G. Hagen et al., Physical Review C **89**, 10.1103/physrevc.89.014319 (2014).

Recent *Ab Initio* Developments

Has not been used
for realistic NM-EOS studies :(

- MBPT, and non-perturbative methods CC, UCC, IMSRG—polynomial scaling[1,2,3]



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Project Goals

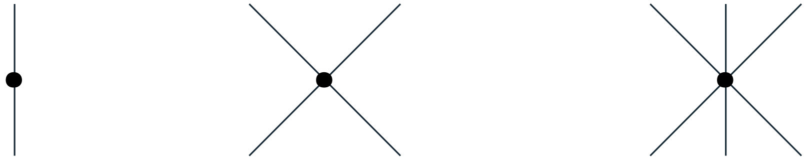
Unlike MBPT and CC, the IMSRG has *not* been applied to study NM-EOS with realistic nucleon forces.

- ✔ We will extend it to infinite nuclei matter using multiple nuclear forces.
- ✔ We will tackle computational challenges that limit our achievable A and model space sizes.

SRG Theory

Consider[4]

$$H = \sum_{pq} T_{pq} a_p^\dagger a_q + \frac{1}{(2!)^2} \sum_{pqrs} V^{(2)}_{pqrs} a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{(3!)^2} \sum_{pqrstu} V^{(3)}_{pqrstu} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$



[4] H is normal-ordered relative to the true vacuum: $\langle 0|H|0\rangle = 0$.

SRG Theory

$$H(s) = U(s) H U(s)^{\dagger}$$

$$\frac{dH(s)}{ds} = \left[\eta(s),\, H(s)\right]$$

Induced A-body forces!

3NF evolution alone *very* costly

Driving force

$$\underbrace{\eta(s)}_{\text{Generator}} \equiv \frac{dU(s)}{ds} U(s)^{\dagger} = -\eta(s)^{\dagger}$$

$$\eta^{Wegner}(s) = \left[H_{\text{diagonal}}(s),\, H_{\text{off-diagonal}}(s)\right]$$

Drives $H_{\text{off-diagonal}}(s \to \infty) = 0$

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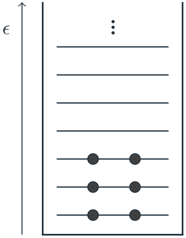
Drives $H_{\text{off-diagonal}}(s \to \infty) = 0$

In-Medium SRG

IMSRG improves SRG by rewriting H *exactly* into a normal-ordered form based on $|\Phi\rangle$.[7,8]

$$H = \underbrace{E}_{\langle\Phi|H|\Phi\rangle} + \sum_{pq} f_{pq} :a_p^\dagger a_q: + \frac{1}{4}\sum_{pqrs}\Gamma_{pqrs} :a_p^\dagger a_q^\dagger a_s a_r: + \frac{1}{36}\sum_{pqrstu} W_{pqrstu} :a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s:$$



$|\Phi\rangle$

[7] G. C. Wick, Phys. Rev. **80**, 268 (1950).
[8] H. Hergert et al., Physics Reports **621**, 165 (2016).

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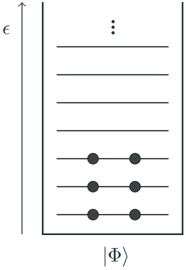

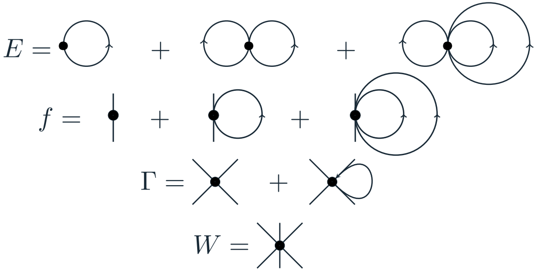

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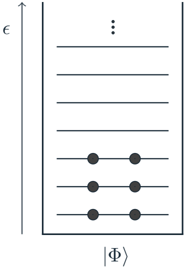

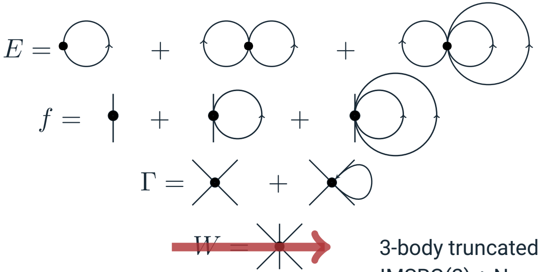

3-body truncated
IMSRG(2) + Normal-ordered 3NF

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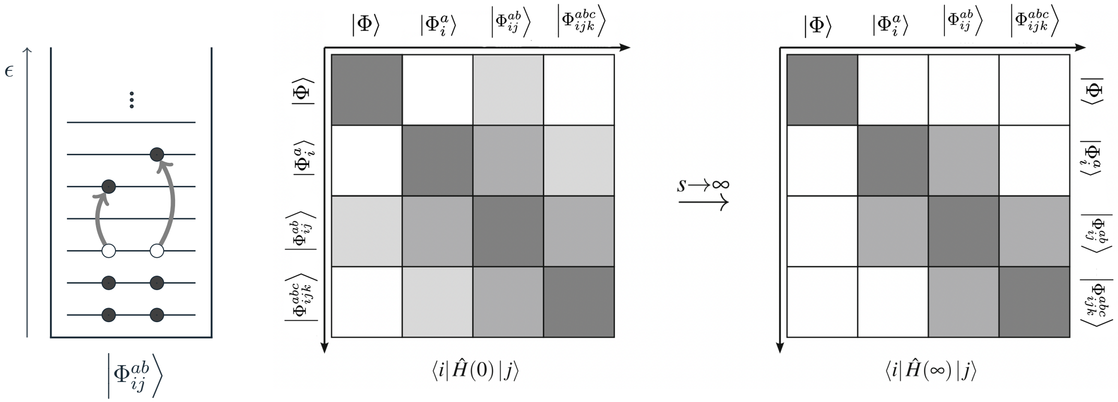
[8] H. Hergert et al., Physics Reports **621**, 165 (2016).

In-Medium SRG Diagonalization

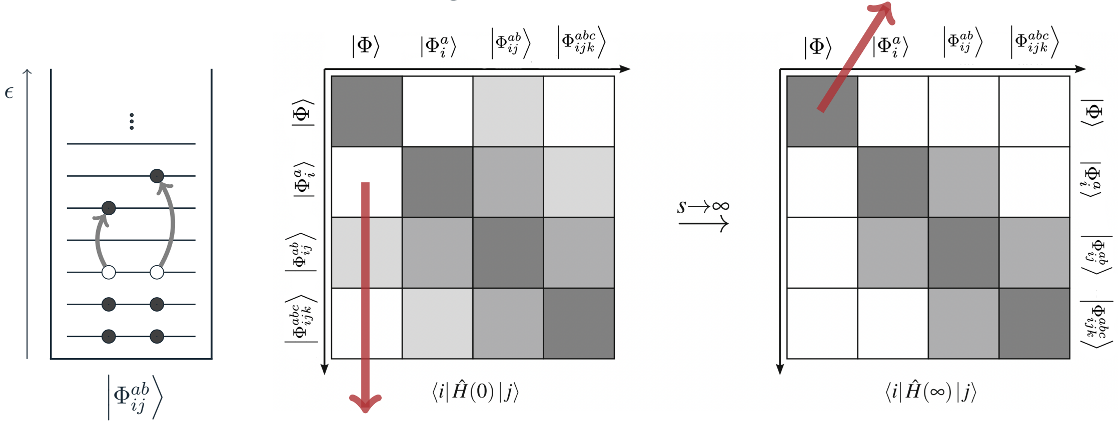


[9] M. Hjorth-Jensen et al., "An advanced course in computational nuclear physics: bridging the scales from quarks to neutron stars", in (Springer Nature, Jan. 2017), pp. 521–529.

In-Medium SRG Diagonalization

(Zero temperature EOS)

Ground state energy



Momentum conservation (infinite matter)

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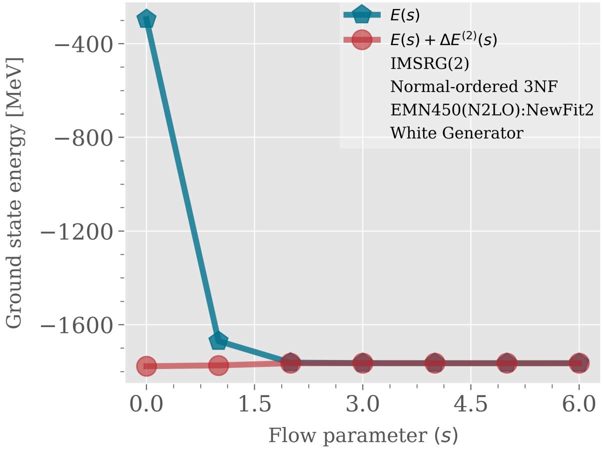
In-Medium SRG Evolution



$N = Z = 66$, $\rho = 0.13\,\mathrm{fm}^{-3}$, $N_{\text{orbitals}} = 3700$

Magnus Expansion in the In-Medium SRG

$$\frac{dH(s)}{ds} = \Big[\eta(s),\, H(s)\Big] \iff \left\{ \begin{array}{c} dU(s)/ds = \eta(s)U(s) \\ \downarrow \\ H(s) = U(s)HU(s)^\dagger \end{array} \right\}$$

$$U(s) = e^{\Omega(s)}$$

$$\Omega(s) = \text{Some complicated expression}$$

Advantages:[10]

- ❏ $\Omega(s \to \infty)$ can be cached for observables beyond energies
- ❏ Memory efficient with built-in unitarity (crude 1st-order Euler solver)
- ❏ *Reminiscent of UCC (can we borrow ideas from UCC?)*

[10] T. D. Morris et al., Physical Review C **92**, 10.1103/physrevc.92.034331 (2015).

Project Goals

Physics objectives

Develop a new IMSRG codebase to carry out non-perturbative NM-EOS calculations with realistic internucleon interactions

- ✔ Calculate NM-EOS at multiple proton fractions
- ✔ Use multiple 2 and 3-body chiral forces
- ✔ Lay groundwork for future directions
  - ❖ NM-EOS studies with EFT uncertainty quantification, finite temperature IMSRG, momentum distributions...

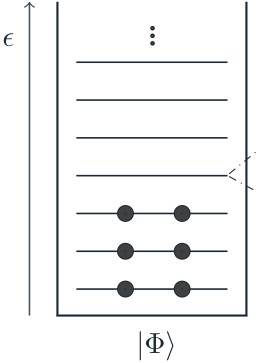
Project Goals

Computational objectives

- ✔ Ensure IMSRG codebase is high-performant
  - ❖ Exploit symmetries of IMSRG operators
  - ❖ Cast tensor contractions into matrix-matrix multiplication
  - ❖ Write contraction algorithms to best utilize CPU cache and thread parallelism
  - ❖ Use approximations in contraction algorithms when feasible
- ✔ Accelerate IMSRG's convergence for computational speedup
  - ❖ Novel UCC-Inspired generators
  - ❖ IMSRG extrapolation using Shanks + Padé transforms (see dissertation)

Modeling Infinite Nuclear Matter in a Cubic Box

We confine N identical neutrons and Z identical protons in a periodic box of volume $\mathcal{V} = \mathcal{L}^3$.



$$\psi(\vec{r}) = \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{\mathcal{V}}} \left|\downarrow\uparrow\right\rangle_{\sigma_z} \left|\downarrow\uparrow\right\rangle_{\tau_z}$$

$$\vec{k} = \frac{2\pi}{\mathcal{L}}\vec{n}, \quad \vec{n} \in \mathbb{R}^3$$

$$\epsilon = \frac{(\hbar c)^2}{2m_{\tau_z}}\vec{k}\cdot\vec{k}$$

Modeling Infinite Nuclear Matter in a Cubic Box

Index	Occ	n_x	n_y	n_z	σ_z	τ_z	k [fm^{-1}]	ϵ [MeV]
0	1	0	0	0	$\downarrow\uparrow$	$\downarrow$	0.000	0.000
2	1	0	0	0	$\downarrow\uparrow$	$\uparrow$	0.000	0.000
4	1	-1	0	0	$\downarrow\uparrow$	$\uparrow$	1.458	44.121
6	1	0	-1	0	$\downarrow\uparrow$	$\uparrow$	1.458	44.121
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
74	0	1	1	0	$\downarrow\uparrow$	$\downarrow$	2.062	88.121

Closed shell system with $N_{\text{orbitals}} = 76$ containing $N = 2$ and $Z = 14$ nucleons with $\mathcal{L} = 4.308\,\text{fm}$, $\rho = 0.20\,\text{fm}^{-3}$

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Closed shell system with $N_{\text{orbitals}} = 76$ containing $N = 2$ and $Z = 14$ nucleons with $\mathcal{L} = 4.308\,\text{fm}$, $\rho = 0.20\,\text{fm}^{-3}$

Finite basis introduces errors in our calculations.

Nuclear Matter Code

We've written a C++ nuclear matter IMSRG code with the following features:

- ✔ Compatible with semi-arbitrary Z/A
- ✔ Implemented with density-dependent 3-body forces
- ✔ Equipped with Shanks + Padé extrapolators[11]
- ✔ Equipped with canonical and novel generators[12]
- ✔ Multi-threaded and MPI capable
- ✔ Based on Eigen C++ library with BLAS and Intel MKL support
- ✔ Equipped with tools to address finite basis errors (IMSRG-MBPT correlation, compute power for brute-force approach)

[11] See dissertation
[12] See slide 22

Nuclear Matter Code

Highlights

- ✔ Written with care—verbose, unit tested
- ✔ Modernized with C++ features (classes, templates, etc.)
- ✔ Extendable to other systems (e.g. finite nuclei, e^- gas)
- ✔ Integrated with a wide range of NN and 3N chiral interactions
- ✔ *Fast*: ~ 10 hour runtime for $A = 132$, $N_{\text{orbitals}} \sim 3700$ at IMSRG(2)
- ✔ Memory efficient: RAM ~ 1 TB for $A = 132$, $N_{\text{orbitals}} \sim 3700$
- ✔ Modernized with automated data compilation—file parsing for plots

High Performance Optimizations

Operator Symmetries

$$H = \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r : + \ldots$$

Matrix representation

$$\begin{array}{c|cc} & (r < s) & (r > s) \\ \hline (p < q) & \Gamma & -\Gamma \\ (p > q) & -\Gamma & +\Gamma \end{array}$$

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$\sim$ 4X memory + compute savings

High Performance Optimizations

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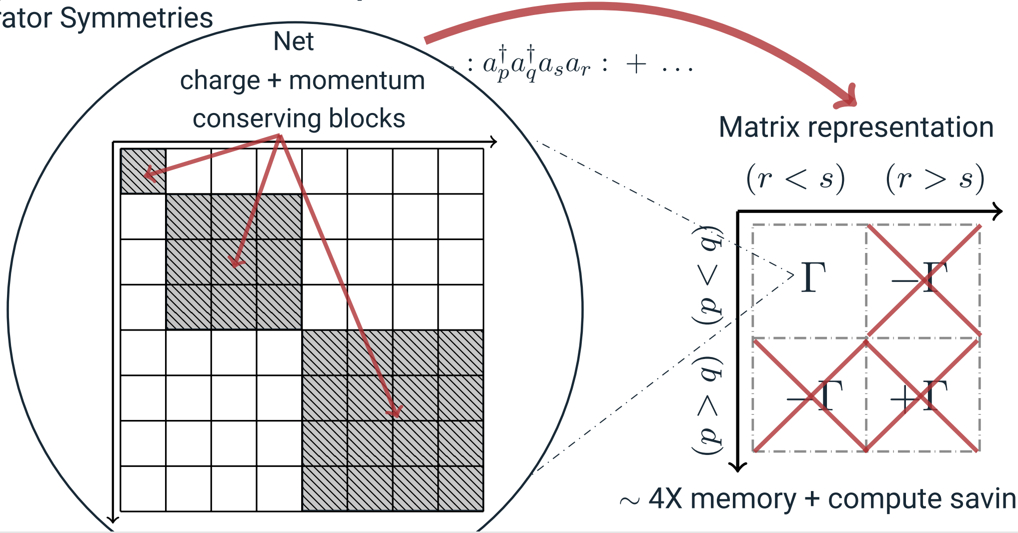

$\sim$ 4X memory + compute savings

High Performance Optimizations
Particle-Hole Contractions

Commutators are the most expensive computations in the IMSRG(2).

$$\Big[\Omega, B\Big]_{pqrs} \mathrel{+}= \sum_{tu} \Omega_{ptur} \times O_{tutu} \times B_{uqst}$$

$$\Omega_{ptur} = \tilde{\Omega}_{prut}$$

$$B_{uqst} = \tilde{B}_{utsq}$$

$$\Big[\Omega, B\Big]_{pqrs} \mathrel{-}= (\tilde{\Omega} O \tilde{B})_{prsq}$$

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Performance optimizations offloaded to BLAS/MKL

High Performance Optimizations

Particle-Hole Contractions

$$O = \begin{bmatrix} O_{\mathbb{P}\mathbb{P}} & O_{\mathbb{P}\mathbb{Q}} = 0 \\ O_{\mathbb{Q}\mathbb{P}} = 0 & O_{\mathbb{Q}\mathbb{Q}} = 0 \end{bmatrix}$$

$$\tilde{\Omega} O \tilde{B} = \begin{bmatrix} \tilde{\Omega}_{\mathbb{P}\mathbb{P}} \times O_{\mathbb{P}\mathbb{P}} \times \tilde{B}_{\mathbb{P}\mathbb{P}} & \tilde{\Omega}_{\mathbb{P}\mathbb{P}} \times O_{\mathbb{P}\mathbb{P}} \times \tilde{B}_{\mathbb{P}\mathbb{Q}} \\ \tilde{\Omega}_{\mathbb{Q}\mathbb{P}} \times O_{\mathbb{P}\mathbb{P}} \times \tilde{B}_{\mathbb{P}\mathbb{P}} & \tilde{\Omega}_{\mathbb{Q}\mathbb{P}} \times O_{\mathbb{P}\mathbb{P}} \times \tilde{B}_{\mathbb{P}\mathbb{Q}} \end{bmatrix}$$

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$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & \ddots \end{bmatrix}$$

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High Performance Optimizations

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$$\left\| \tilde{\Omega}_{\mathbb{QP}} \right\| \approx 0$$

$$\left\| \tilde{B}_{\mathbb{PQ}} \right\| \approx 0$$ (Magnus expansion)

High Performa[nce Optimizations]

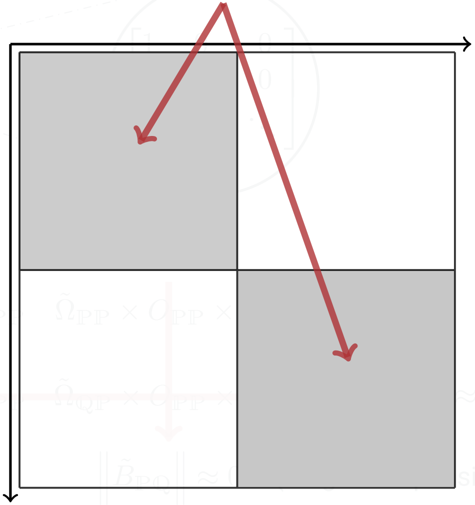
Particle-Hole Contra[ctions]

$$O = \begin{bmatrix} O_{\mathbb{PP}} & \\ O_{\mathbb{QP}} = 0 & \end{bmatrix}$$

$$\tilde{\Omega} O \tilde{B} = \begin{bmatrix} \tilde{\Omega}_{\mathbb{PP}} & \\ \tilde{\Omega}_{\mathbb{QP}} \times & \end{bmatrix}$$

Relative charge

\+ momentum conserving blocks



High Performa

Particle-Hole Contra

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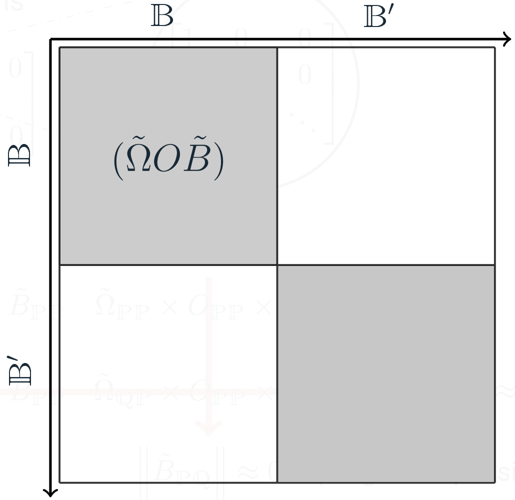
Every block $\mathbb{B}$ containing (p, r)
is mirrored by $\mathbb{B}'$ containing (r, p)



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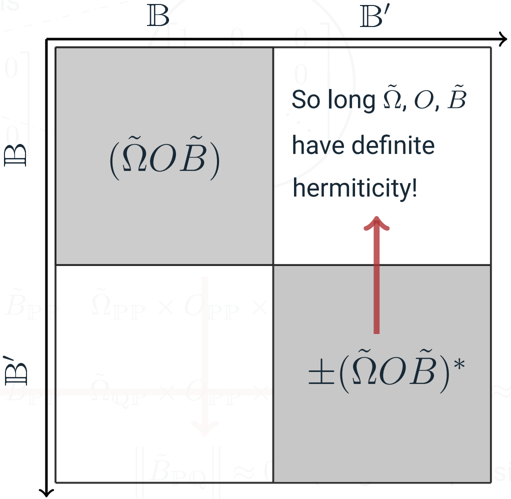

High Performance Optimizations
Particle-Hole Contractions

$$O = \begin{bmatrix} O_{\mathbb{PP}} & O_{\mathbb{PQ}} = 0 \\ O_{\mathbb{QP}} = 0 & O_{\mathbb{QQ}} = 0 \end{bmatrix}$$

$$\tilde{\Omega} O \tilde{B} = \begin{bmatrix} \tilde{\Omega}_{\mathbb{PP}} \times O_{\mathbb{PP}} \times \tilde{B}_{\mathbb{PP}} & \tilde{\Omega}_{\mathbb{PP}} \times O_{\mathbb{PP}} \times \cdots \\ \cancel{\tilde{\Omega}_{\mathbb{QP}} \times O_{\mathbb{PP}} \times \tilde{B}_{\mathbb{PP}}} & \cancel{\tilde{\Omega}_{\mathbb{QP}} \times O_{\mathbb{PP}} \times \cdots} \end{bmatrix}$$

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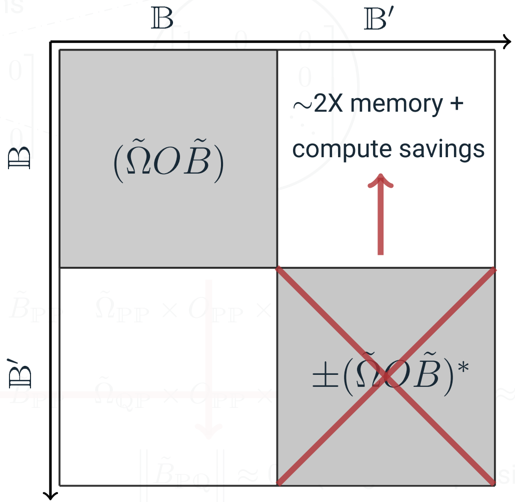

High Performance Optimizations
Tensor Contractions - Cache Misses :>

$$\left[\Omega, H\right]_{pqrs} \mathrel{-}= \sum_t \left(f_{pt}\,\Omega_{tqrs} + f_{qt}\,\Omega_{ptrs} - f_{tr}\,\Omega_{pqts} - f_{ts}\,\Omega_{pqrt} \right)$$

Largest block size $\sim N^2_{\text{orbitals}} \times \frac{16}{1e6}$ Megabytes $= \underbrace{144 \text{ Megabytes}}_{N_{\text{orbitals}}=3000}$

Assume: $f_{p\neq q} \approx 0$

$$\Downarrow$$

$$\left[\Omega, H\right]_{pqrs} \mathrel{-}= \left(f_{pp} + f_{qq} - f_{rr} - f_{ss} \right) \times \Omega_{pqrs}$$

$\sum_t$ eliminated with less cache misses!

High Performance Optimizations

Tensor Contractions - Cache Misses :>

$$\left[\Omega, H\right]_{pqrs} -= \sum_t \left(f_{pt}\,\Omega_{tqrs} + f_{qt}\,\Omega_{ptrs} - f_{tr}\,\Omega_{pqts} - f_{ts}\,\Omega_{pqrt} \right)$$

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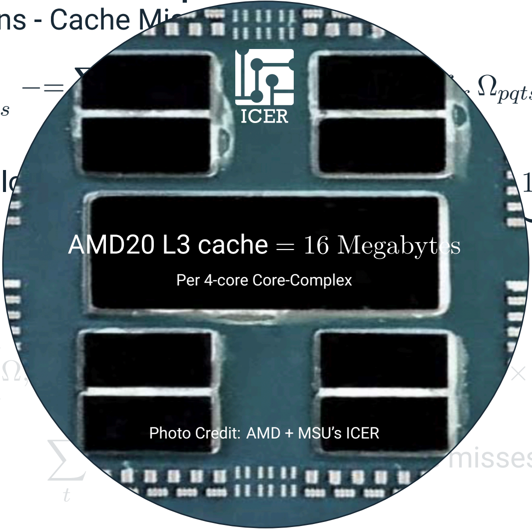

High Performance Optimizations

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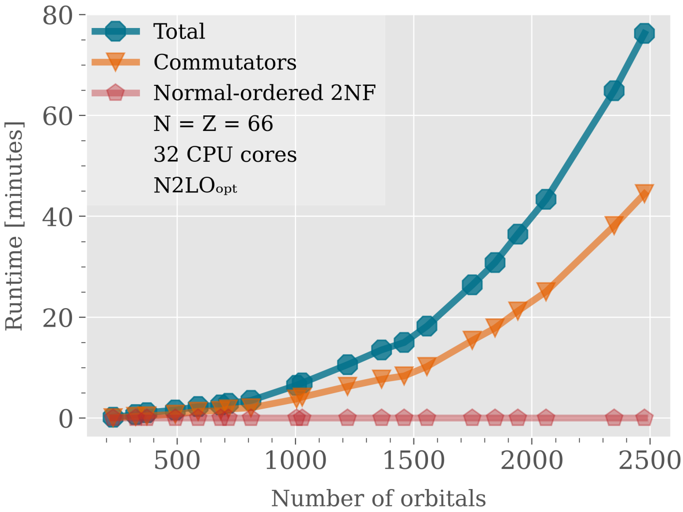
Performance Results



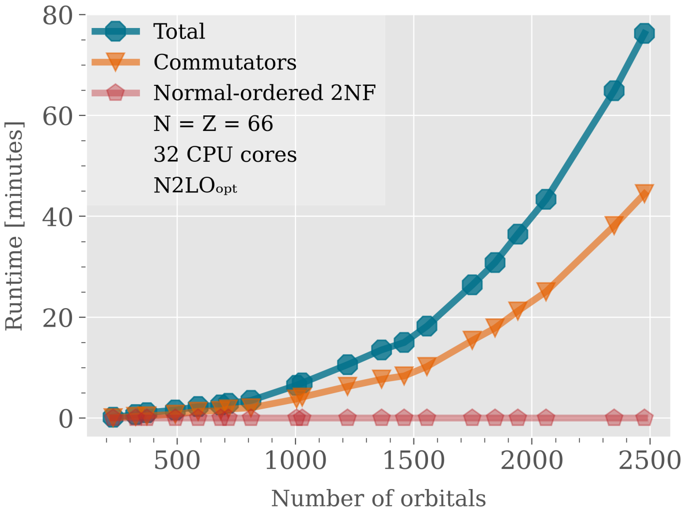
Automated data handling:

-Labeled data

-Auto-generated figures

-Accessible to everyone

Performance Results



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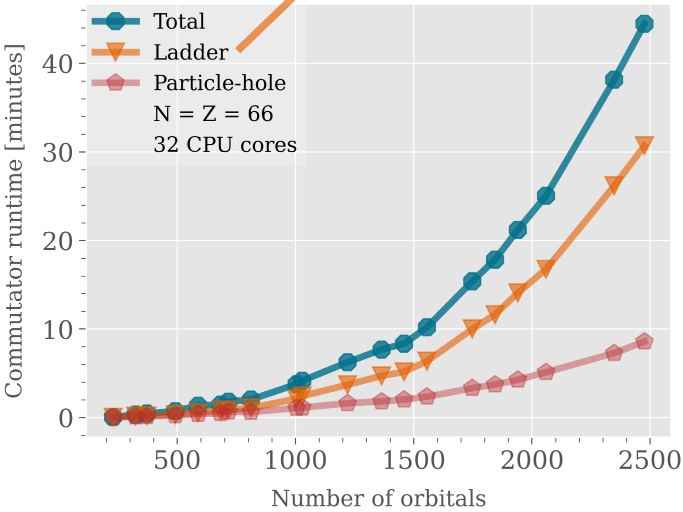
Performance Results

Easier to optimize (already in matrix multiplication form)



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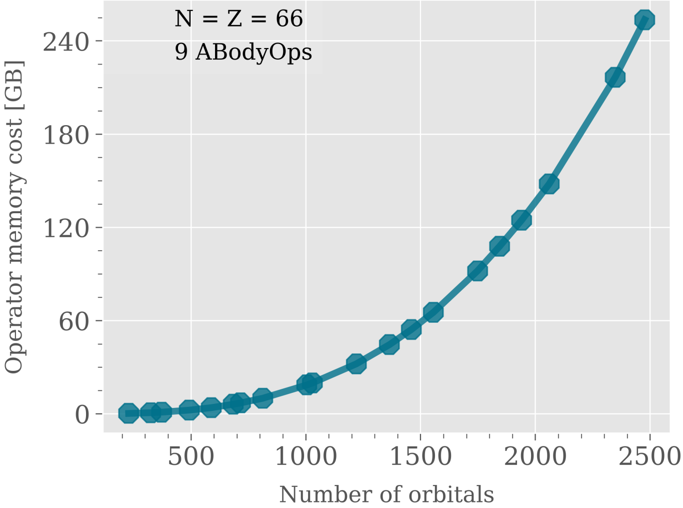
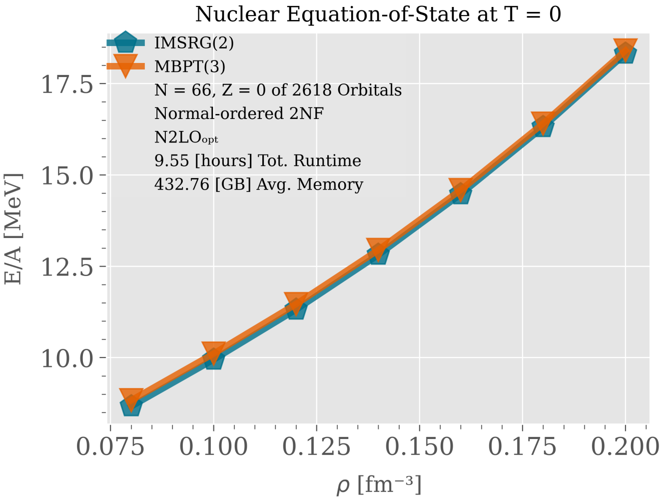


Nuclear Matter Equation-of-State Results



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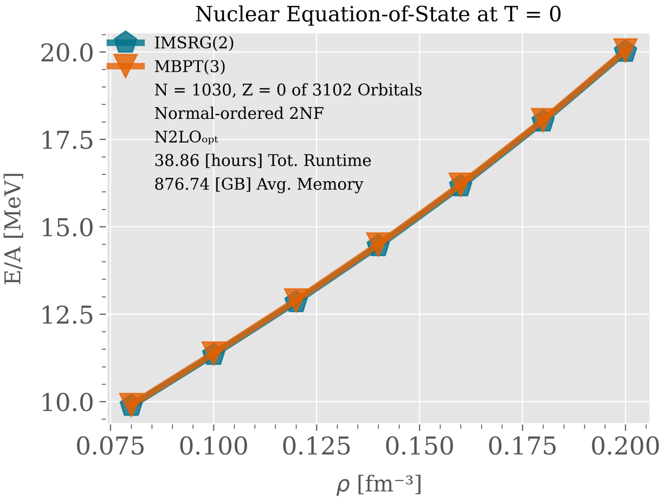

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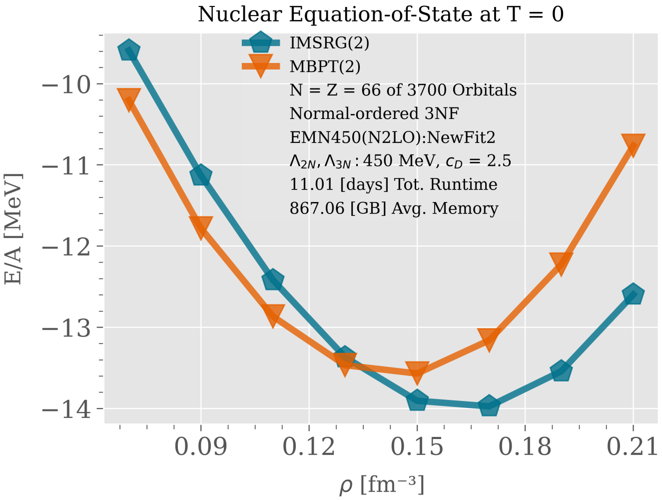
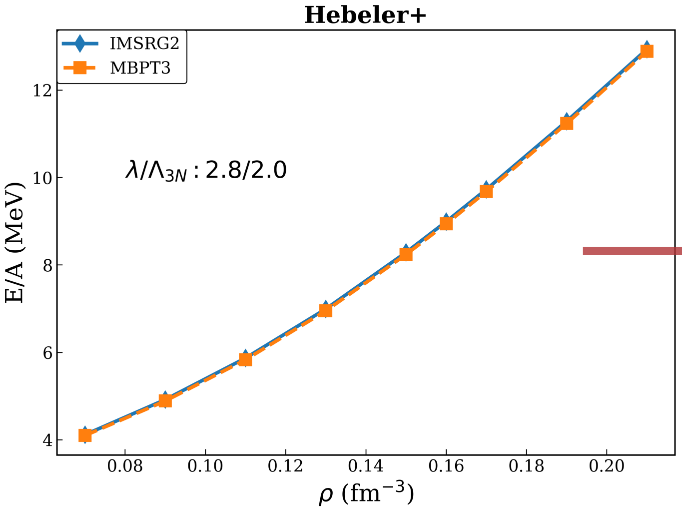


Nuclear Matter Equation-of-State Results

Proton fraction = 0.05

Normal-ordered 3NF



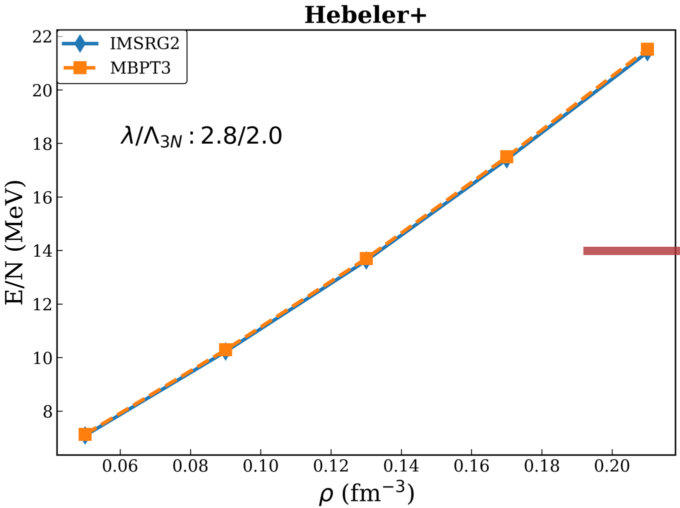
Great IMSRG

& MBPT agreement

Nuclear Matter Equation-of-State Results

Proton fraction = 0

Normal-ordered 3NF



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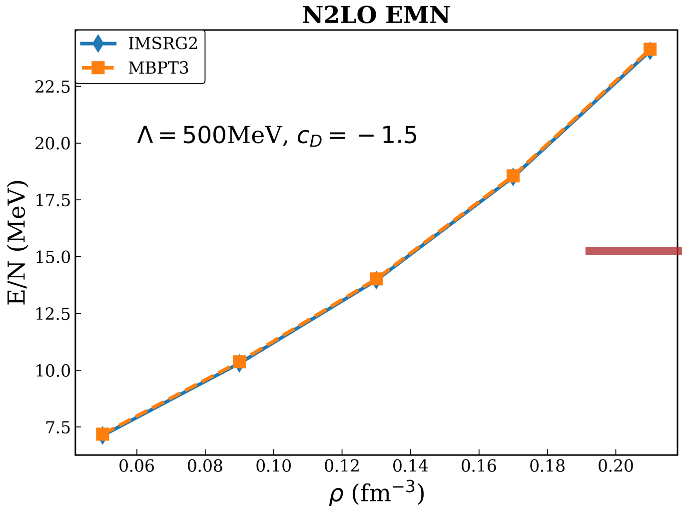

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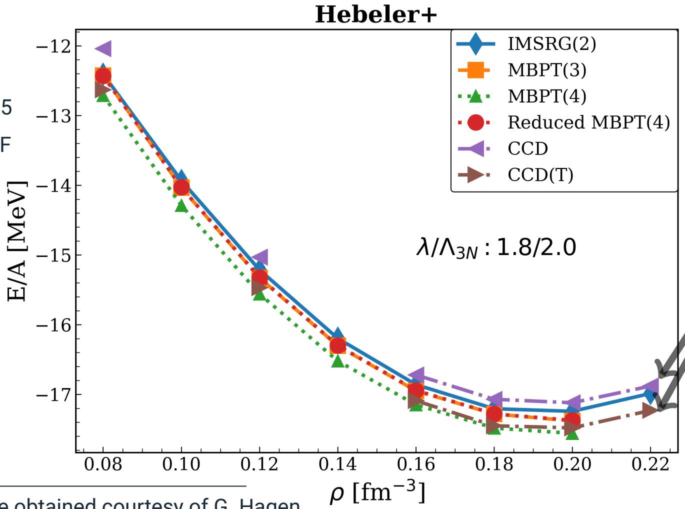

IMSRG(2) between CCD and CCD(T)

[14] CC results were obtained courtesy of G. Hagen.

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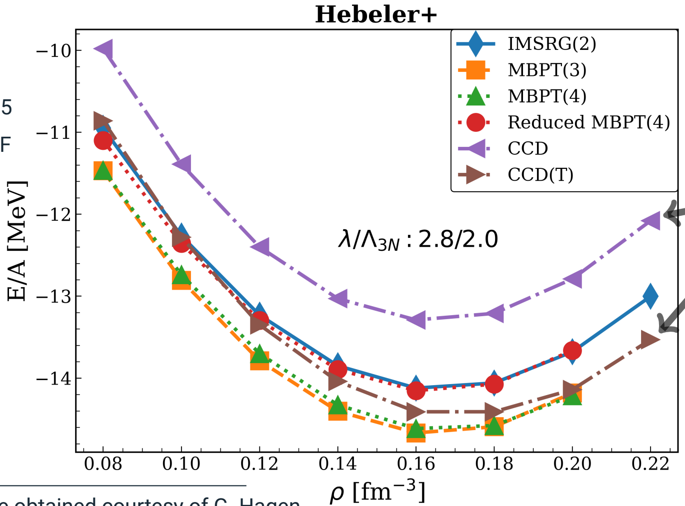

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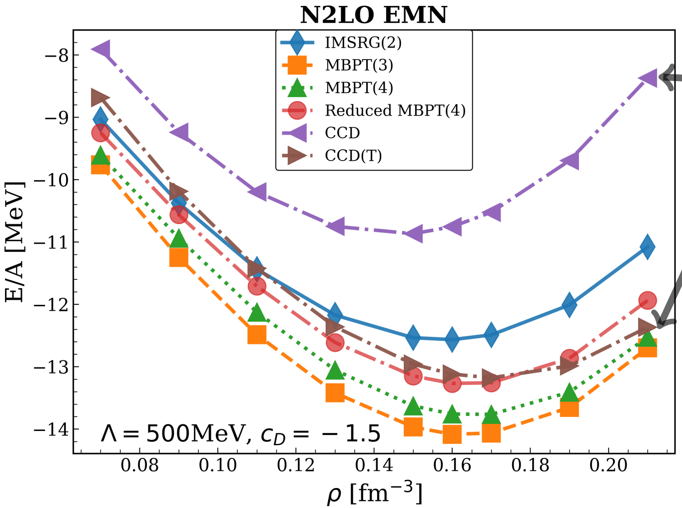


IMSRG(2) between CCD and CCD(T)

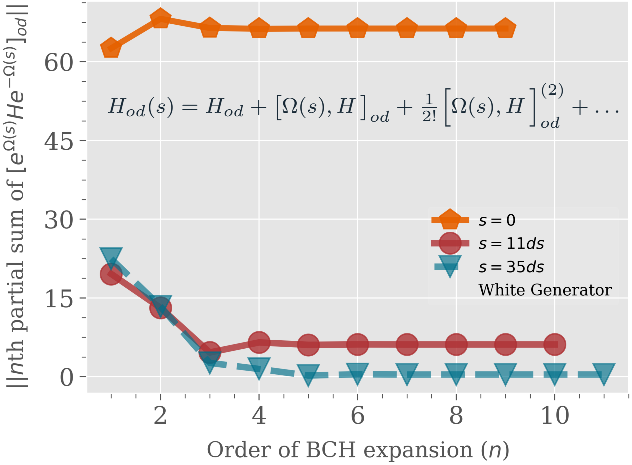
Nuclear Matter Equation-of-State Results

Key takeaways

- ❑ Excellent agreement between IMSRG and MBPT in PNM
- ❑ Sizable energy disagreements between methods in SNM with harder forces
  - ❖ Differences understood with perturbative analysis of CC and IMSRG(2)[14]
  - ❖ IMSRG(2) generally falls between CCD and CCD(T)—consistent with finite nuclei!
- ❑ All methods saturate near the same point.
- ❑ Triples in CC become sizable with increasing ρ.

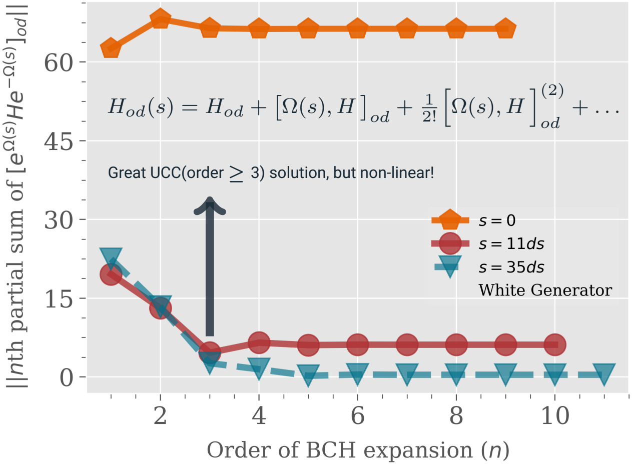
[14] H. Hergert et al., Physics Reports **621**, 165 (2016).

UCC-Inspired IMSRG Generators: General Idea



$N = Z = 14$, $\rho = 0.11\,\mathrm{fm}^{-3}$, $N_{\text{orbitals}} = 76$

UCC-Inspired IMSRG Generators: General Idea



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UCC-Inspired IMSRG Generators: Motivation

- $\mathcal{O}(N^6_{\text{orbitals}})$ commutator evaluations are the most compute limiting IMSRG(2) operations (without 3-body forces).
- The IMSRG can sometimes require hundreds of commutator evaluations to converge—detrimental in large systems.

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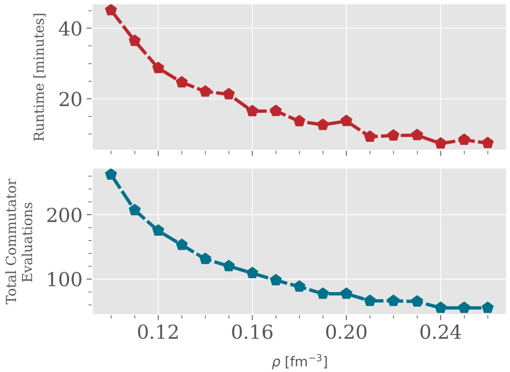
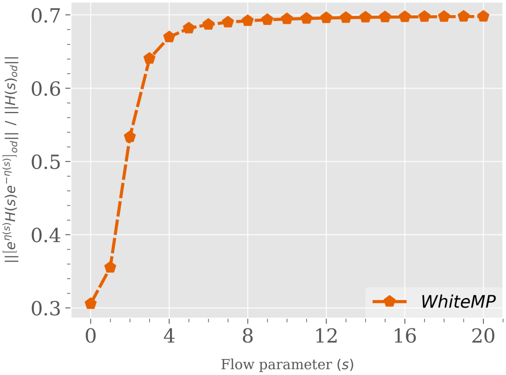


IMSRG performance costs using $\eta^{WhiteMP}(s)$,[a] $N = Z = 14$, and $N_{\text{orbitals}} = 1556$.

[a] S. R. White, The Journal of Chemical Physics **117**, 7472 (2002).

UCC-Inspired IMSRG Generators: Observation

- $\eta(s)$ *partially* diagonalizes $H(s)$
- Magnitude of diagonalization largest early in flow where $\Delta E^{(2)}(s)/E(s)$ is largest and IMSRG is far from convergence



Comparison of $H(s)_{od}$ and its unitary equivalent, where $\eta(s) = \eta^{WhiteMP}(s)$, $N = Z = 14$, $\rho = 0.12$, and $N_{\text{orbitals}} = 228$.

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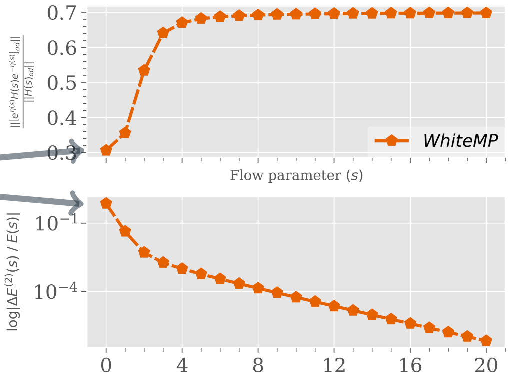

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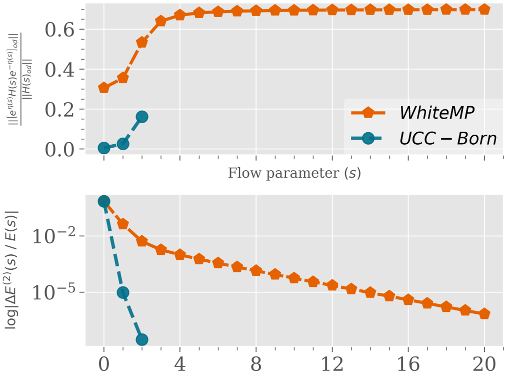
UCC-Inspired IMSRG Generators: Hypothesis

- Convergence acceleration achievable by improving diagonalizing power of $\eta(s)$
- Look towards UCC for better diagonalizers $\eta(s)$



Post-hoc comparison of $H(s)_{od}$ and its unitary equivalent, where $N = Z = 14$, $\rho = 0.12$, and $N_{\text{orbitals}} = 228$.

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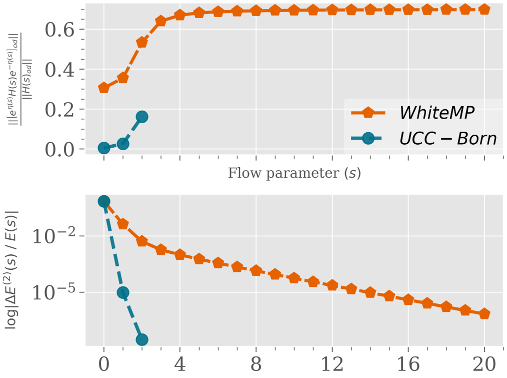

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UCC Theory

Consider a given Hamiltonian H. We aim to find η such that

$$\left[e^{\eta} H e^{-\eta}\right]_{od} = 0, \qquad \eta = -\eta^{\dagger}$$

$$\Downarrow$$

$$-H_{od} = \Big[\eta\,,\ H\Big]_{od} + \frac{\Big[\eta\,,\ H\Big]^{(2)}_{od}}{2!} + \frac{\Big[\eta\,,\ H\Big]^{(3)}_{od}}{3!} + \ldots \qquad \text{(BCH expansion)}$$

$$-H_{od} = \left[\eta,\ \underbrace{\sum_{m=0}^{\infty} \frac{[\eta,\ H]^{(m)}}{(m+1)!}}_{H^{RG}(\eta)}\right]_{od} \qquad \text{Invertible?}^{15}$$

[15] The view of UCC as a nonlinear commutator inversion problem was partly inspired by Kutzelnigg [10].

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Commutator Inversion via Born Series

Suppose we are tasked with inverting the following commutator[16]

$$-H_{abij} = \left[\eta,\ H^{RG}\right]_{abij}$$

$$\Gamma_{abij} \qquad\qquad E^{RG} + f^{RG} + \Gamma^{RG}$$

$$-\Gamma_{abij} = \cancel{\left[\eta,\ E^{RG}\right]}_{abij} + \left[\eta,\ f^{RG}\right]_{abij} + \left[\eta,\ \Gamma^{RG}\right]_{abij}$$

$$\left[\eta,\ f^{RG}\right]_{abij} = -\Delta^{RG}_{abij} \times \eta_{abij}$$

See slide 38

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Commutator Inversion via Born Series

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$$\eta_{abij} = \frac{\Gamma_{abij}}{\Delta^{RG}_{abij}} + \frac{\left[\eta,\ \Gamma^{RG}\right]_{abij}}{\Delta^{RG}_{abij}}$$

Adopting the following notation for any A-body operator O[16]

$$\left(O_*\right)_{abij} \equiv \frac{O_{abij}}{\Delta^{RG}_{abij}}$$

$$\eta = \Gamma_* + \left[\eta,\ \Gamma^{RG}\right]_* \qquad \text{(Lippmann-Schwinger Eq.!)}$$

[16] All sectors of O_* other than $\left(O_*\right)_{abij}$ are defined to be zero. For example, $\left(O_*\right)_{abcd} \equiv 0 \ \ \forall abcd$.

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Commutator Inversion via Born Series

$$\eta \approx \Gamma_* + \Big[\Gamma_*\,,\ \Gamma^{RG}\Big]_* + \bigg[\Big[\Gamma_*,\ \Gamma^{RG}\Big]_*,\ \Gamma^{RG}\bigg]_* + \dots$$

Dr. Max Born
University of Göttingen
(1882-1970)

Preconditioning the Born Series

- All novel generators strongly rely on the Born series
  - Its convergence behaviour is paramount
  - We seek to accelerate its convergence when possible[16]

$$-H_{abij} = \left[\underbrace{\eta}_{\eta^{Guess} + \delta\eta} \; , \; H^{RG} \right]_{abij}$$

$$-\left(H_{abij} + \left[\eta^{Guess}, \; H^{RG} \right]_{abij} \right) = \left[\delta\eta, \; H^{RG} \right]_{abij}$$

[16] Preconditioning the Born series is reminiscent of the Newton-Krylov method [11].

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Estimating $H^{RG}(\eta)$

Recall, we aim to solve: $-H_{abij} = \left[\eta,\ \underbrace{H + \frac{1}{2!}\left[\eta,\ H\right] + \frac{1}{3!}\left[\eta,\ H\right]^{(2)} + \dots}_{H^{RG}(\eta)}\right]_{abij}$

Novel generators estimate $H^{RG}(\eta)$ differently:

$$-H_{abij} = \left[\eta^{Born},\ H\right]_{abij}$$

$$-H_{abij} = \left[\underbrace{\eta^{UCC-Born}}_{\eta^{Born}+\delta\eta},\ H + \frac{2}{3}\left[\eta^{Born},\ H\right] + \frac{1}{3}\left[\eta^{Born},\ H\right]^{(2)} + \dots\right]_{abij}$$

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$$-H_{abij} = \left[\underbrace{\eta^{UCC-Born}}_{\eta^{Born} + \delta\eta},\ H + \frac{2}{3}\left[\eta^{Born},\ H\right] + \frac{1}{3}\left[\eta^{Born},\ H\right]^{(2)} + \ldots\right]_{abij}$$

Estimating $H^{RG}(\eta)$

Recall, we aim to solve: $-H_{abij} = \Bigg[\eta,\ \underbrace{H + \frac{1}{2!}[\eta,\ H] + \frac{1}{3!}[\eta,\ H]^{(2)} + \ldots}_{H^{RG}(\eta)}\Bigg]_{abij}$

Novel generators estimate $H^{RG}(\eta)$ differently:

$$-H_{abij} = \left[\eta^{Born},\ H\right]_{abij}$$

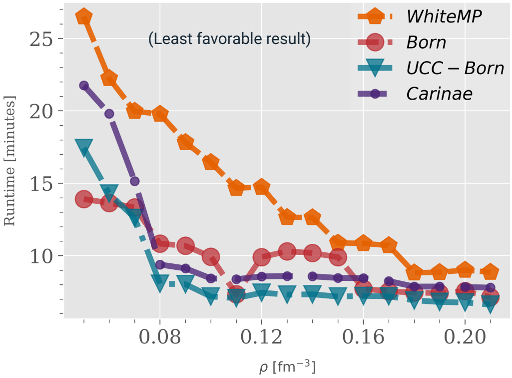
$$-H_{abij} = \Bigg[\underbrace{\eta^{UCC-Born}}_{\eta^{Born}+\delta\eta},\ H + \frac{2}{3}[\eta^{Born},\ H] + \frac{1}{3}[\eta^{Born},\ H]^{(2)} + \ldots\Bigg]_{abij}$$

Estimating $H^{RG}(\eta)$

$$-H_{abij} = \Big[\underbrace{\eta^{\{k^*+1\}}}_{\eta^{Carinae}},\ H^{RG}\big(\eta^{\{k^*\}}\big)\Big]_{abij}$$

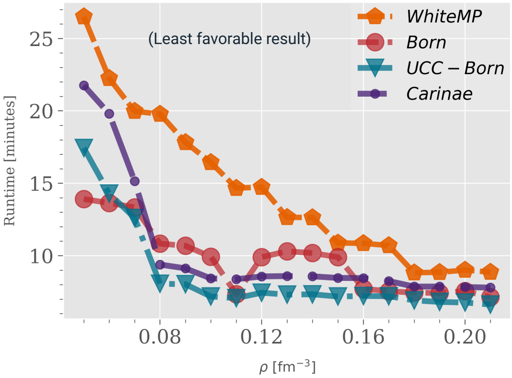
(Successive approximations)

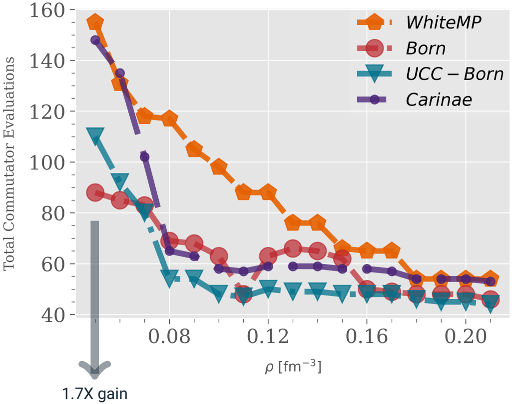
Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 66$, $Z = 54$, $N_{\text{orbitals}} = 1460$

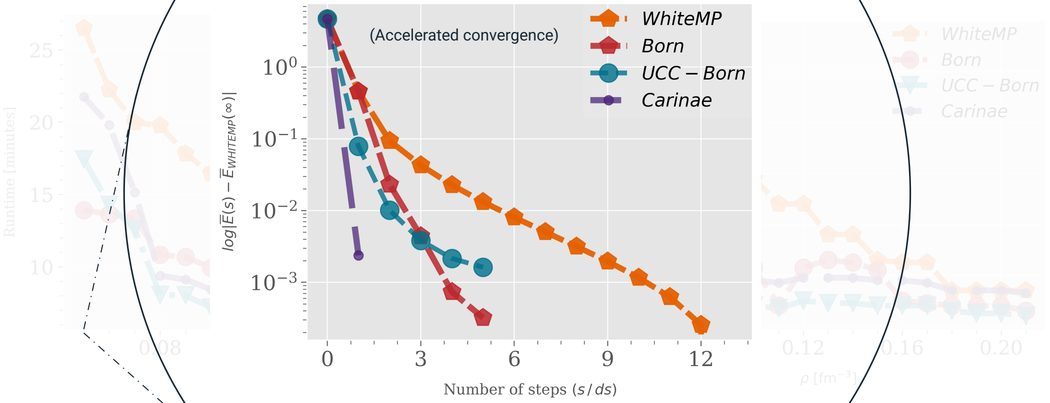
Results: Generator Comparisons





N2LO$_{\text{opt}}$, $N = 66$, $Z = 54$, $N_{\text{orbitals}} = 1460$

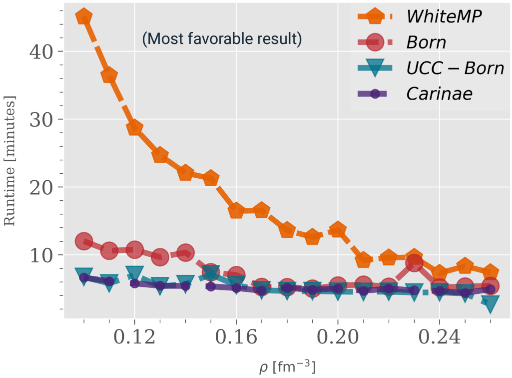
Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 66$, $Z = 54$, $N_{\text{orbitals}} = 1460$

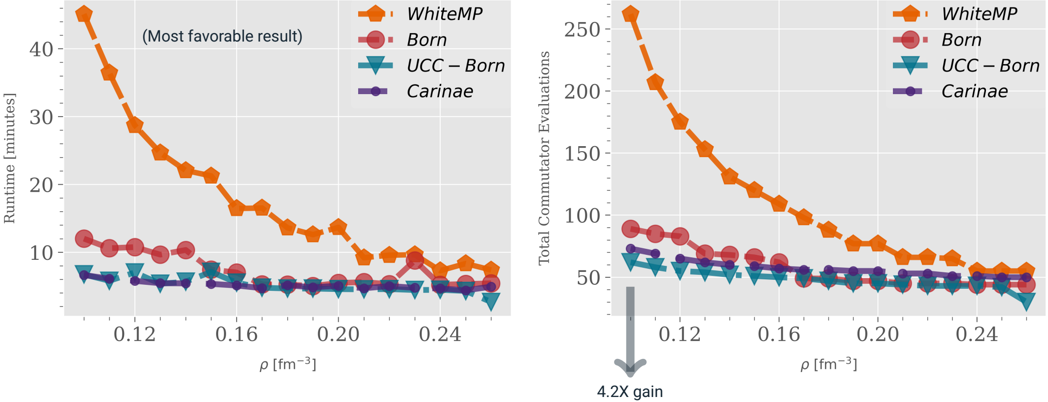
$\rho = 0.05\ \text{fm}^{-3}$

Results: Generator Comparisons



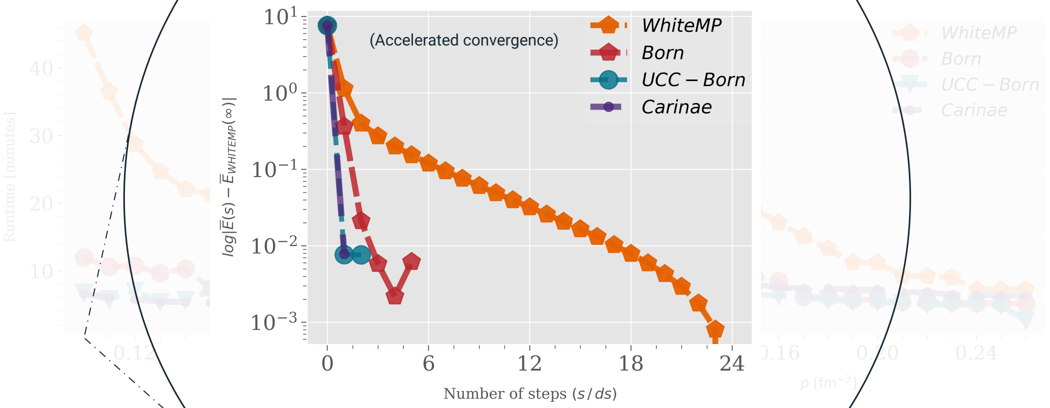
N2LO$_{\text{opt}}$, $N = 14$, $Z = 14$, $N_{\text{orbitals}} = 1556$

Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 14$, $Z = 14$, $N_{\text{orbitals}} = 1556$

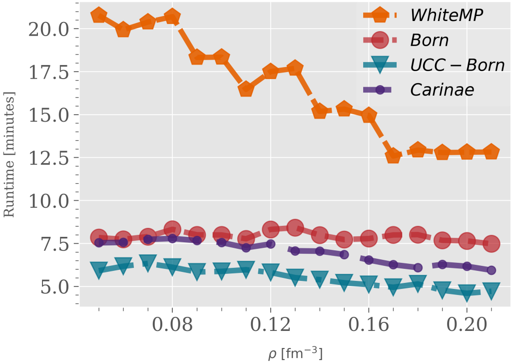
Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 14$, $Z = 14$, $N_{\text{orbitals}} = 1556$

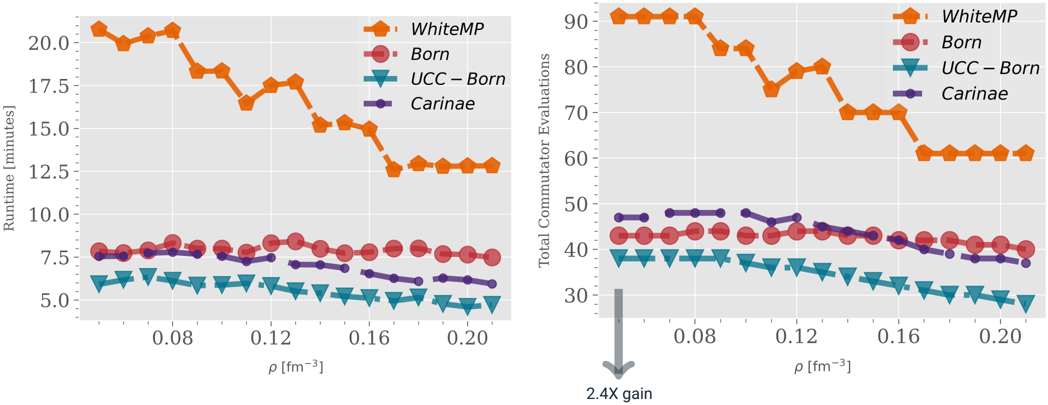
$\rho = 0.1 \text{ fm}^{-3}$

Results: Generator Comparisons



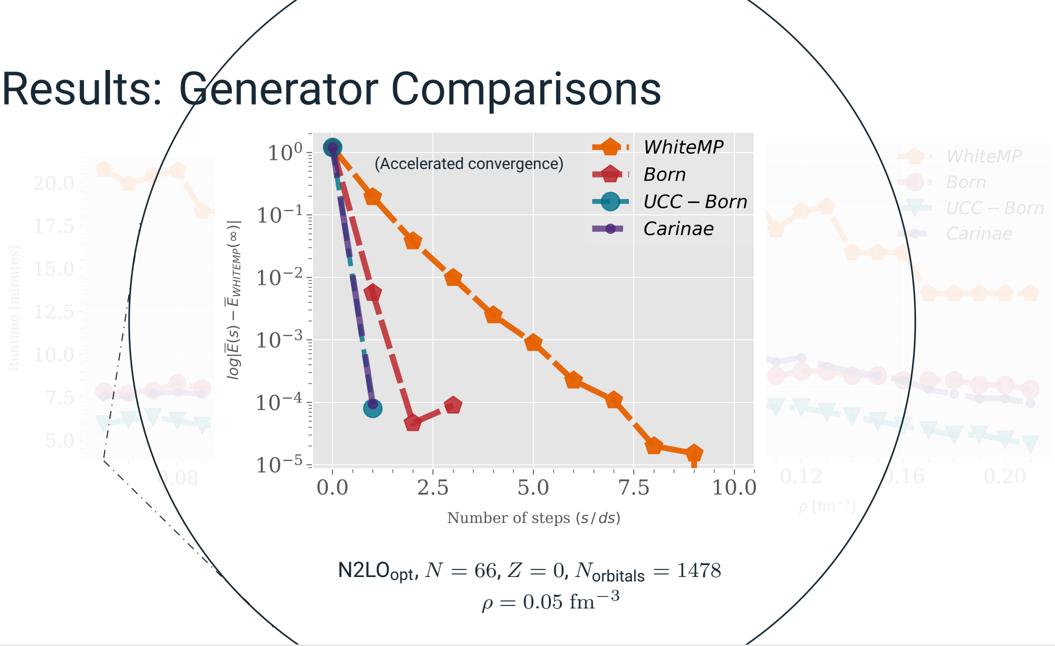
N2LO$_{\text{opt}}$, $N = 66$, $Z = 0$, $N_{\text{orbitals}} = 1478$

Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 66$, $Z = 0$, $N_{\text{orbitals}} = 1478$

Results: Generator Comparisons



N2LO$_{\text{opt}}$, $N = 66$, $Z = 0$, $N_{\text{orbitals}} = 1478$
$\rho = 0.05\ \text{fm}^{-3}$

Results: Generator Comparisons

Key takeaways

- ❑ Novel generators accelerate IMSRG's convergence.
- ❑ We generally see reductions in commutator evaluations sometimes translating to 2–4X IMSRG speedup.
- ❑ Speedup with novel generators is strongly system dependent.
  - ❖ Regardless, runtimes with novel generators are more stable when varying ρ.

Summary

- ❑ We extended the IMSRG to compute realistic NM-EOS with three chiral forces.
  - ❖ Developed a state-of-the-art, high-performant nuclear matter IMSRG program with access to a multitude of two- and three-body forces
  - ❖ Made comparisons of IMSRG(2) to MBPT and CC obtained NM-EOS
    - ✻ Observed notable disparities in SNM due to non-perturbative physics
- ❑ IMSRG NM-EOS computations are *very* computationally expensive. Thus, we:
  - ❖ Accelerated the IMSRG using three novel UCC-inspired IMSRG generators
    - ✻ Used approximate UCC solutions as IMSRG generators
    - ✻ Introduced the preconditioned Born series in UCC
  - ❖ Applied known nonlinear methods—i.e., Shanks and Padé transforms to accelerate the IMSRG (see dissertation)

Outlook

- ❏ Three chiral forces at N2LO are used in this work. More are needed, going up to N3LO, to determine EFT truncation errors.[17]
- ❏ Excited to see possible emulation of IMSRG computed NM-EOS. See works of Lee and König *et al.* [13], Ekström and Hagen [14], Davidson [15], and Cook *et al.* [16].
- ❏ We look forward to incorporating triples into the nuclear matter IMSRG.[18]
- ❏ Exciting developments on the horizon by Kang Yu for IMSRG computed momentum distributions, static structure factors, etc. in nuclear matter
- ❏ Finite temperature IMSRG extensions[19]

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Assumptions Used in This Work

For all Hamiltonians $H = E + f + \Gamma$:

0. All A-body operators are truncated at the 2-body level.
1. $f_{pq} = \delta_{pq} \times f_{pq} \;\; \forall\, pq \quad \longrightarrow \quad H_{od} = \cancel{f_{ai}} + \Gamma_{abij} \;\; \forall\, abij$.
2. $\Delta_{abij} \equiv f_{aa} + f_{bb} - f_{ii} - f_{jj} \neq 0 \;\; \forall\, abij$.
3. We denote approximate diagonalizers of H by

$$\eta(H) \equiv \sum_{ai} \cancel{\eta_{ai}(H)} : a_a^\dagger a_i : + \frac{1}{4} \sum_{abij} \eta_{abij}(H) : a_a^\dagger a_b^\dagger a_j a_i : - \text{H.c.}$$

where H.c. denotes the Hermitian conjugate of $\eta(H)$. $\eta(H)$ is assumed to be zero in its diagonal sectors. We also assume $\eta_{ai}(H) \propto f_{ai}$, and $f_{ai} = 0$.