



Nuclear Matter Equation of State from In-Medium Similarity Renormalization Group

INT/N3AS Workshop EOS Measurements with Next-Generation Gravitational-Wave Detectors

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Outline

- Introduction
- IMSRG-EOS Framework
- Preliminary EOS Results
- Summary and Outlook

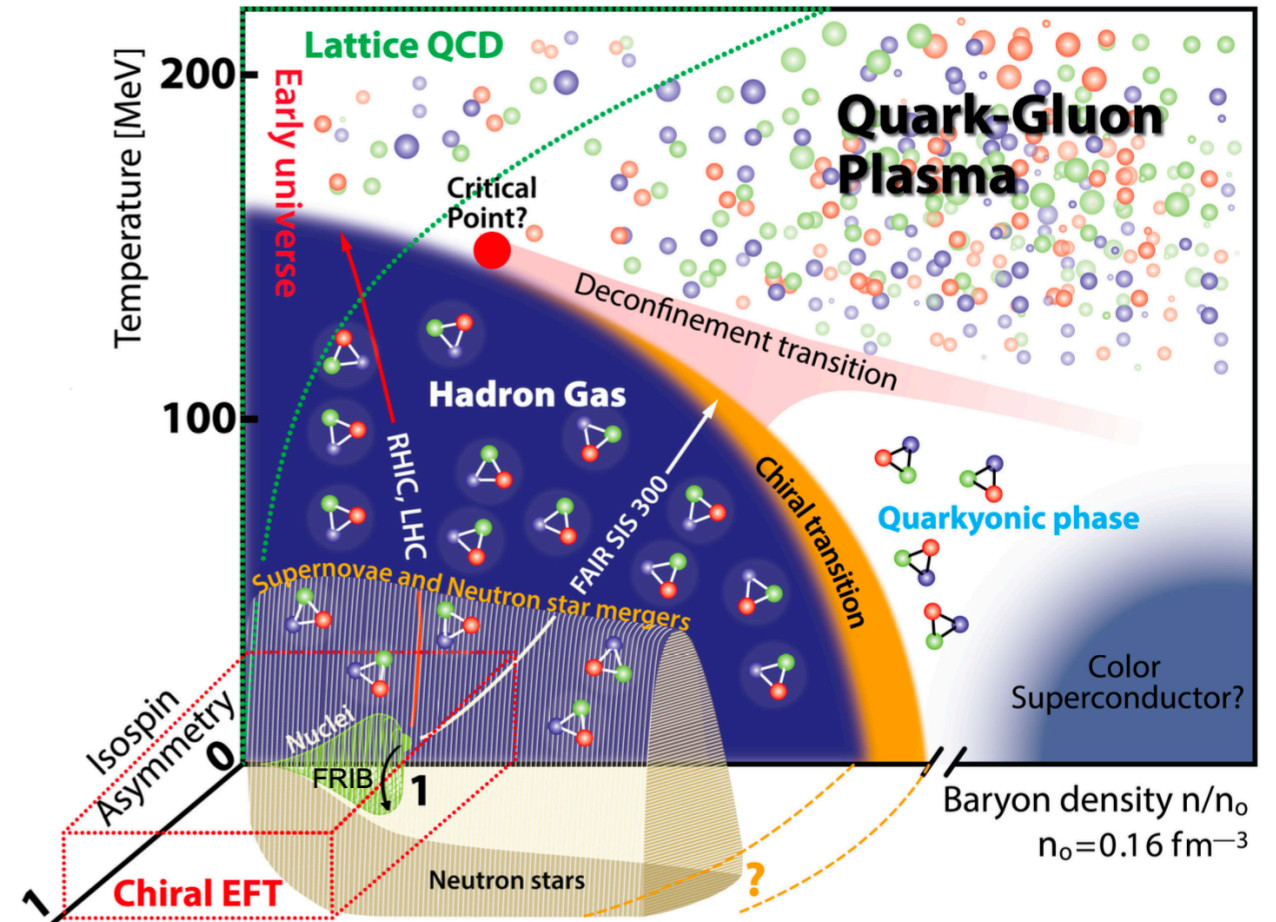


Introduction - Nuclear Matter and Equation of State

- Nuclear Matter: an idealized system of interacting nucleons in the thermodynamical limit

Why is it interesting to us:

- Testing ground for many body methods
- Strongly related to dense astronomical objects like neutron stars, offers a link between nuclear physics and astrophysical observables



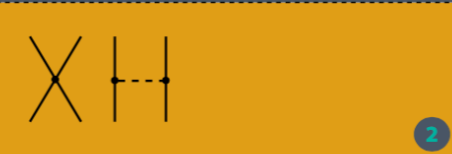





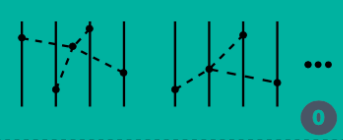


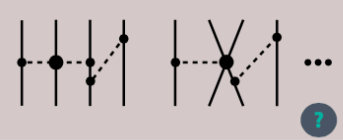
Introduction - Chiral EFT & Ab Initio Nuclear Theory

■ Chiral effective field theory:

- Consistent NN, NNN, ... interactions
- Systematic low-momentum expansion
- Link with underlying QCD

■ Ab initio nuclear theory \equiv

systematically improvable approach for quantitatively describing nuclei and nuclear matter using the finest resolution scale possible while maximizing its predictive capabilities

	NN forces	3N forces	4N forces
LO (Q^0)	 2	—	—
NLO (Q^2)	 7	—	—
N ² LO (Q^3)	 0	 2	—
N ³ LO (Q^4)	 12	 0	 0
N ⁴ LO (Q^5)	 0	 7	 7



Introduction - Similarity Renormalization Group

Basic Idea

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given “uncorrelated” many-body basis



Introduction - Similarity Renormalization Group

- **flow equation** for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:

$$\frac{d}{ds}H(s) = [\eta(s), H(s)], \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

- choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(s) = [H_d(s), H_{od}(s)]$$

to **suppress** (suitably defined) **off-diagonal Hamiltonian**

$$\lim_{s \rightarrow \infty} H_{od}(s) \longrightarrow 0$$

Introduction - In-Medium Similarity Renormalization Group

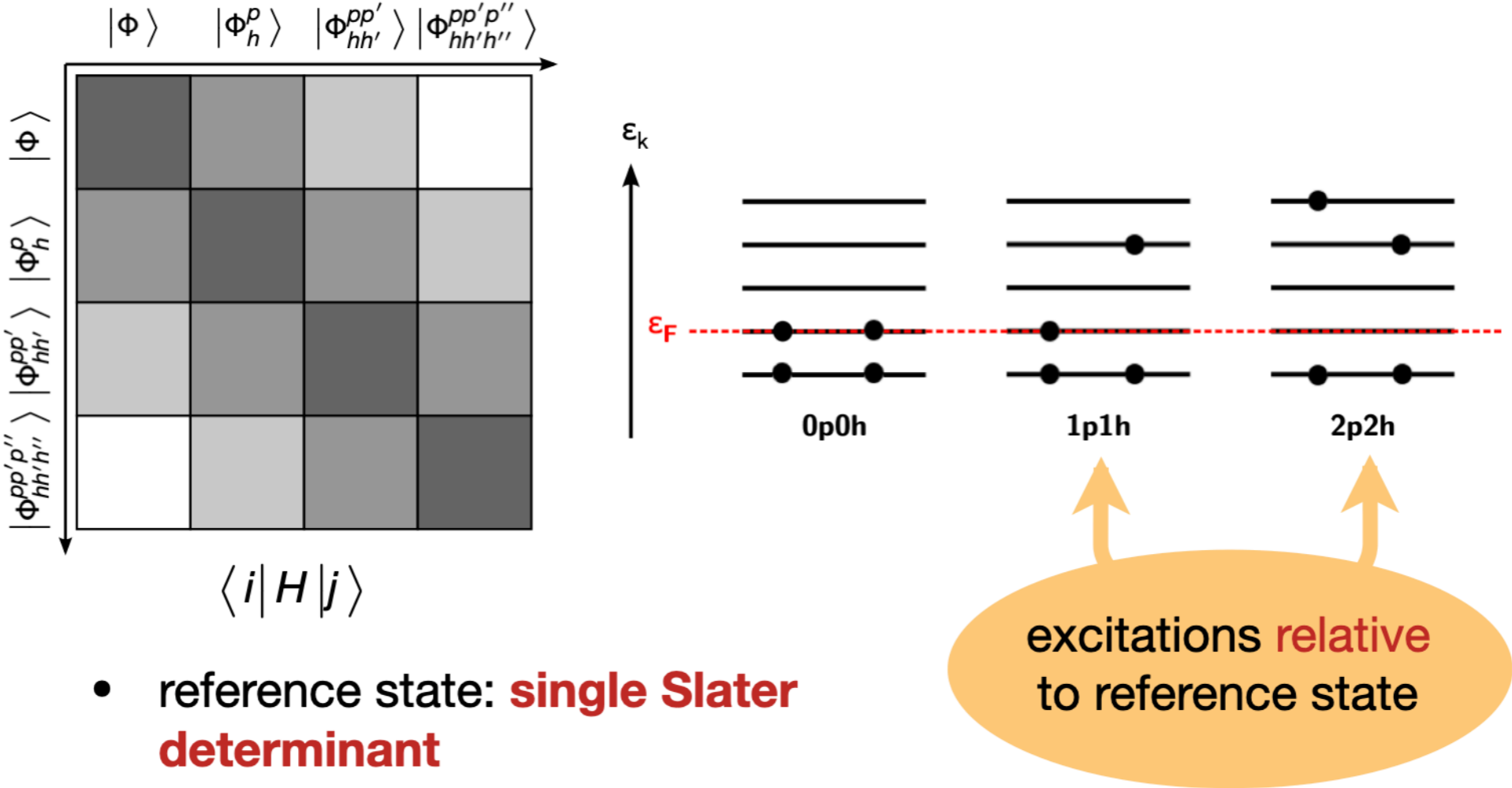
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f_l^k : A_l^k : + \frac{1}{4} \sum_{klmn} \Gamma_{mn}^{kl} : A_{mn}^{kl} : + \frac{1}{36} \sum_{ijklmn} W_{lmn}^{ijk} : A_{lmn}^{ijk} :$$

$$A_{j_1 \dots j_N}^{i_1 \dots i_N} \equiv a_{i_1}^\dagger \dots a_{i_N}^\dagger a_{j_N} \dots a_{j_1}$$

$$\langle \Phi | : A : | \Phi \rangle = 0$$

Introduction - In-Medium Similarity Renormalization Group

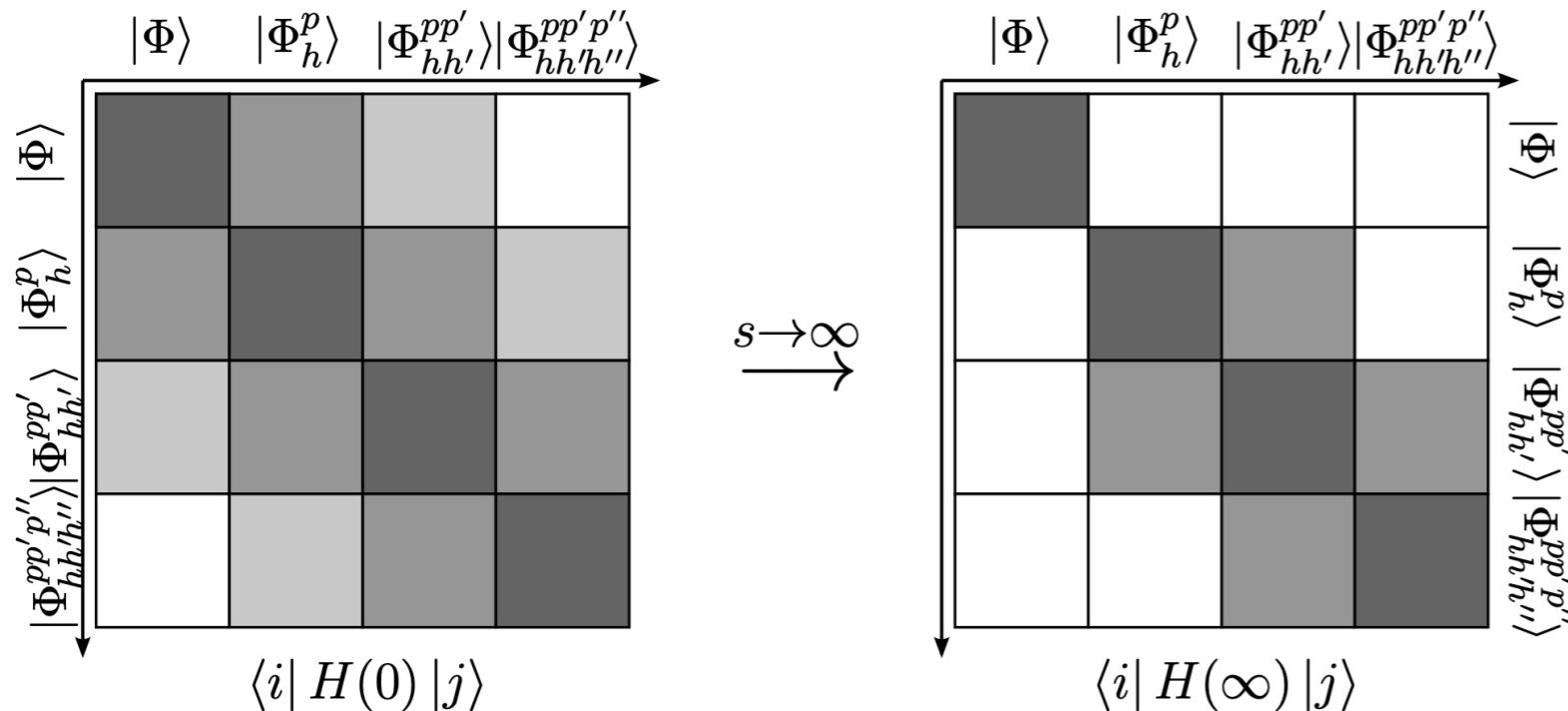


- reference state: **single Slater determinant**

Introduction - In-Medium Similarity Renormalization Group

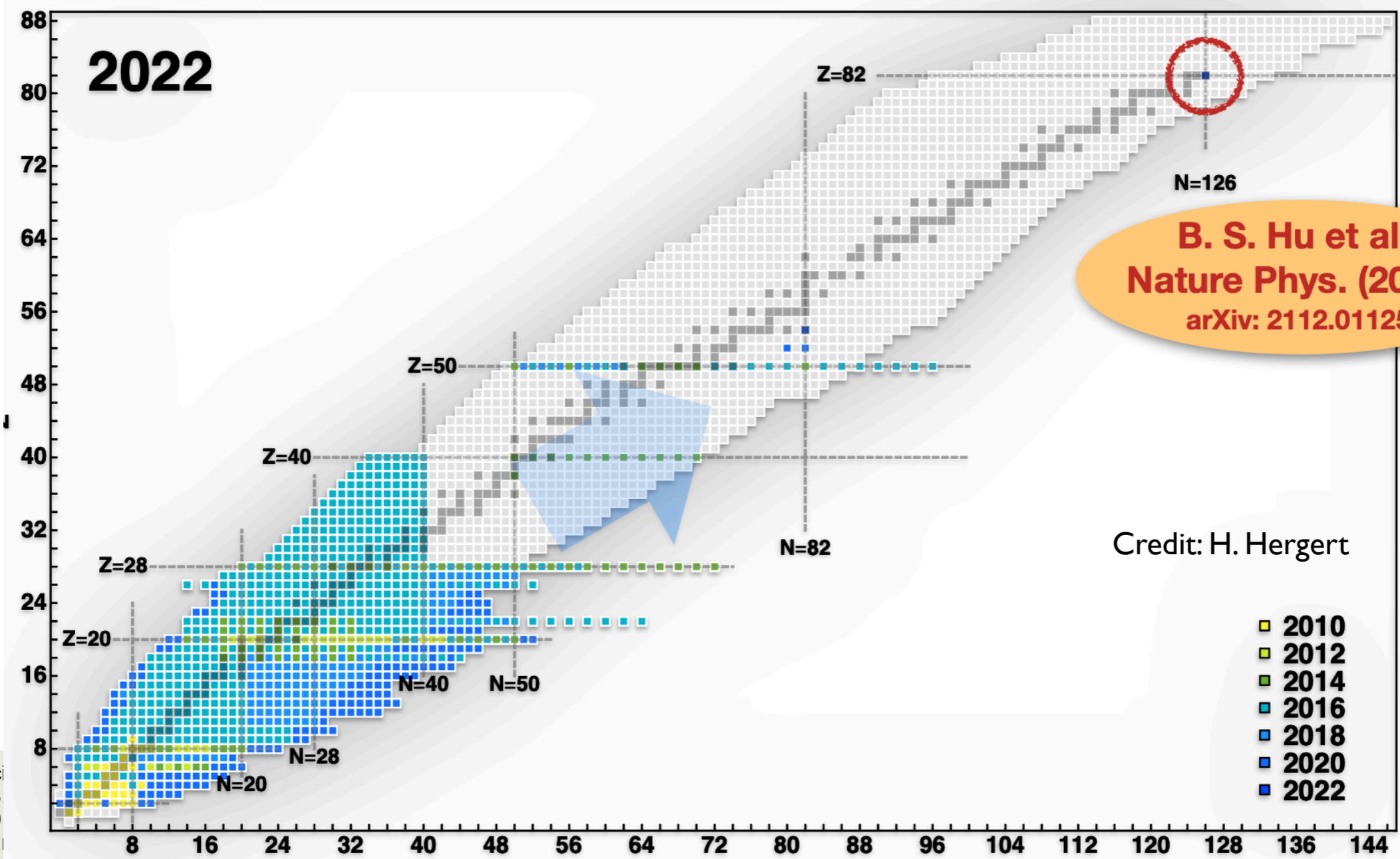
$$\frac{d}{ds}H(s) = [\eta(s), H(s)], \quad \text{e.g.,} \quad \eta(s) \equiv [H_d(s), H_{od}(s)]$$

IM-SRG(2): Truncate $H(s)$, $\eta(s)$ to **normal ordered** 2-body terms

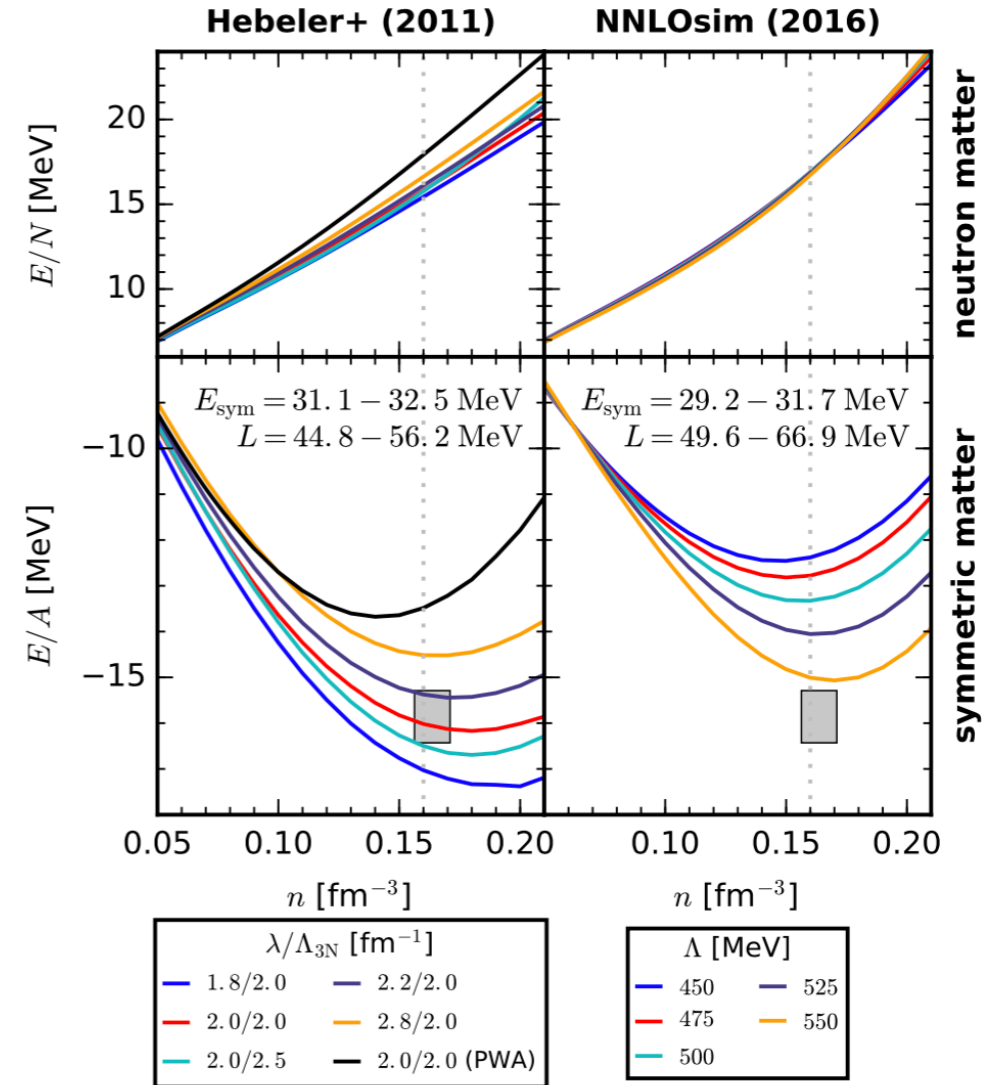
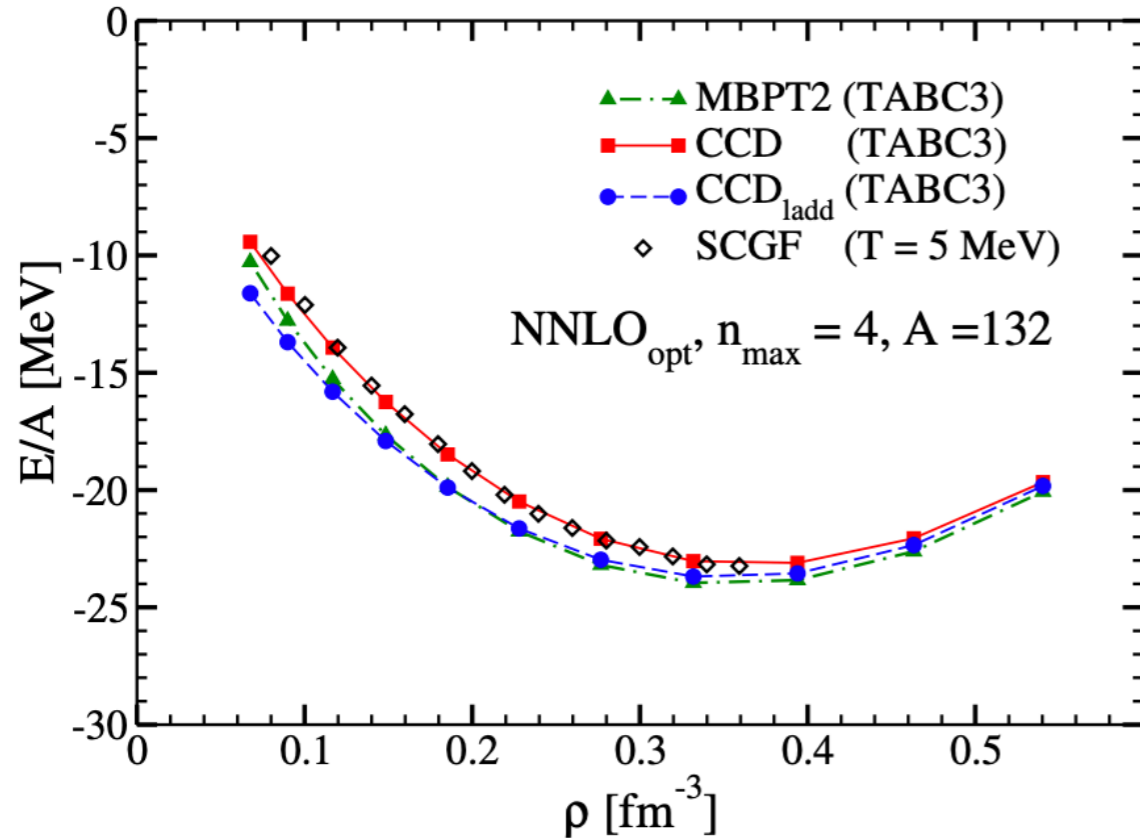


two-body formalism with in-medium contributions from NNN interactions

Introduction - Application of Ab Initio Methods in Nuclear Structure

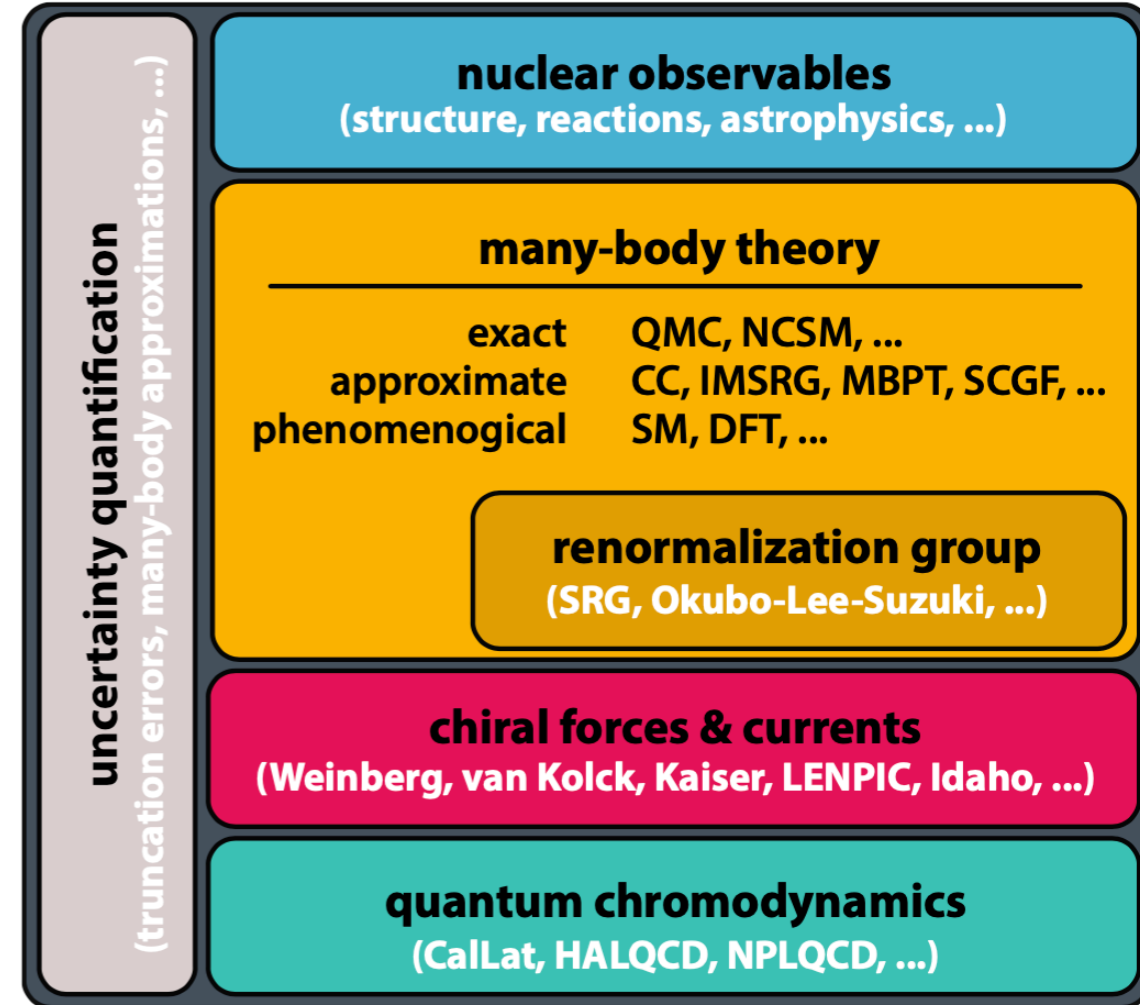


Introduction - Application of Other Ab Initio Methods in NM EOS



IMSRG-EOS Framework - Overview

- Physical System: Nucleons in a finite box
- Framework:
 1. Single particle basis (plane waves w/Periodic boundary condition) -> Many particle basis
 2. Input from chiral EFT -> Hamiltonian Matrix Elements
 3. IMSRG Evolution of the Hamiltonian, NO2B level
- can be easily generalized to study other infinite systems (with arbitrary dimension) such as 2D electron gas



Preliminary Results - Interactions

■ Hebeler Interactions:

- Based on chiral EFT, but not fully consistent NN and 3N interactions
- Starts from N3LO EM 500 MeV NN potential
- NN interaction is softened by SRG evolution
- NNLO 3N interaction adjusted to fit the triton binding energy and He charge radius
- Denoted by λ/Λ_{3N} , where λ is the SRG flow parameter, Λ_{3N} is the 3N cutoff

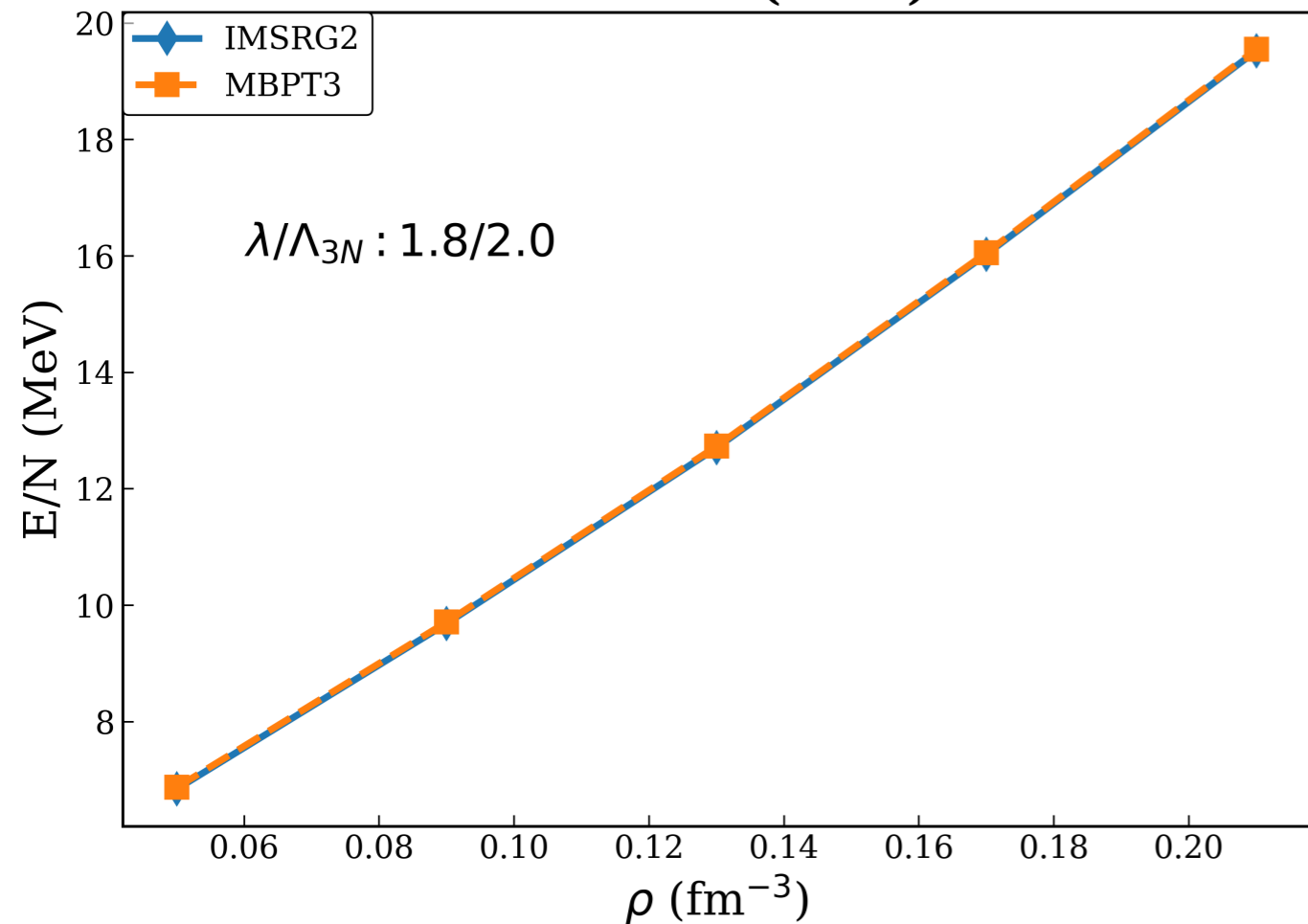
■ N2LO EMN Interactions:

- Not SRG-evolved
- consistent NN and 3N interaction
- c_D and c_E are fitted to the ${}^3\text{H}$ and empirical saturation properties

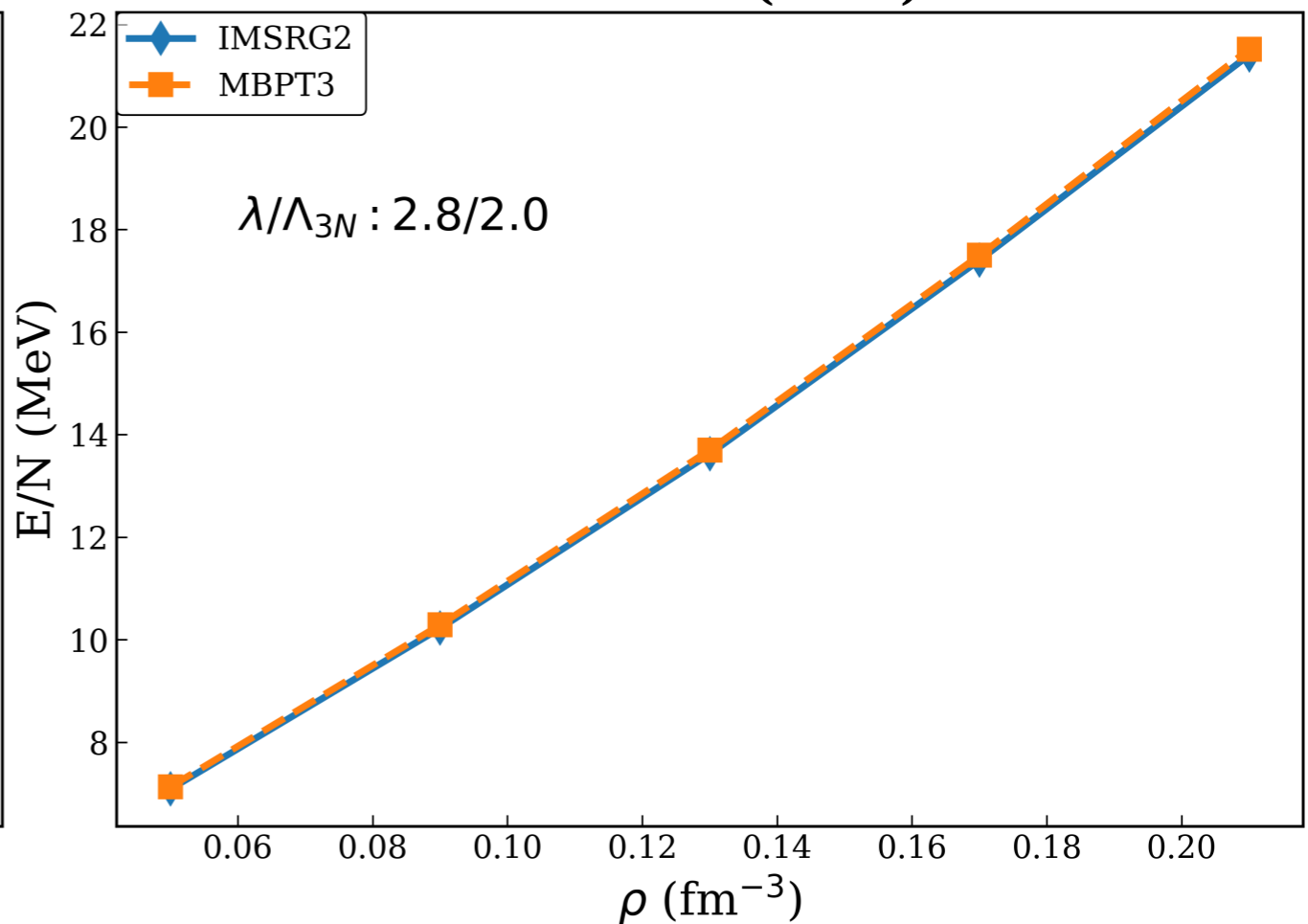


Preliminary Results - PNM EOS with Hebeler Interactions

Hebeler+ (2011)

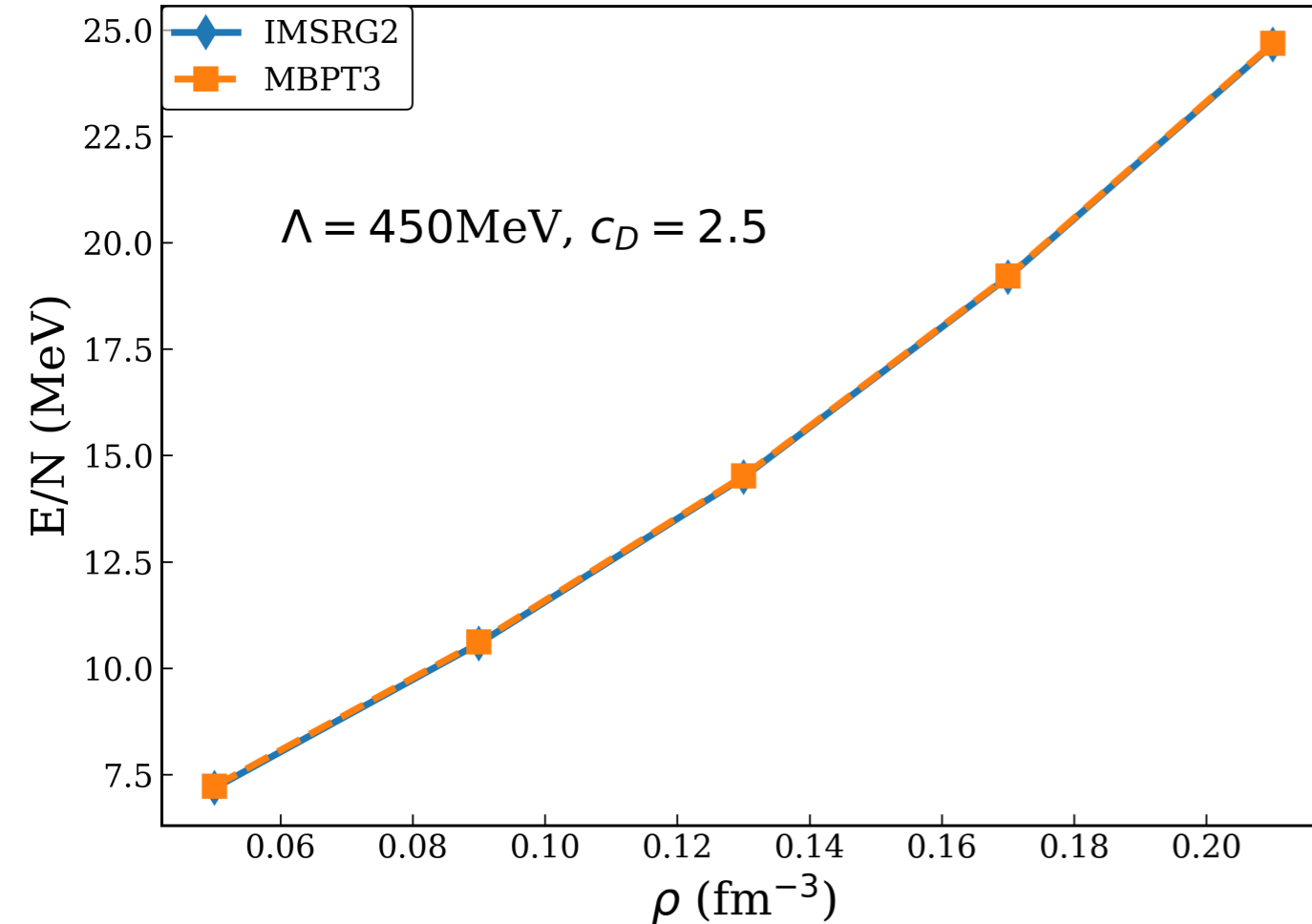


Hebeler+ (2011)

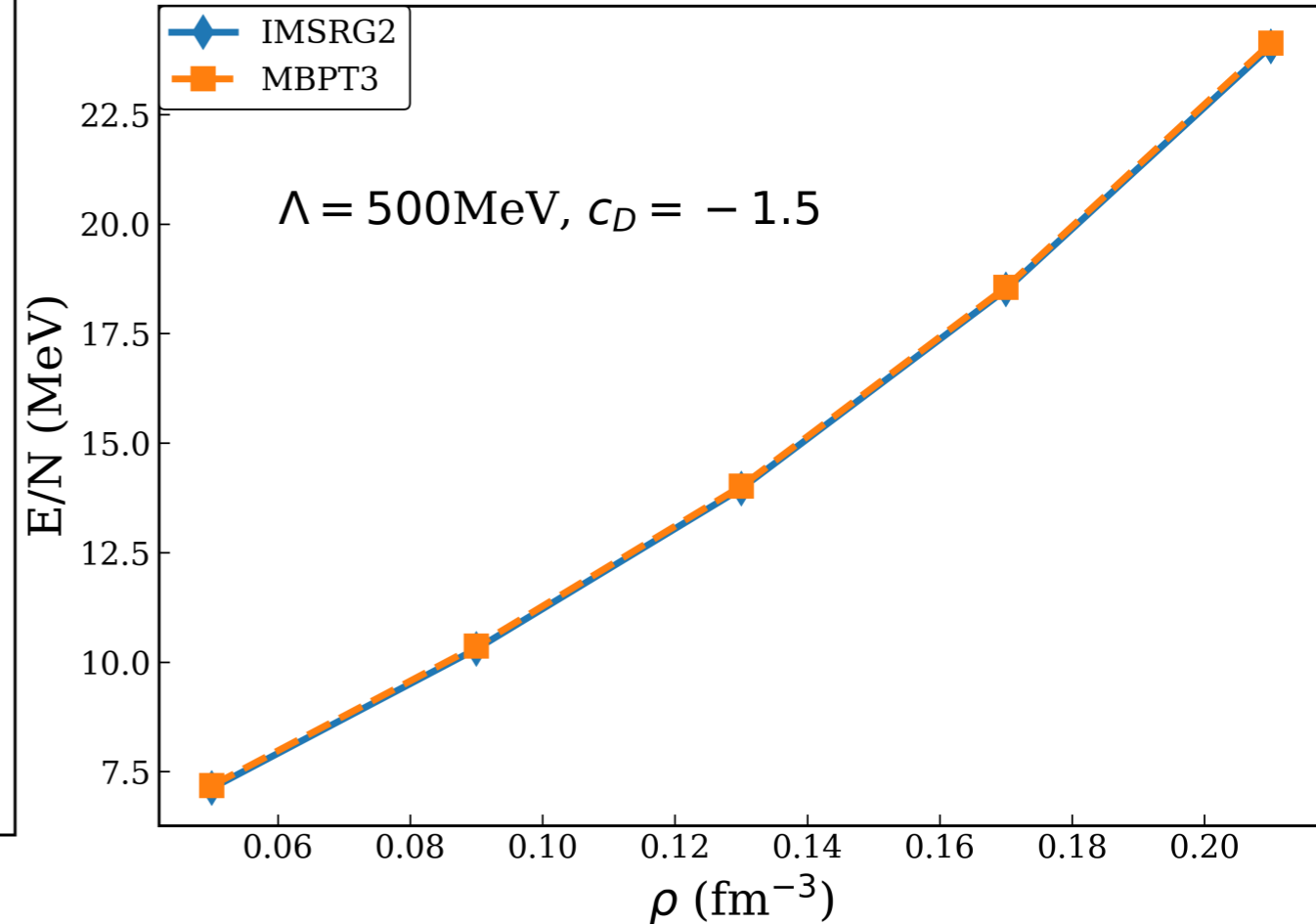


Preliminary Results - PNM EOS with N2LO EMN Interactions

N2LO EMN (2017)

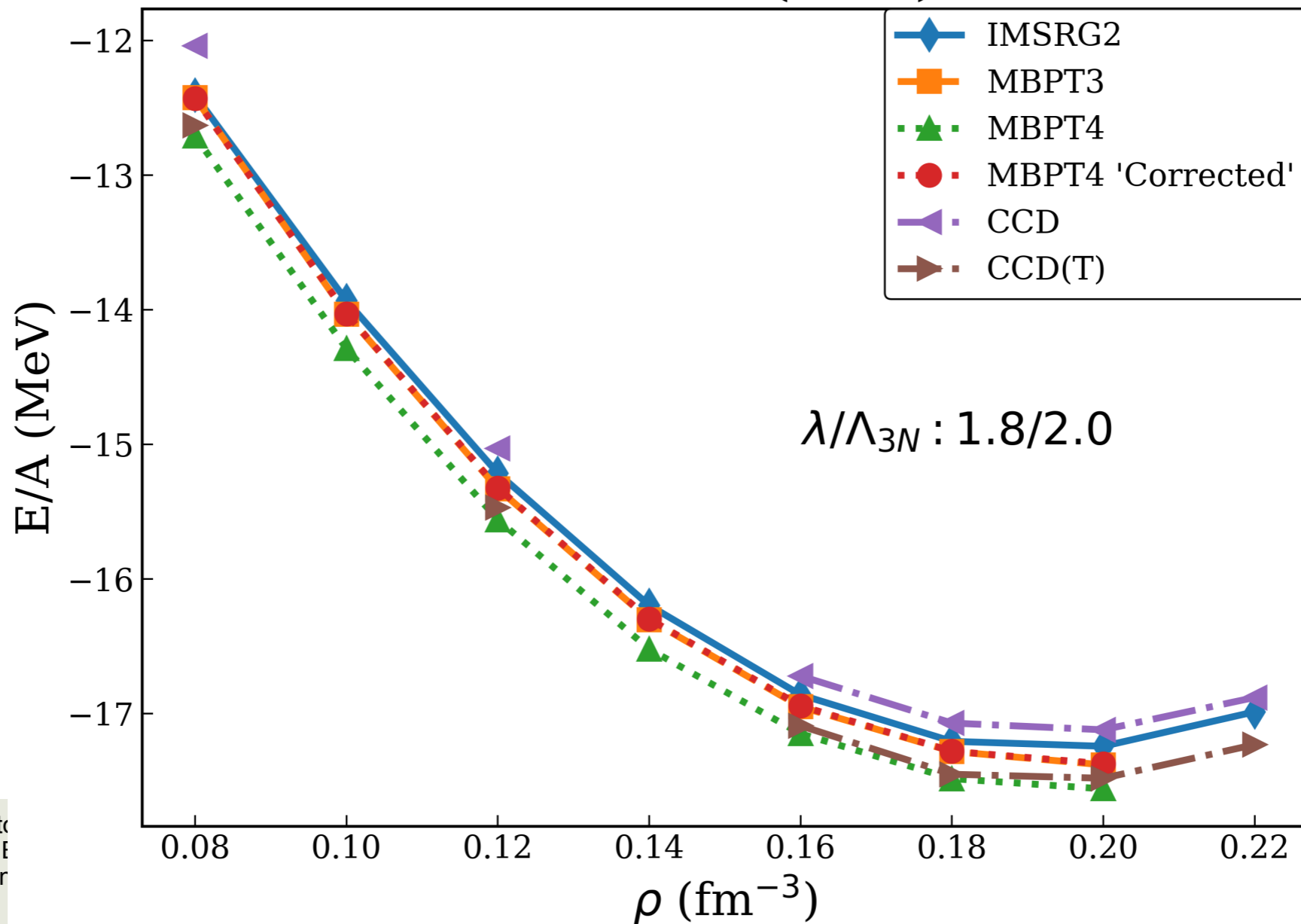


N2LO EMN (2017)



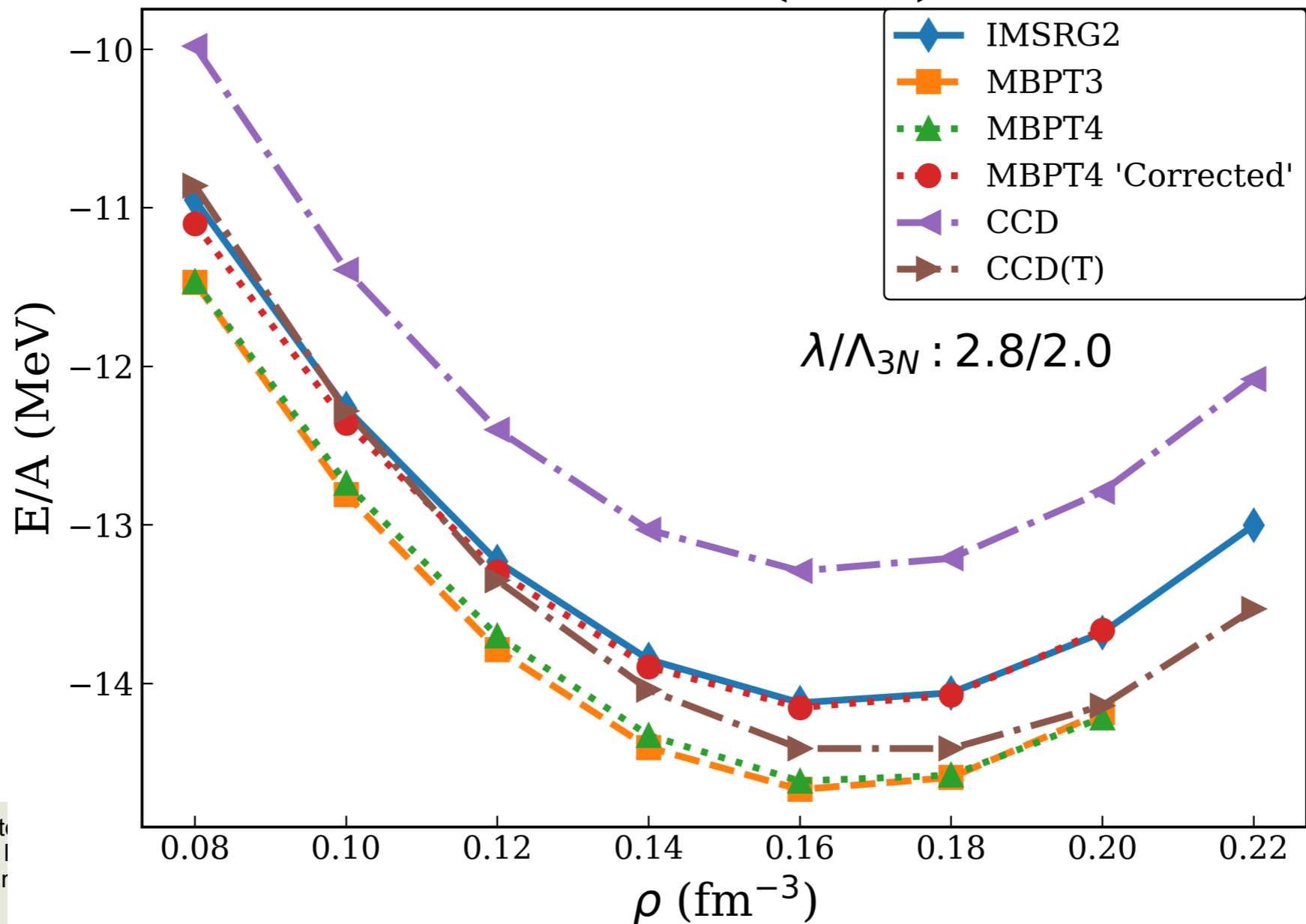
Preliminary Results - SNM EOS with Hebeler Interactions

Hebeler+ (2011)

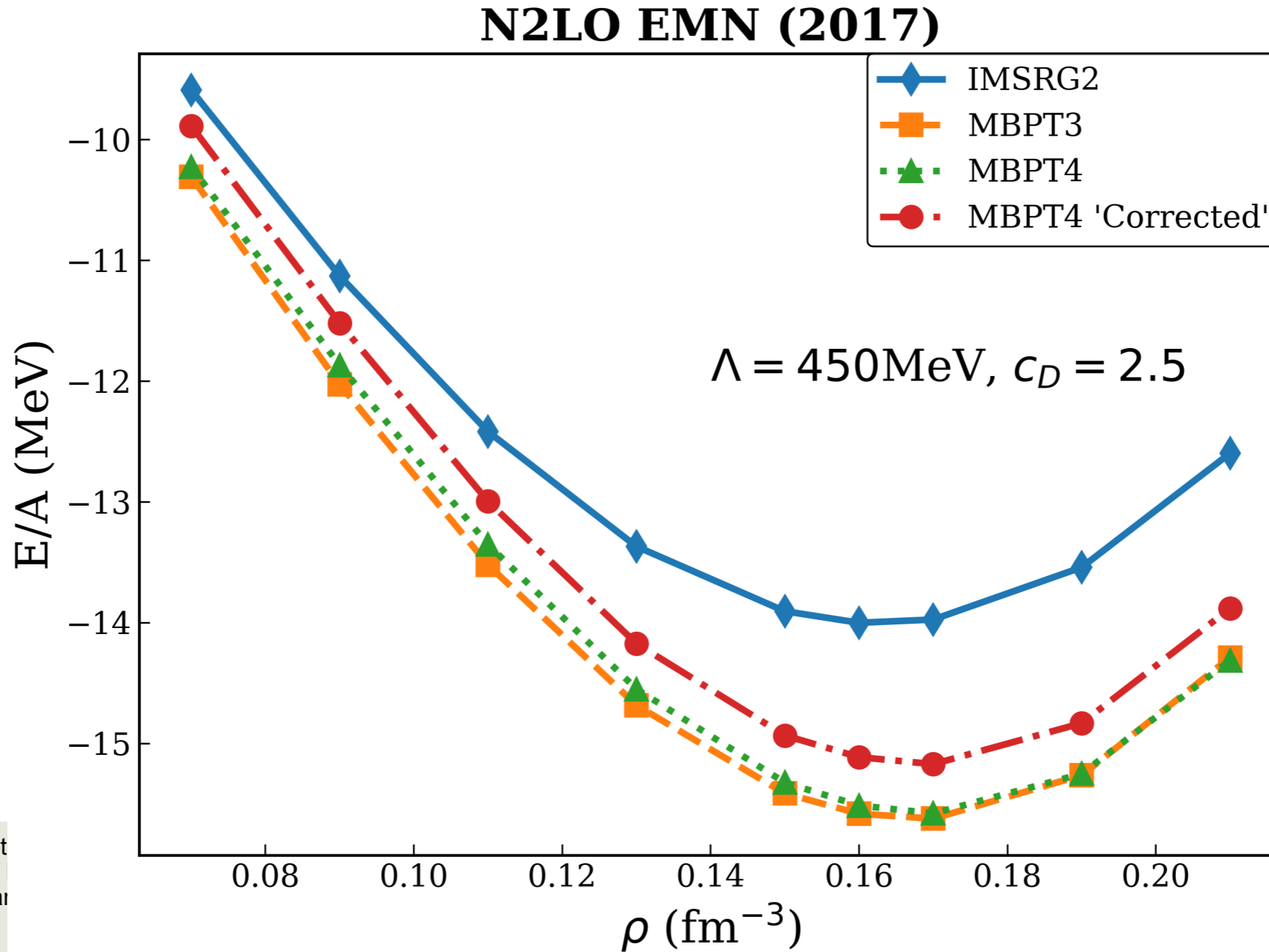


Preliminary Results - SNM EOS with Hebeler Interactions

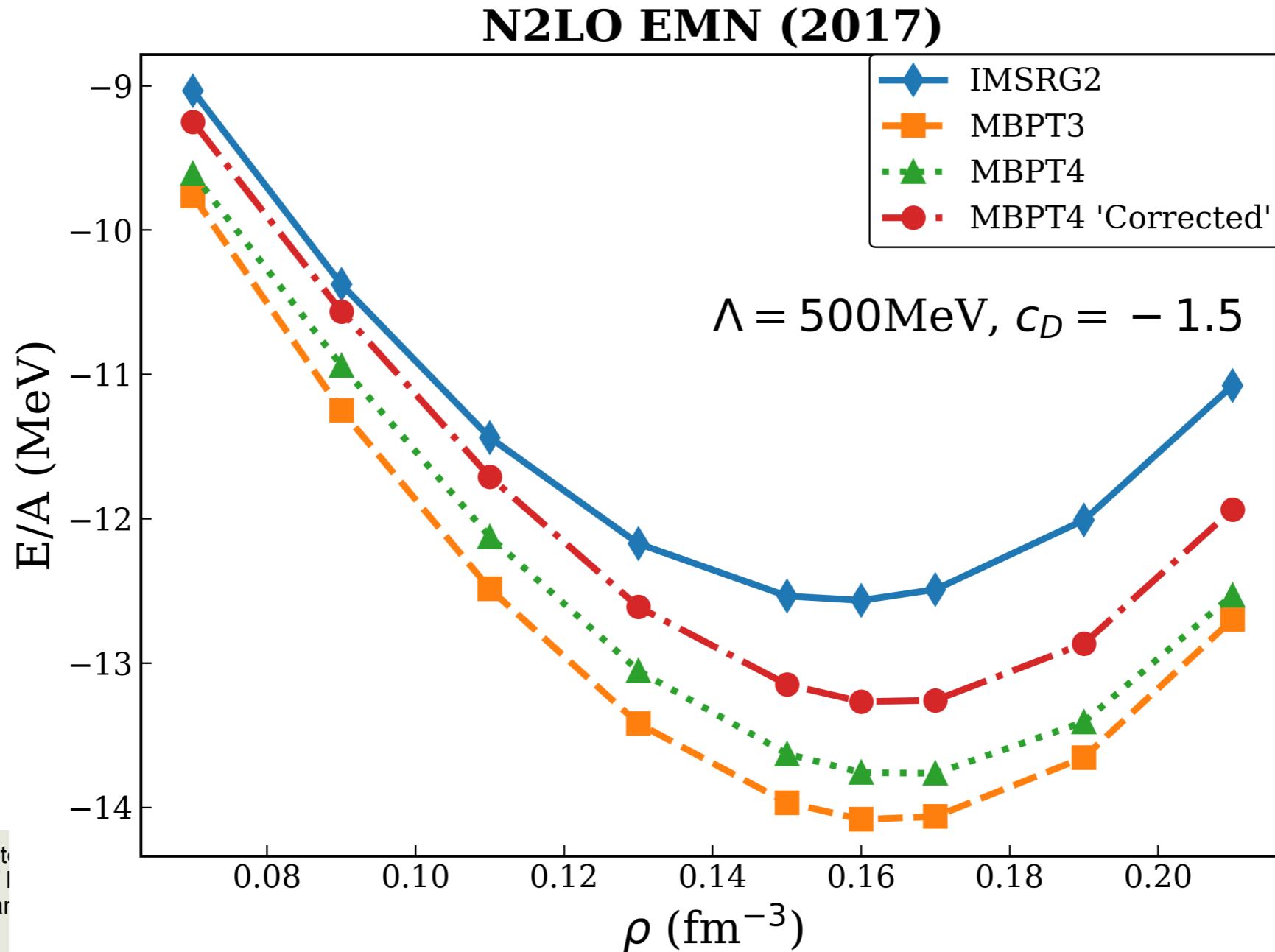
Hebeler+ (2011)



Preliminary Results - SNM EOS with N2LO EMN Interactions

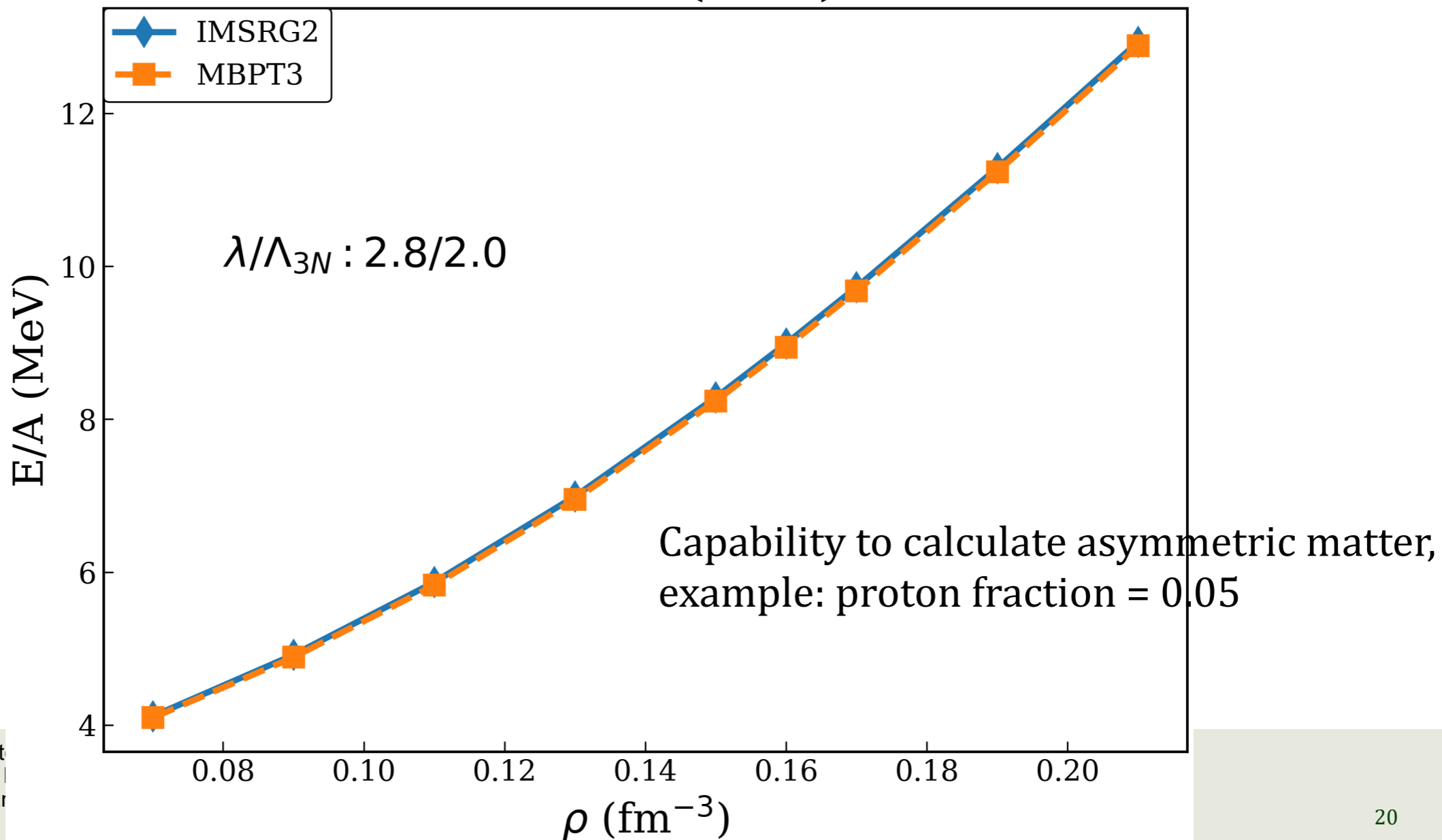


Preliminary Results - SNM EOS with N2LO EMN Interactions



Preliminary Results - ANM EOS with Hebeler Interactions

Hebeler+ (2011)



Summary

We've built a nuclear many-body modeling infrastructure based on IMSRG for EOS calculations.

- Converged calculations for a range of proton fractions
- Good agreement with other many body methods - MBPT and CC for perturbative system (PNM)
- For more correlated system (SNM), the agreement is still good for softer interactions (Hebeler).
- Noticeable discrepancies starts to occur for relatively harder interactions (N2LO EMN)
 - Still working to understand these differences (finite-size corrections, approximate IMSRG(3), etc.)



Outlook

- Computation of other static properties (momentum distributions, static structure factors) in progress
- Large scale EOS calculations at $T = 0$ for different chiral EFT interactions
 - Bayesian analysis of EFT truncation errors (BUQEYE)
 - Comparison of different many body methods
- Explore emulators for IMSRG calculations (Dynamical Mode Decomposition, Parametric Matrix Models)
- Possible extensions
 - Finite T (see Smith et al. <https://arxiv.org/abs/2407.00576>)
 - Approximate IMSRG(3) (see Stroberg et al., <https://arxiv.org/abs/2406.13010>)
 - Response via EOM (and other) techniques





Taste of Xian

Thank you for your attention!



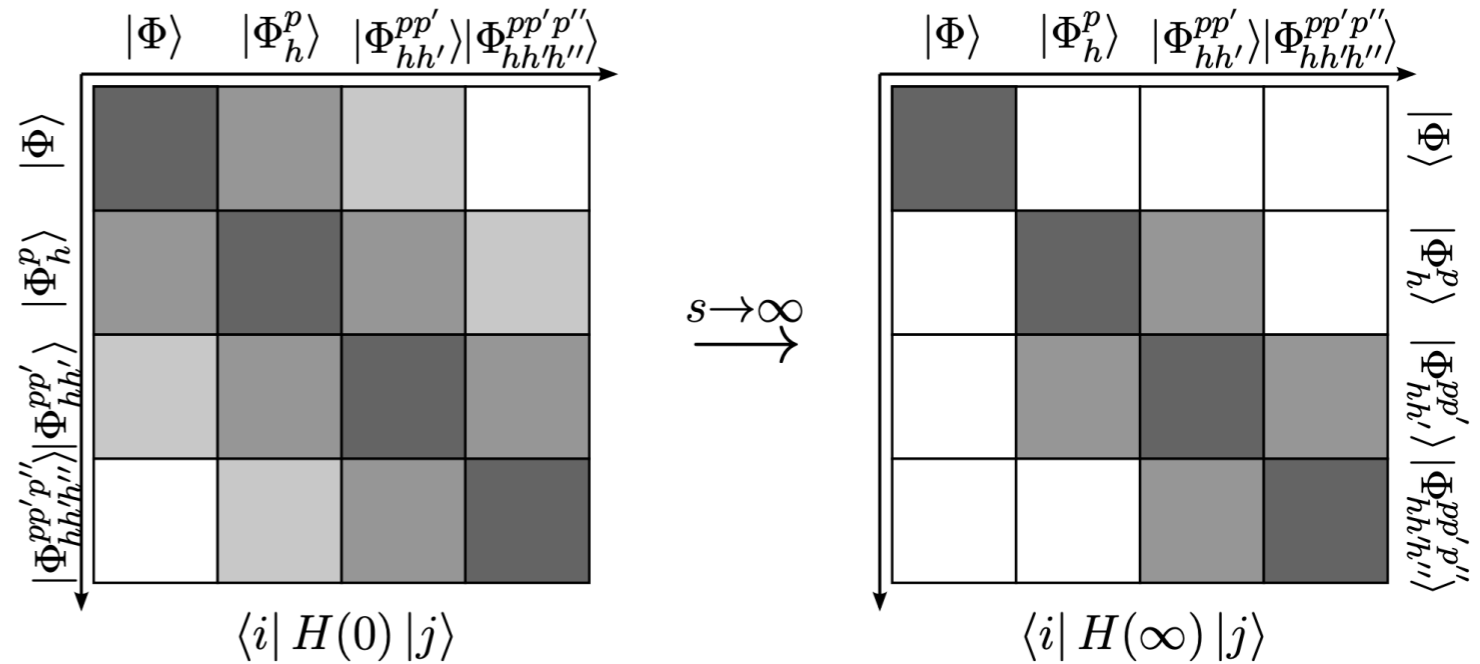
Introduction - In-Medium Similarity Renormalization Group

IMSRG(2) flow equations:

$$\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_{ab} f_{ba} + \frac{1}{2} \sum_{abcd} \eta_{abcd} \Gamma_{cdab} n_a n_b \bar{n}_c \bar{n}_d,$$

$$\begin{aligned} \frac{df_{ij}}{ds} = & \sum_a (1 + P_{ij}) \eta_{ia} f_{aj} + \sum_{ab} (n_a - n_b) (\eta_{ab} \Gamma_{biaj} - f_{ab} \eta_{biaj}) \\ & + \frac{1}{2} \sum_{abc} (n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c) (1 + P_{ij}) \eta_{ciab} \Gamma_{abcj}, \end{aligned}$$

$$\begin{aligned} \frac{d\Gamma_{ijkl}}{ds} = & \sum_a \{ (1 - P_{ij}) (\eta_{ia} \Gamma_{ajkl} - f_{ia} \eta_{ajkl}) - (1 - P_{kl}) (\eta_{ak} \Gamma_{ijal} - f_{ak} \eta_{ijal}) \} \\ & + \frac{1}{2} \sum_{ab} (1 - n_a - n_b) (\eta_{ijab} \Gamma_{abkl} - \Gamma_{ijab} \eta_{abkl}) \\ & + \sum_{ab} (n_a - n_b) (1 - P_{ij}) (1 - P_{kl}) \eta_{aibk} \Gamma_{bjal}. \end{aligned}$$



M Hjorth-Jensen et al, *An Advanced Course in Computational Nuclear Physics: Bridging the Scales from Quarks to Neutron Stars*
 H. Hergert et al, *Nuclear Structure from the In-Medium Similarity Renormalization Group*

Introduction - Magnus Formulation

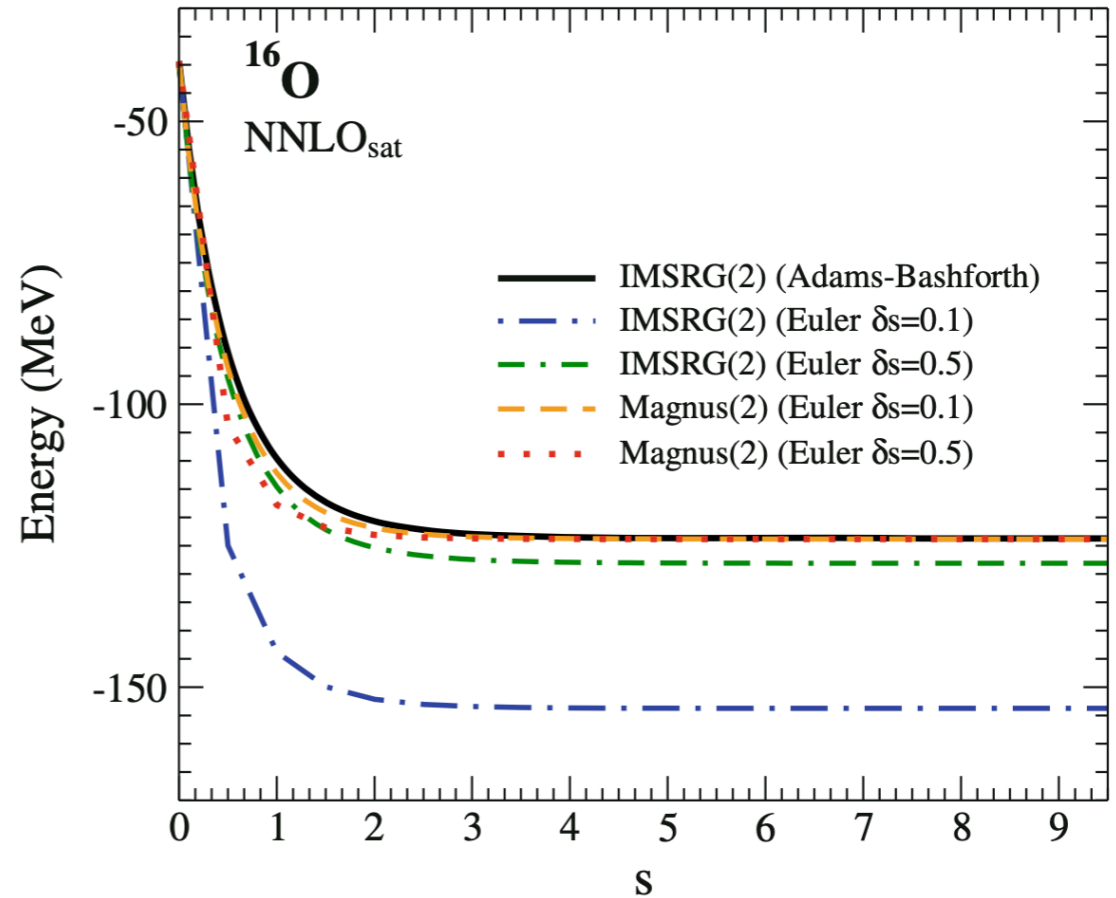
$$\hat{U}(s) \equiv e^{\hat{\Omega}(s)}$$

$$\frac{d\hat{\Omega}}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_{\hat{\Omega}}^k(\hat{\eta})$$

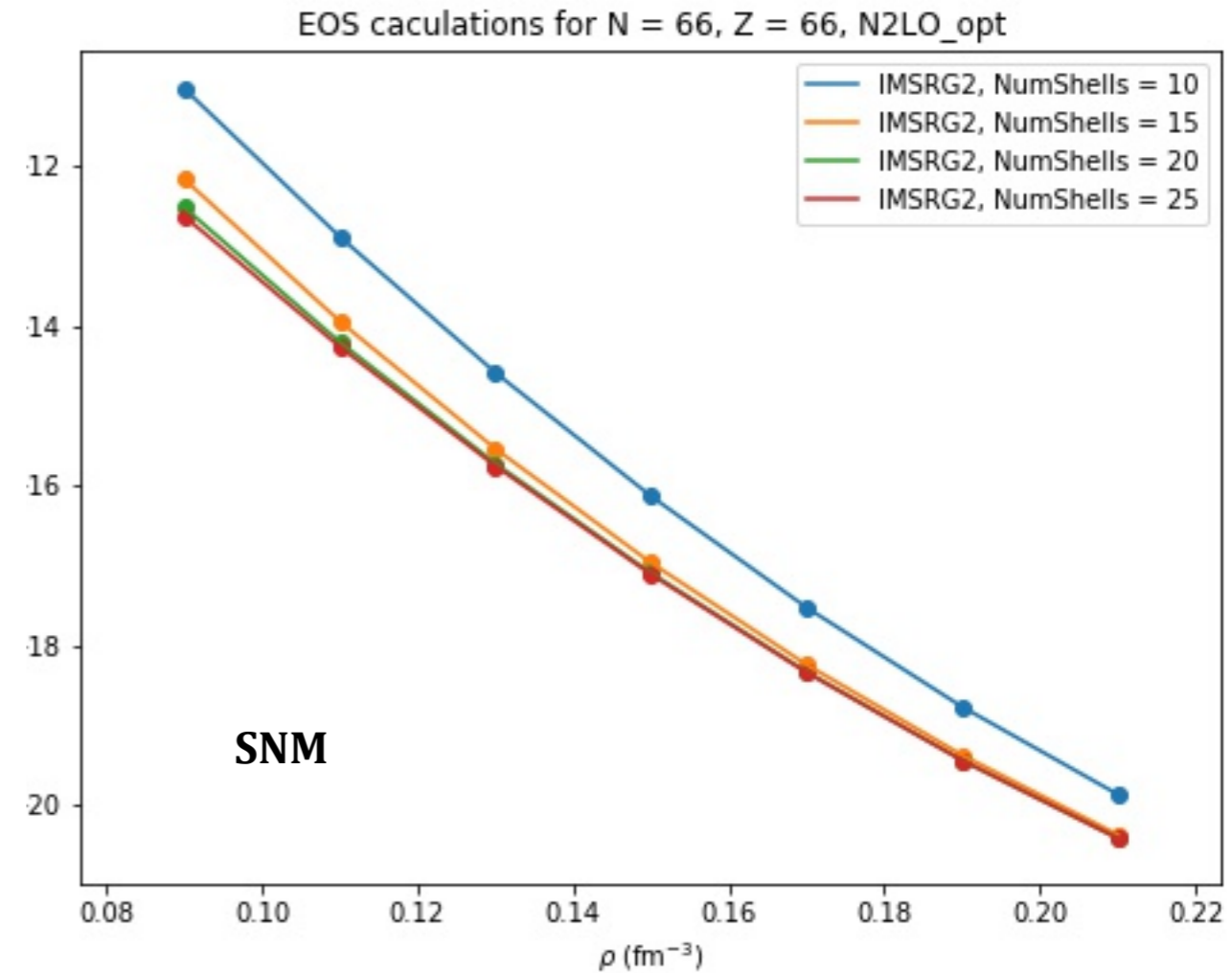
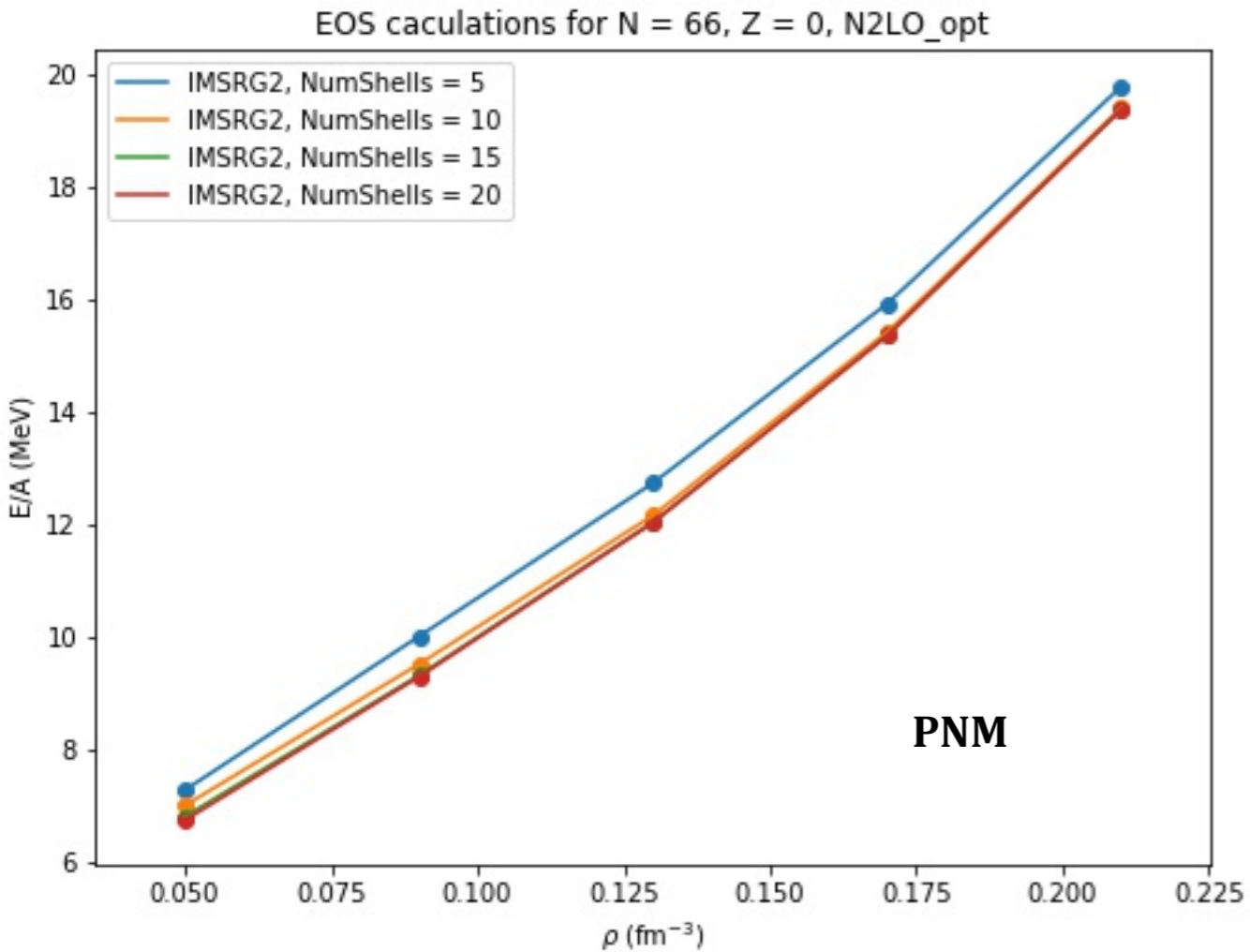
$$\text{ad}_{\hat{\Omega}}^0(\hat{\eta}) = \hat{\eta}$$

$$\text{ad}_{\hat{\Omega}}^k(\hat{\eta}) = [\hat{\Omega}, \text{ad}_{\hat{\Omega}}^{k-1}(\hat{\eta})]$$

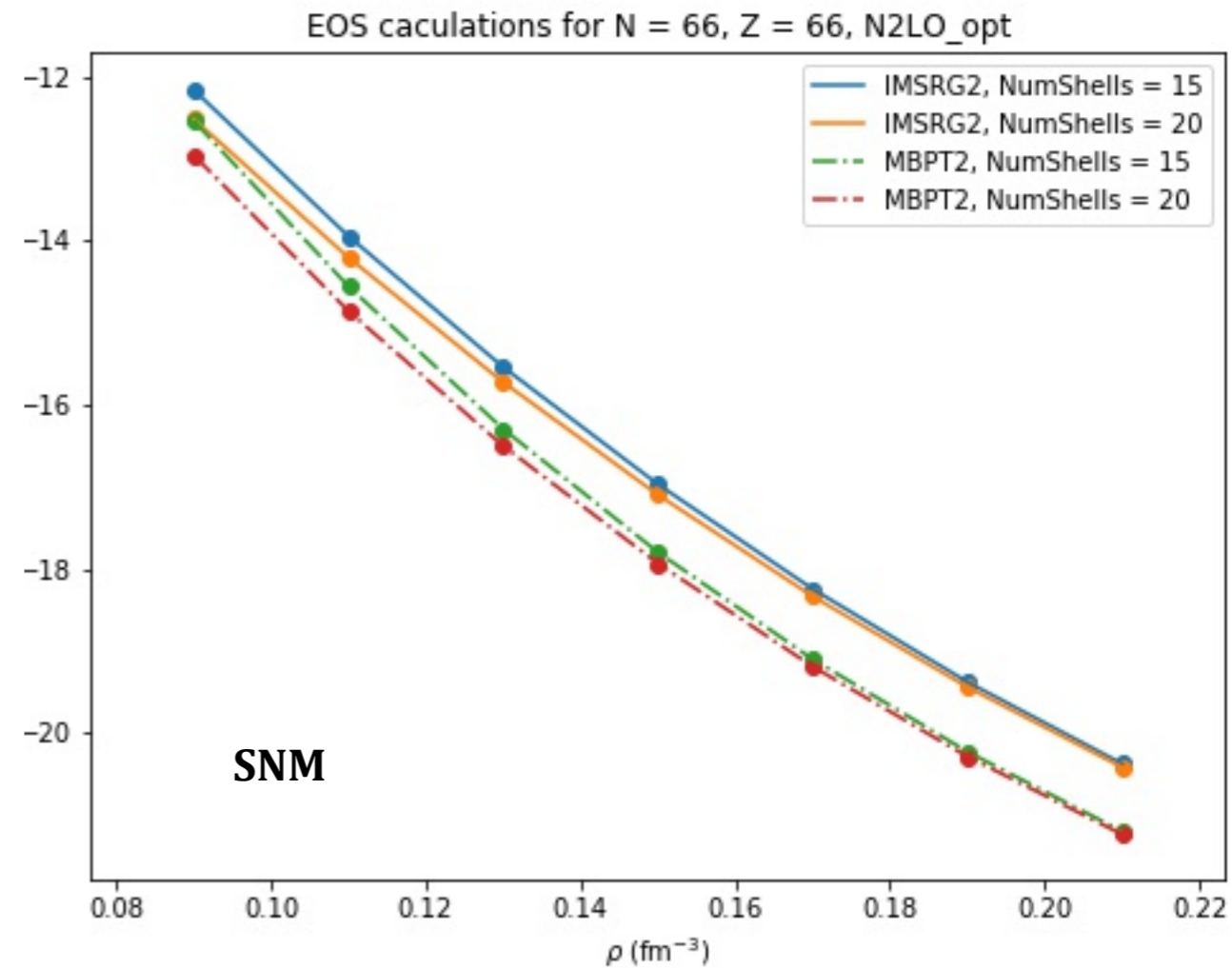
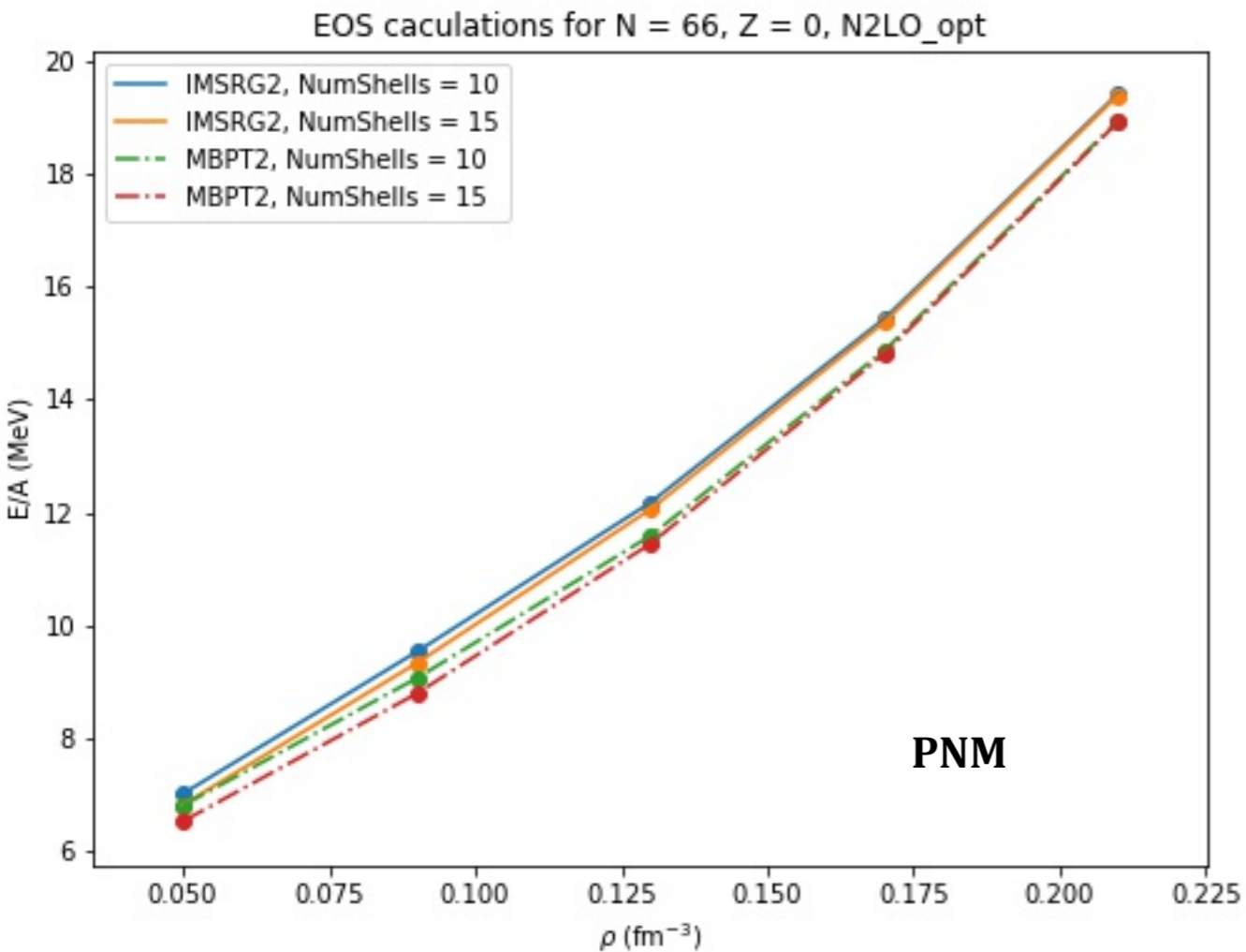
$$\hat{H}(s) \equiv e^{\hat{\Omega}(s)} \hat{H}(0) e^{-\hat{\Omega}(s)} = \sum_{k=0}^{\infty} \frac{1}{k!} \text{ad}_{\hat{\Omega}(s)}^k(\hat{H}(0))$$



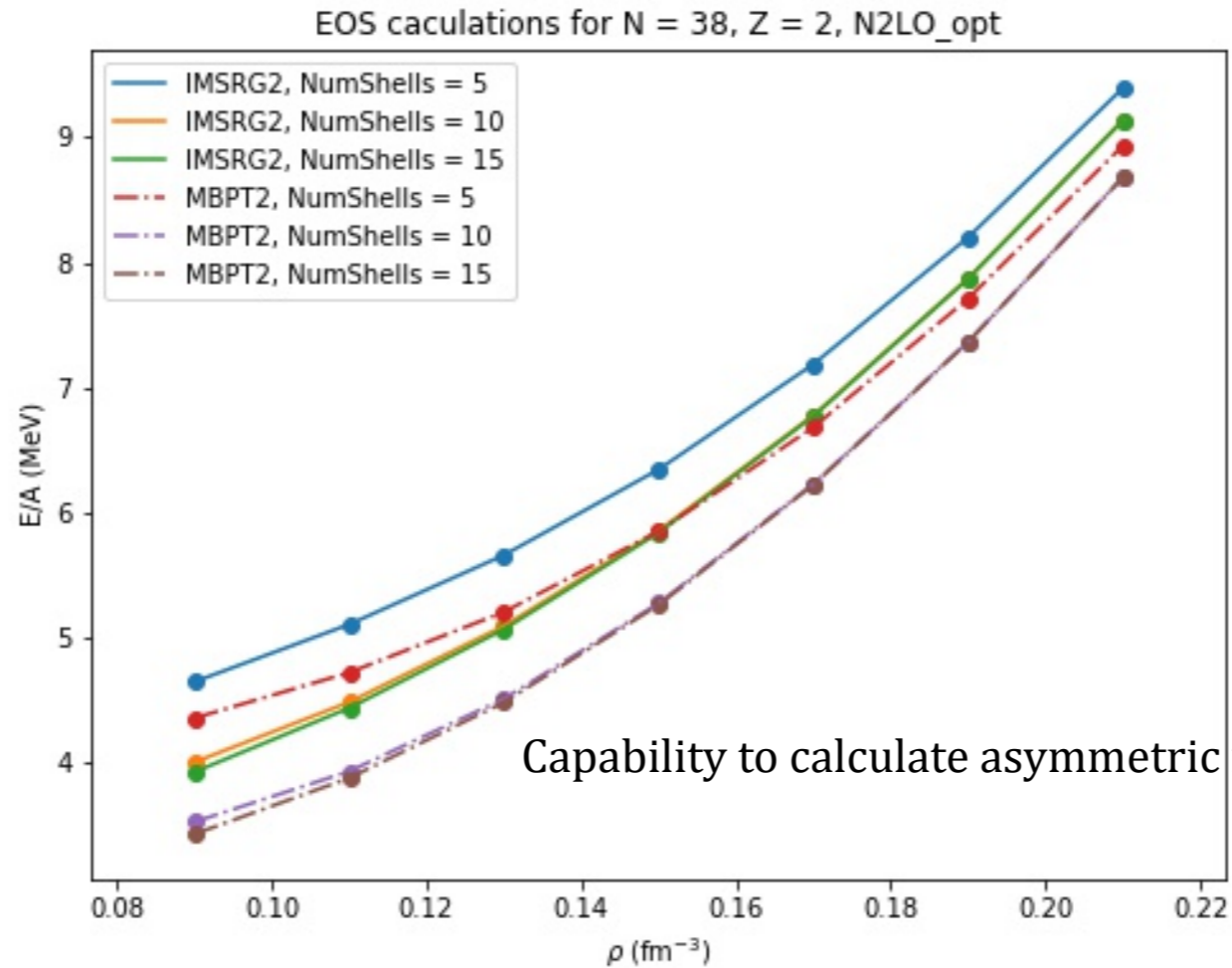
Results - Basis Convergence



Results - Basis Convergence



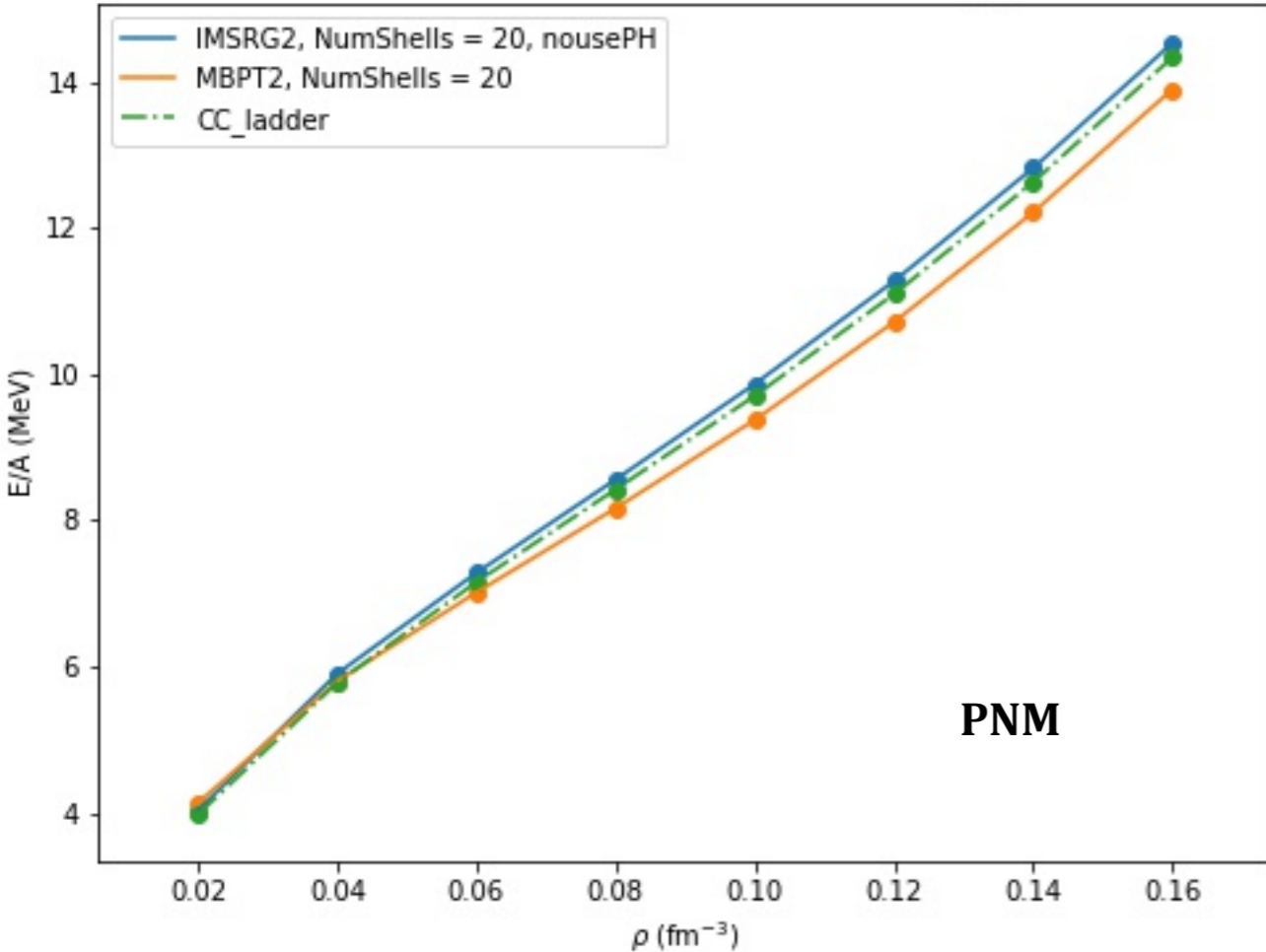
Results - Basis Convergence



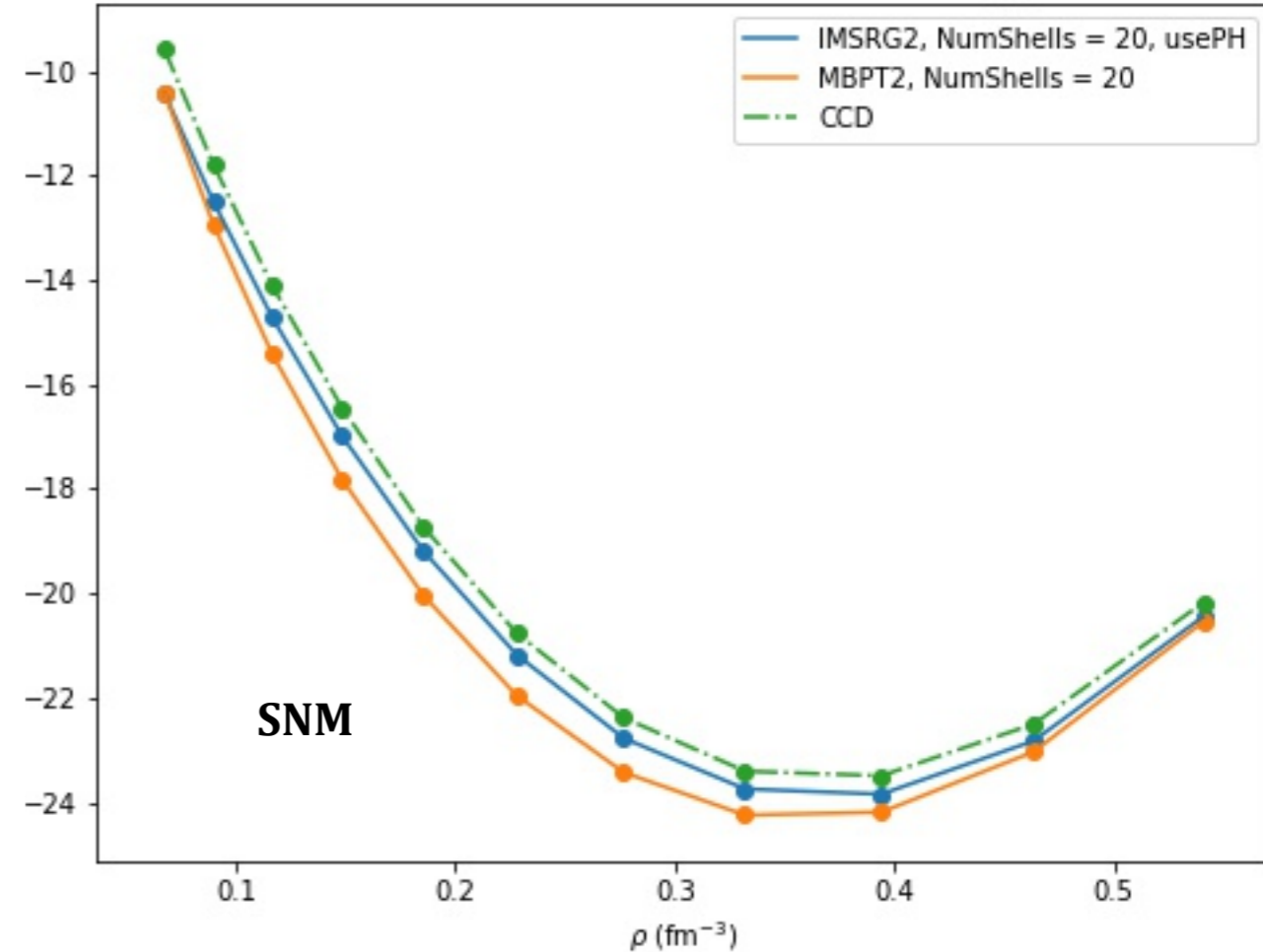
Capability to calculate asymmetric matter, proton fraction = 0.05

Results - Benchmark

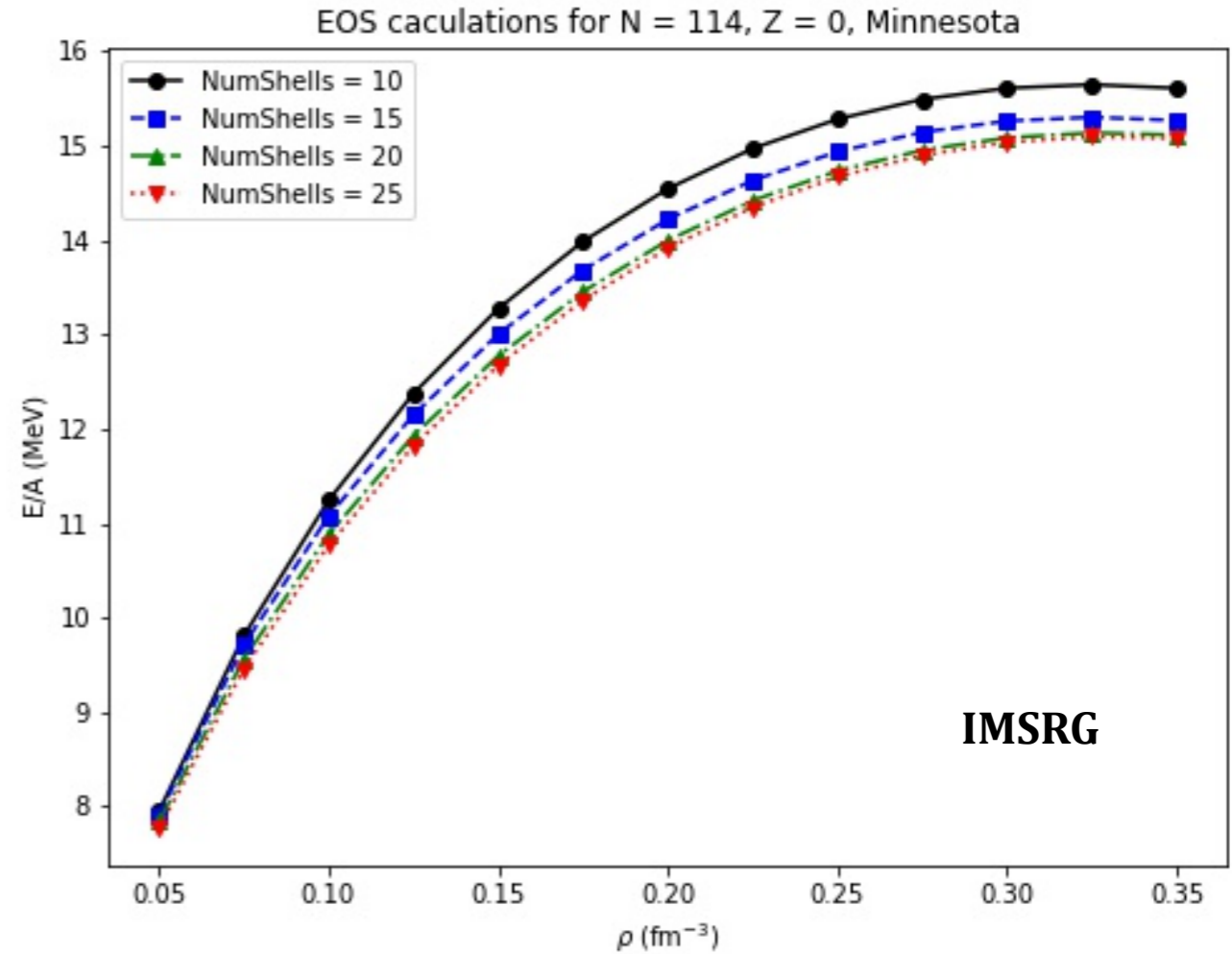
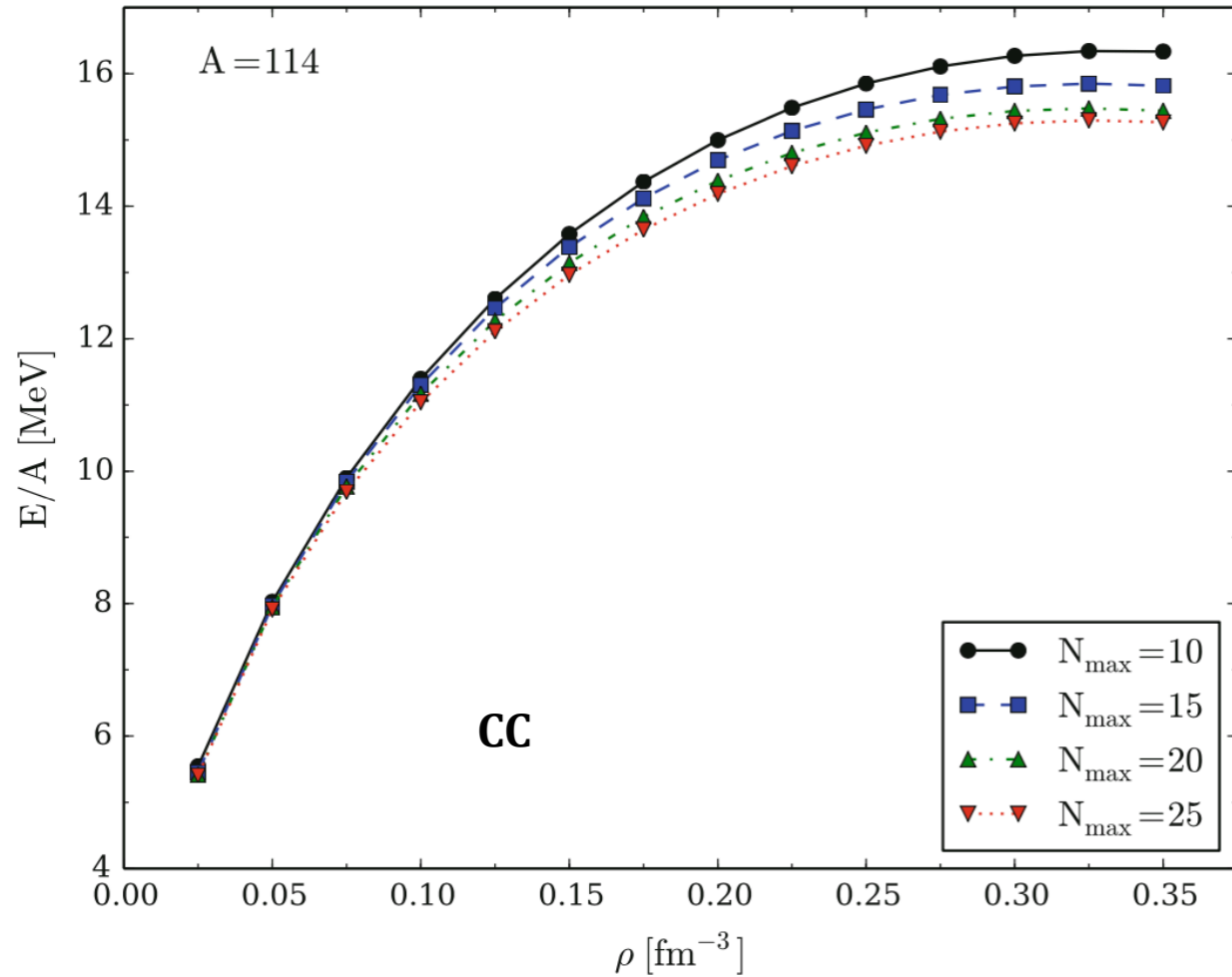
EOS calculations for $N = 66, Z = 0, N2LO_opt$



EOS calculations for $N = 66, Z = 66, N2LO_opt$

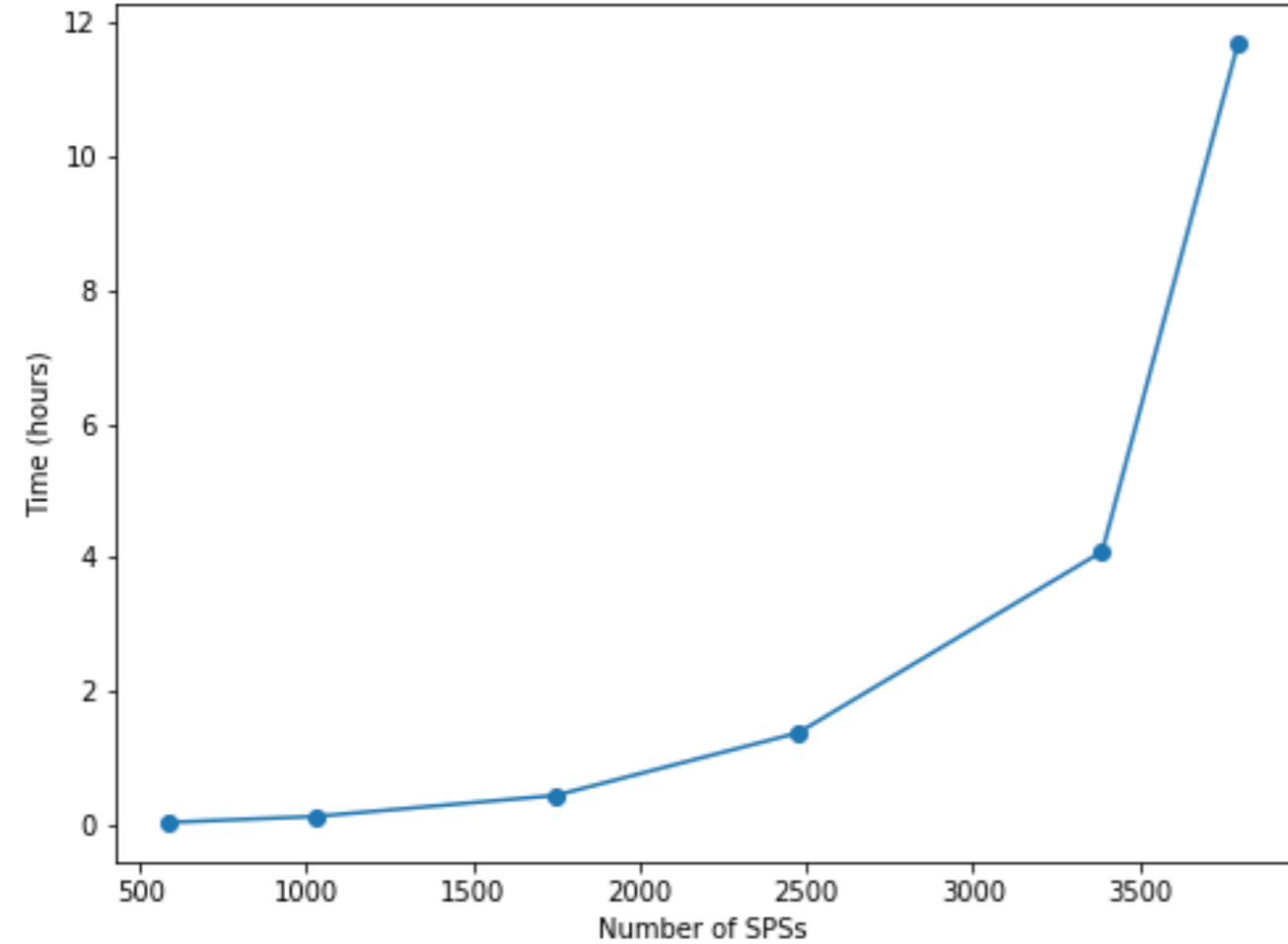


Results - Benchmark

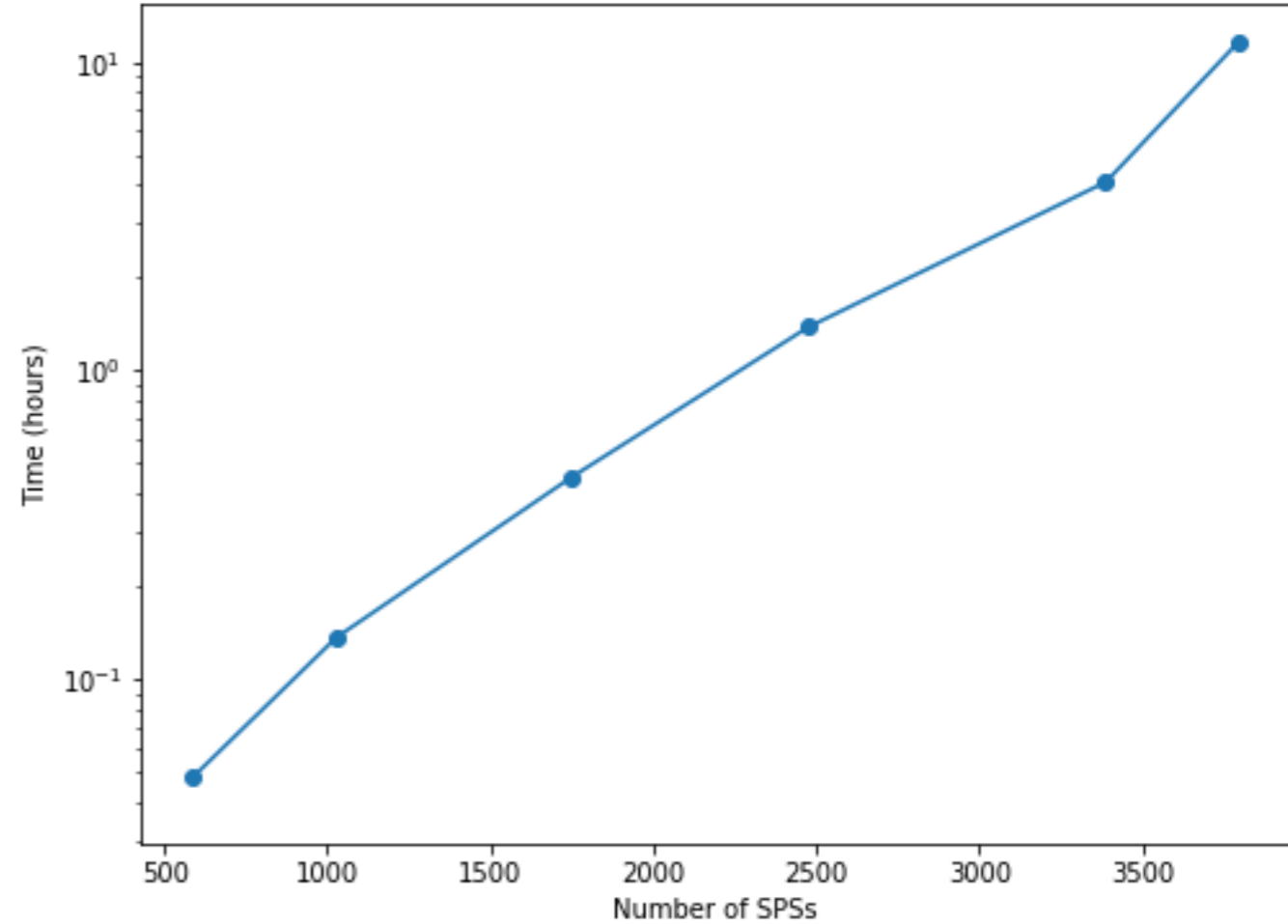


Results - Scaling

Runtime Scaling of Symmetric Nuclear Matter

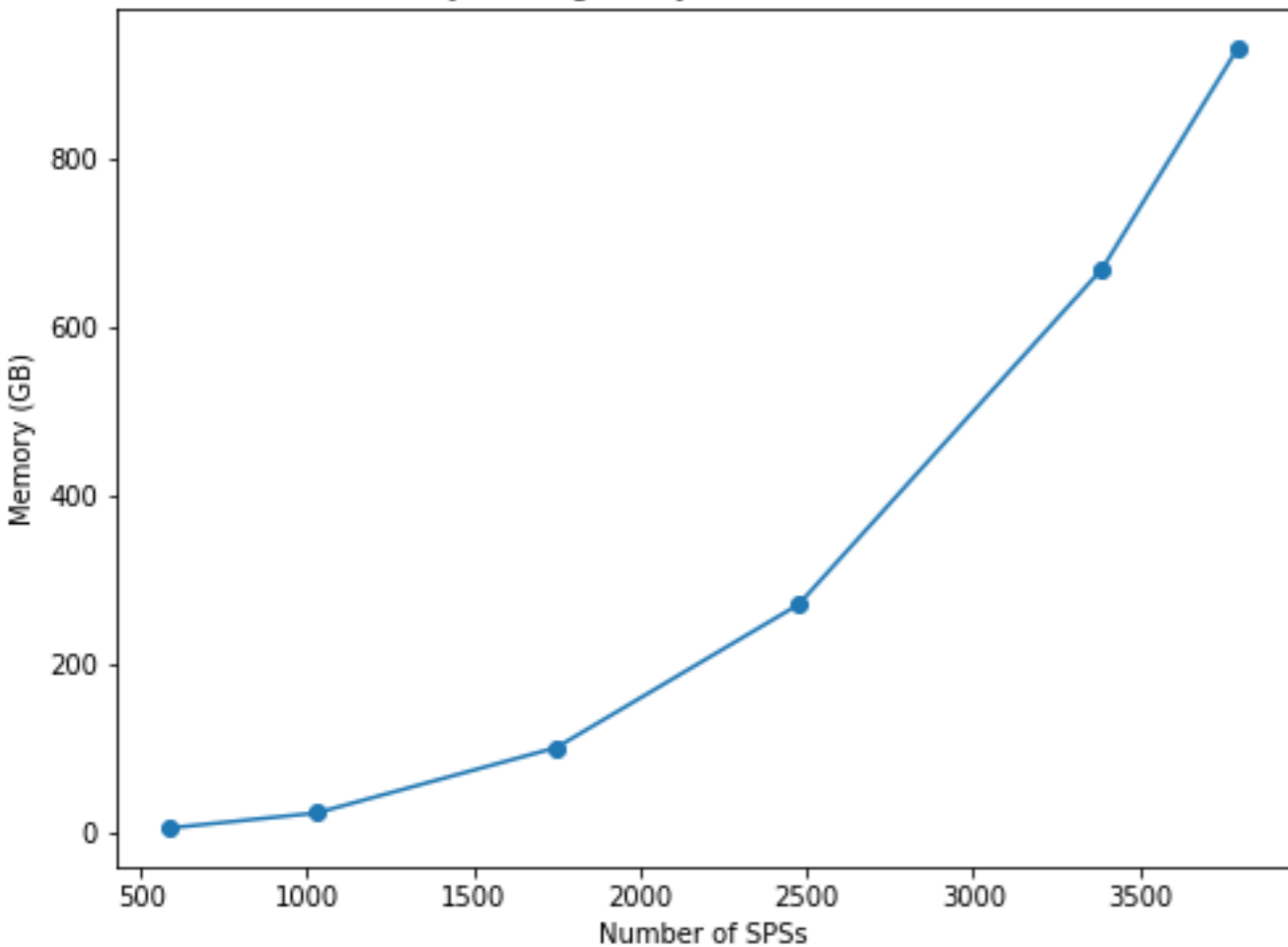


Runtime Scaling of Symmetric Nuclear Matter

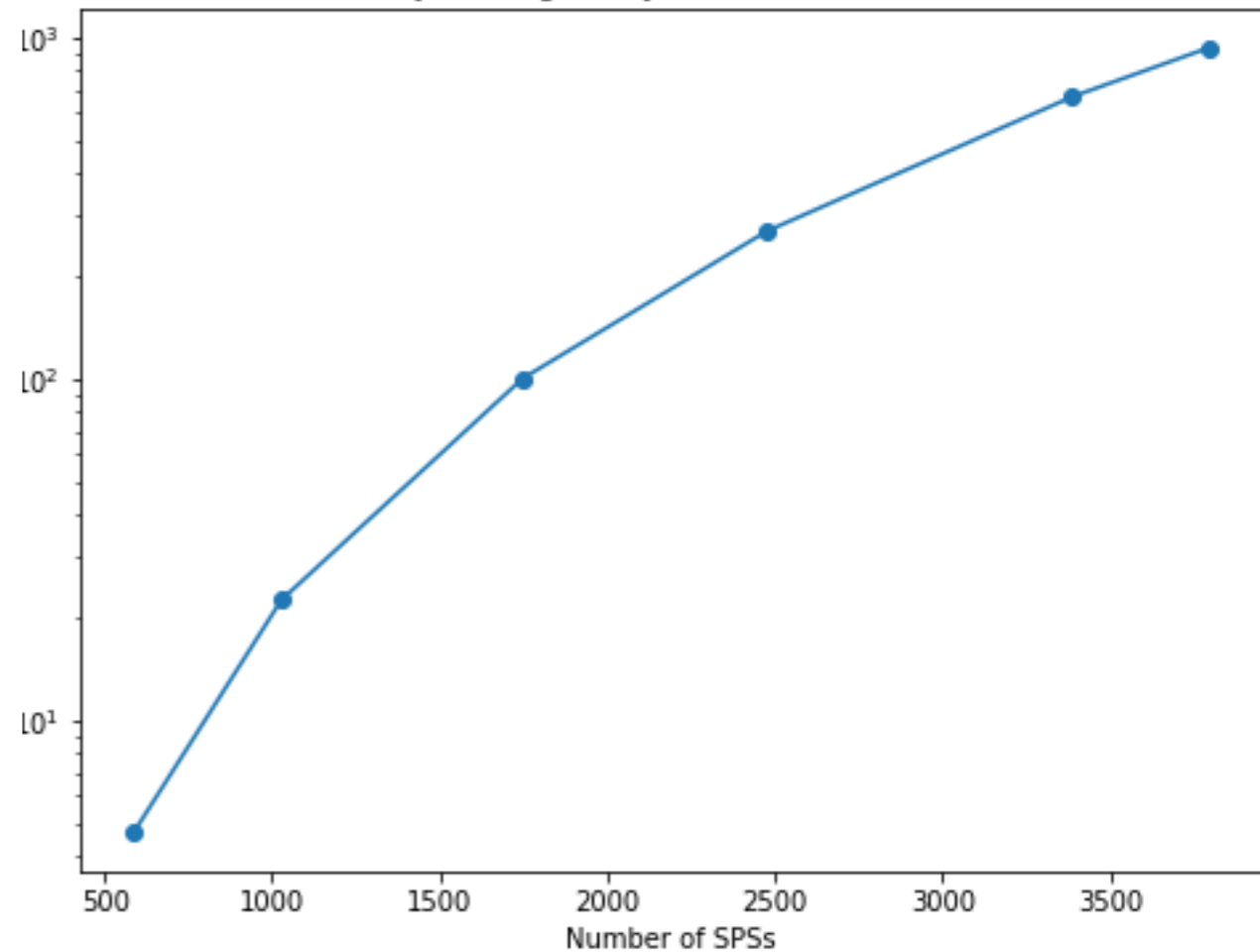


Results - Scaling

Memory Scaling for Symmetric Nuclear Matter

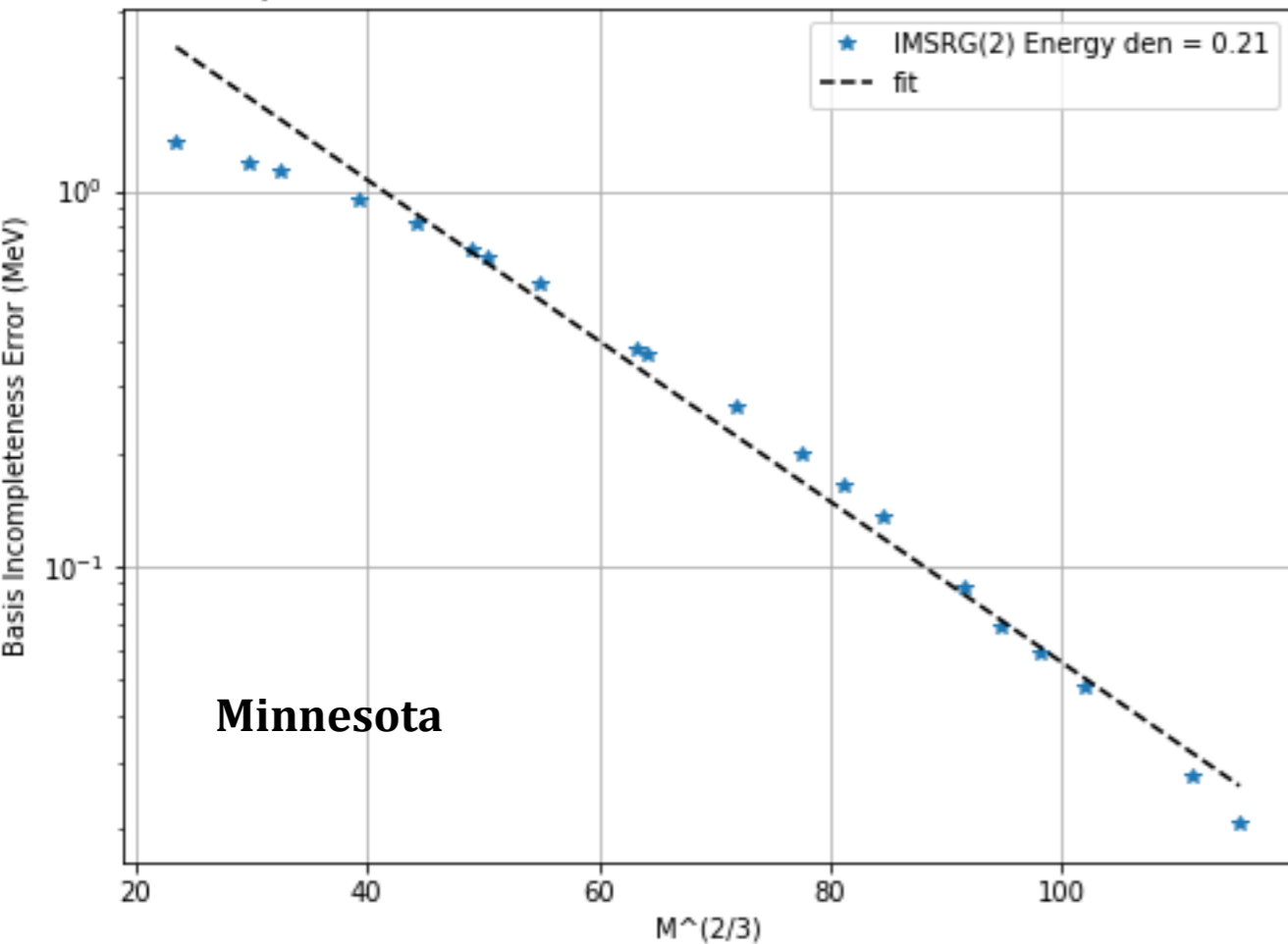


Memory Scaling for Symmetric Nuclear Matter

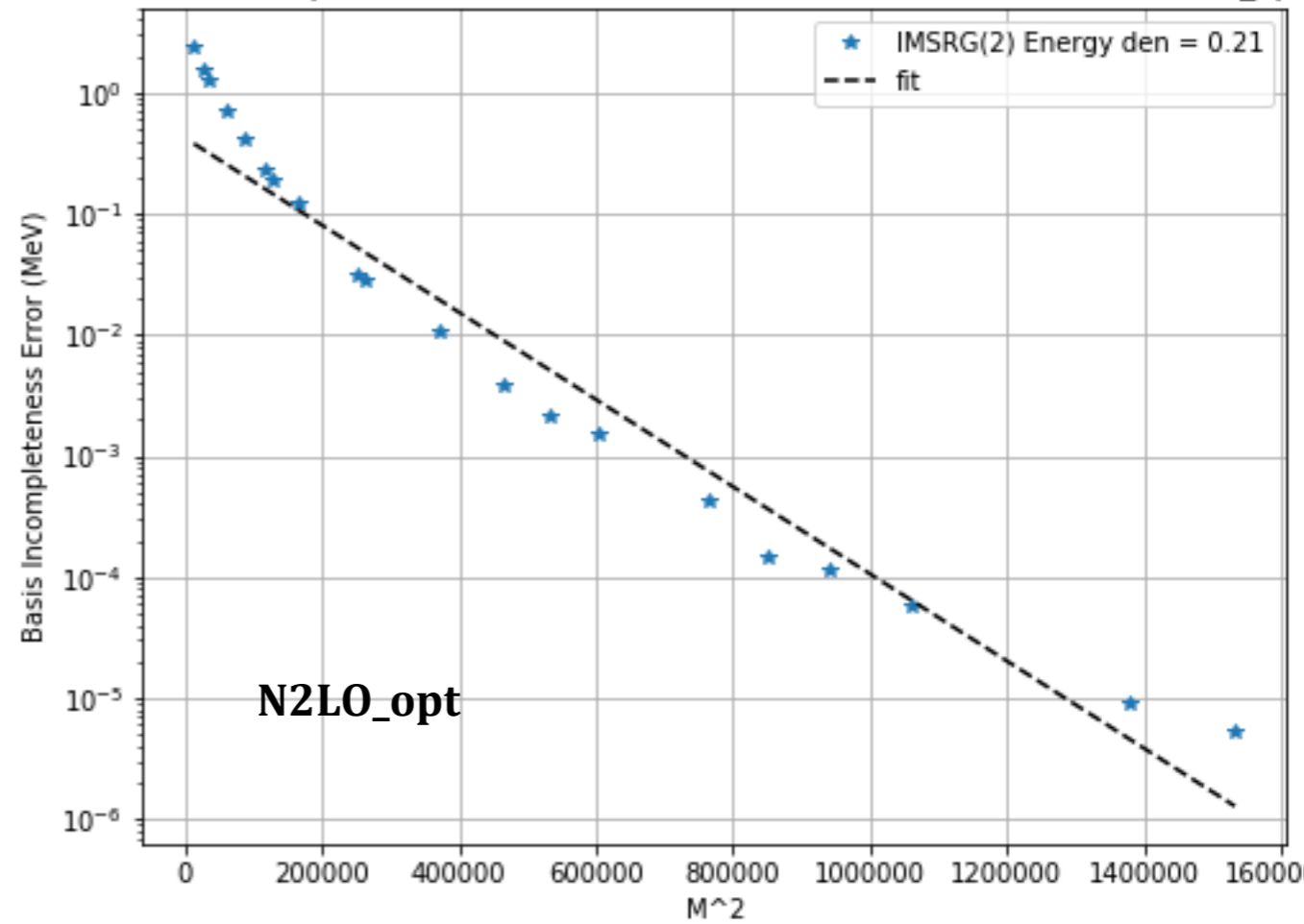


Results - Basis Extrapolation

Basis Incompleteness Error vs $M^{2/3}$ for $N = 66$, $Z = 0$, $\text{den} = 0.21$, Minnesota

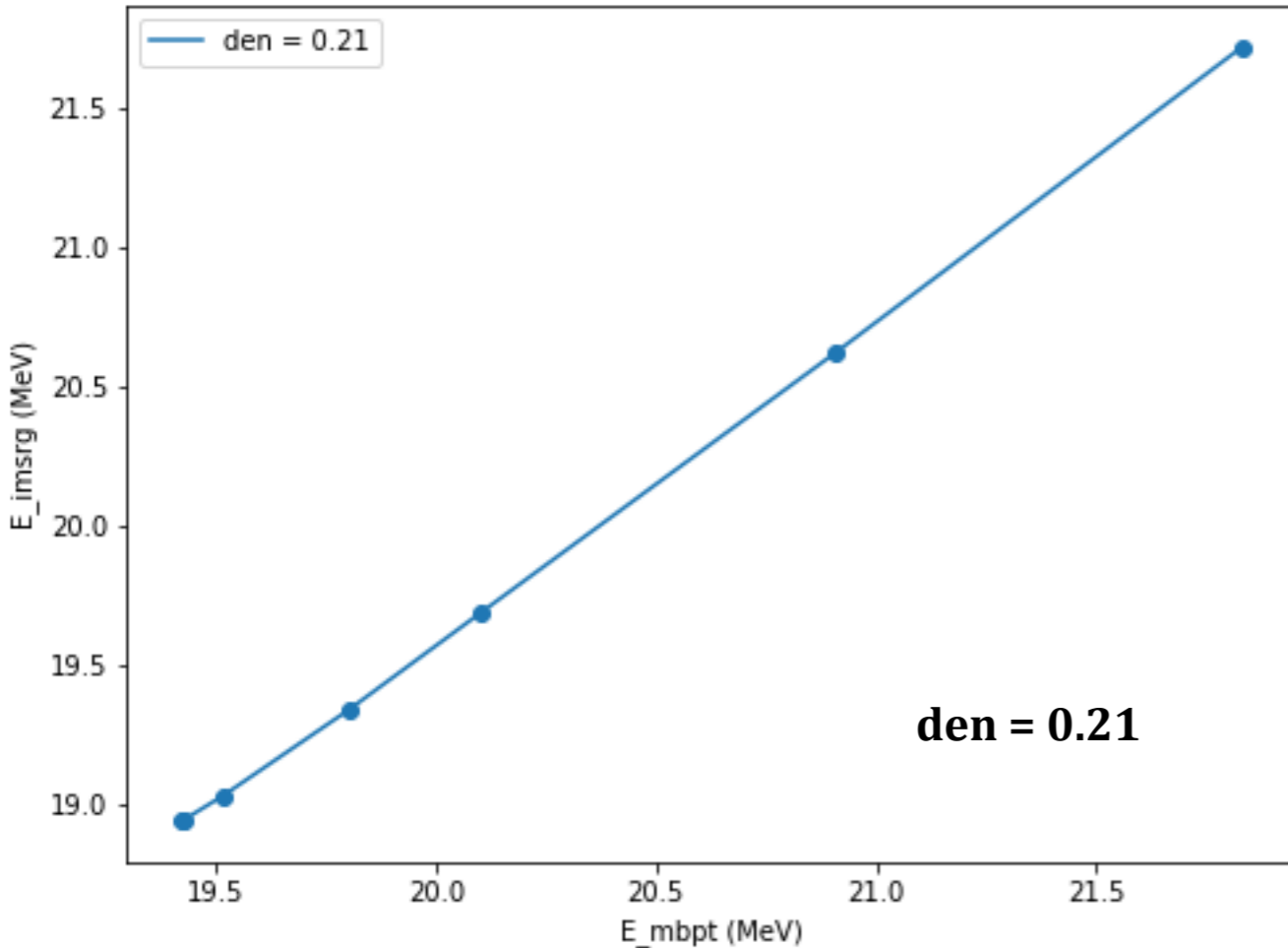


Basis Incompleteness Error vs M^2 for $N = 66$, $Z = 0$, $\text{den} = 0.21$, N2LO_opt

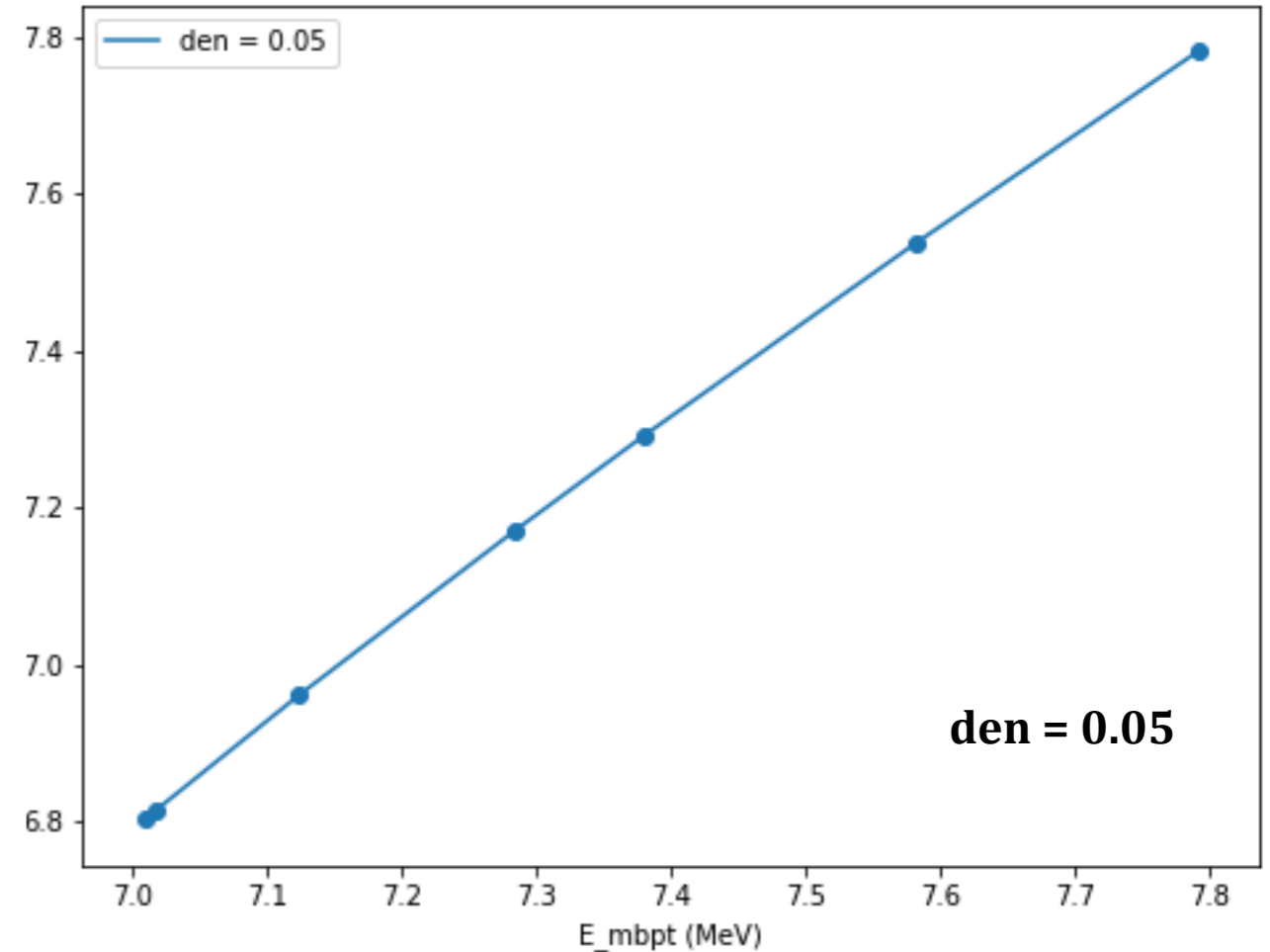


Results - Basis Extrapolation

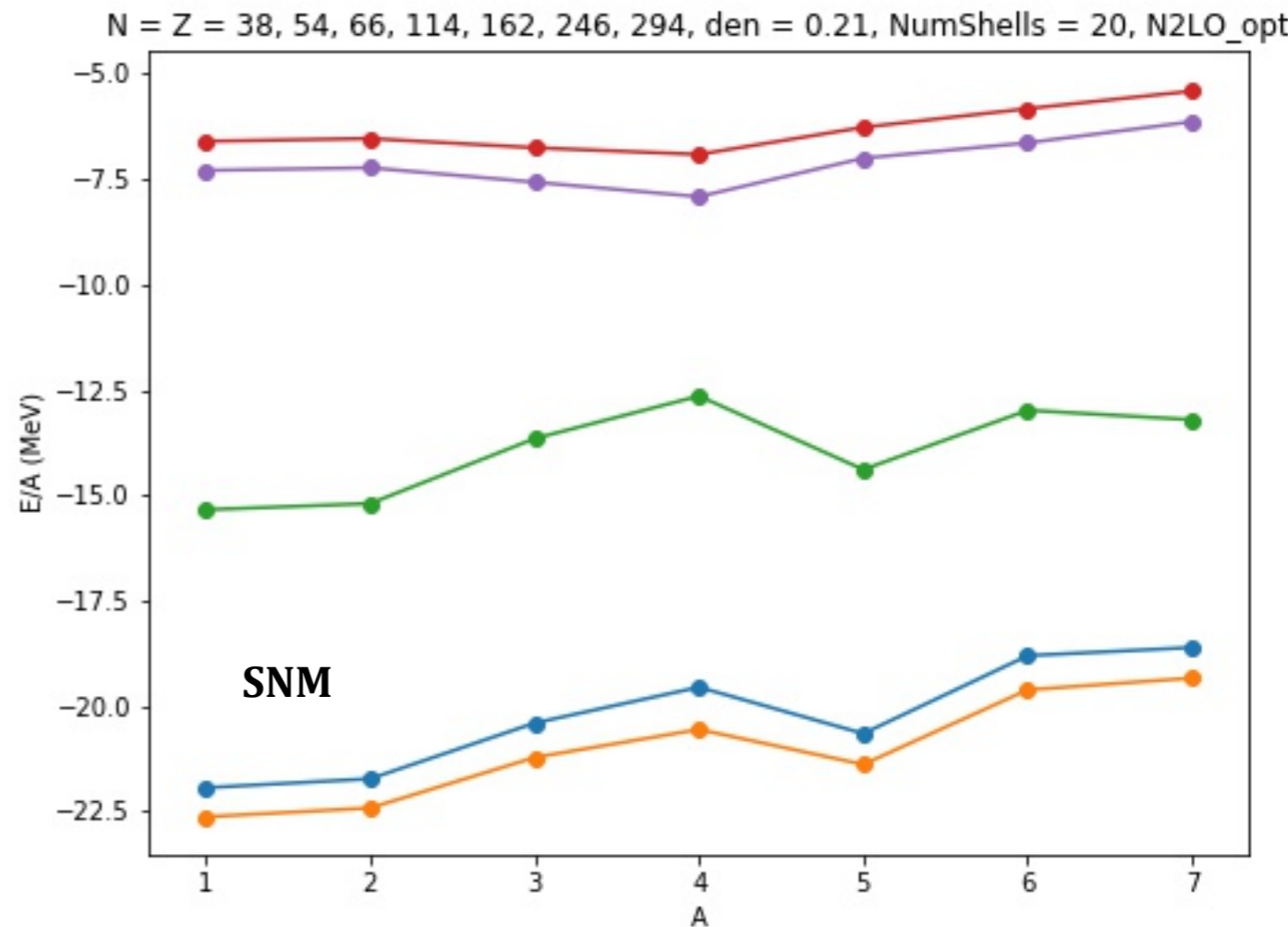
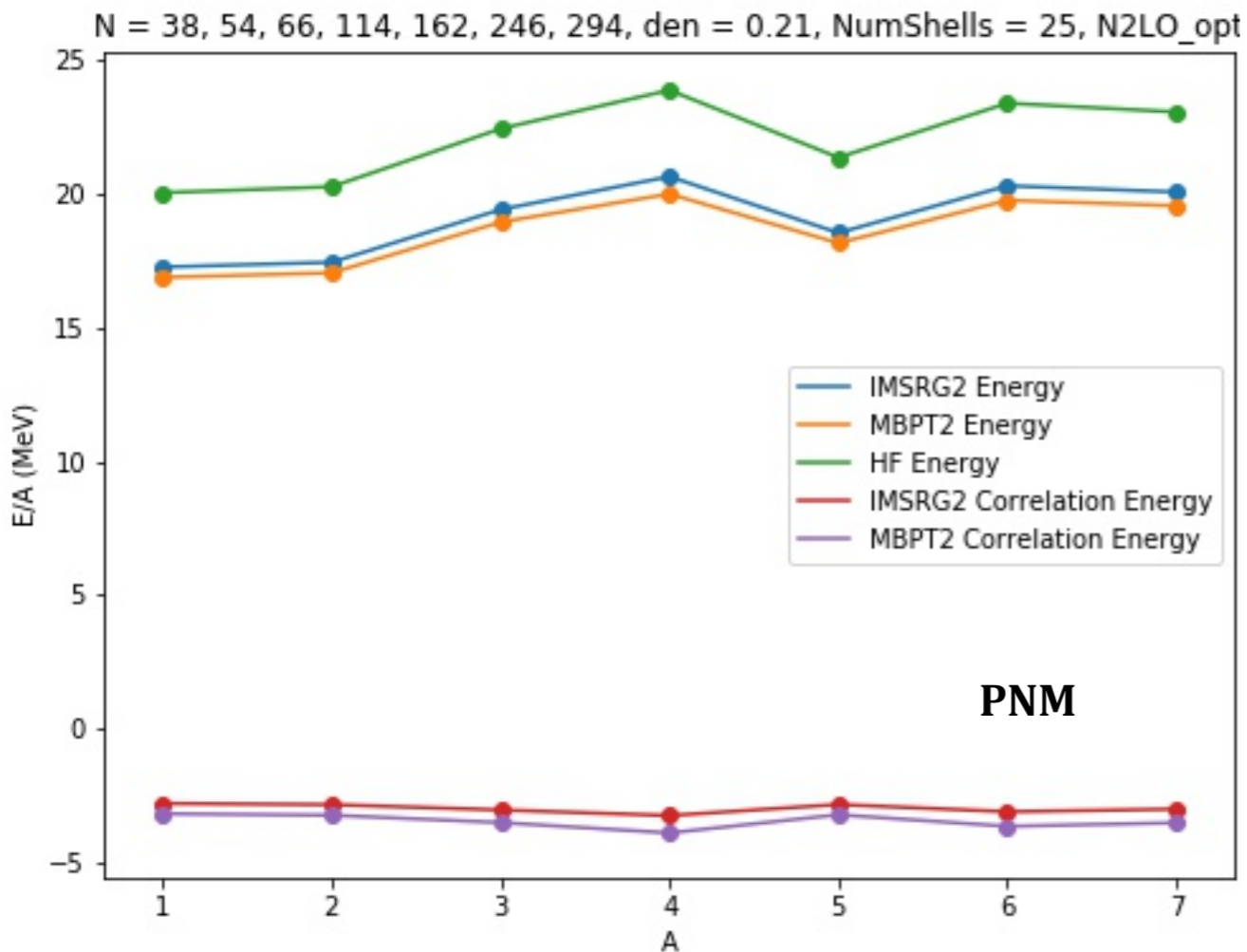
E_{imsrg} vs E_{mbpt} for $N_{\text{max}} = 1,3,5,6,9,10,12$ with $N = 66$, $Z = 0$, $\text{den} = 0.21$, $N2LO_{\text{opt}}$



E_{imsrg} vs E_{mbpt} for $N_{\text{max}} = 1,3,5,6,9,10,12$ with $N = 66$, $Z = 0$, $\text{den} = 0.05$



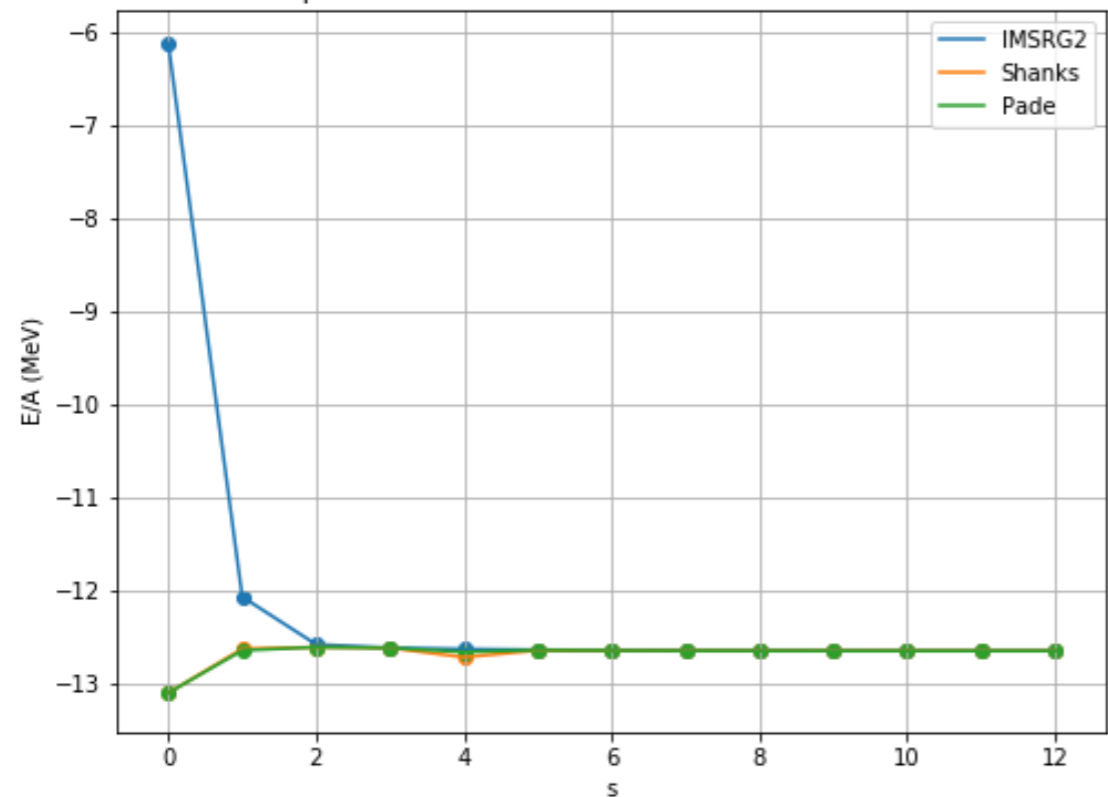
Results - Finite Size Effect



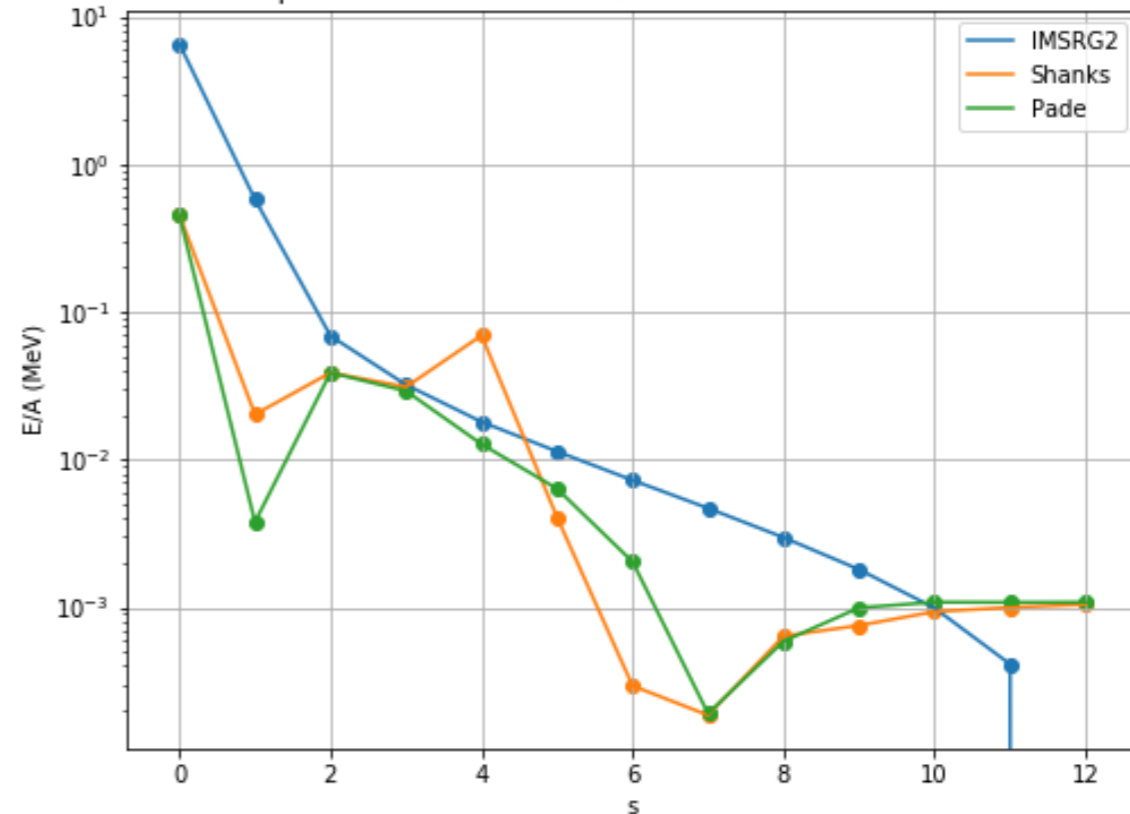
Numerical Techniques

■ Shanks Transformation & Padé Approximation

IMSRG flow and extrapolation for $N = 66$, $Z = 66$, $\text{den} = 0.09$, $\text{NumShells} = 28$, N2LO_{opt}

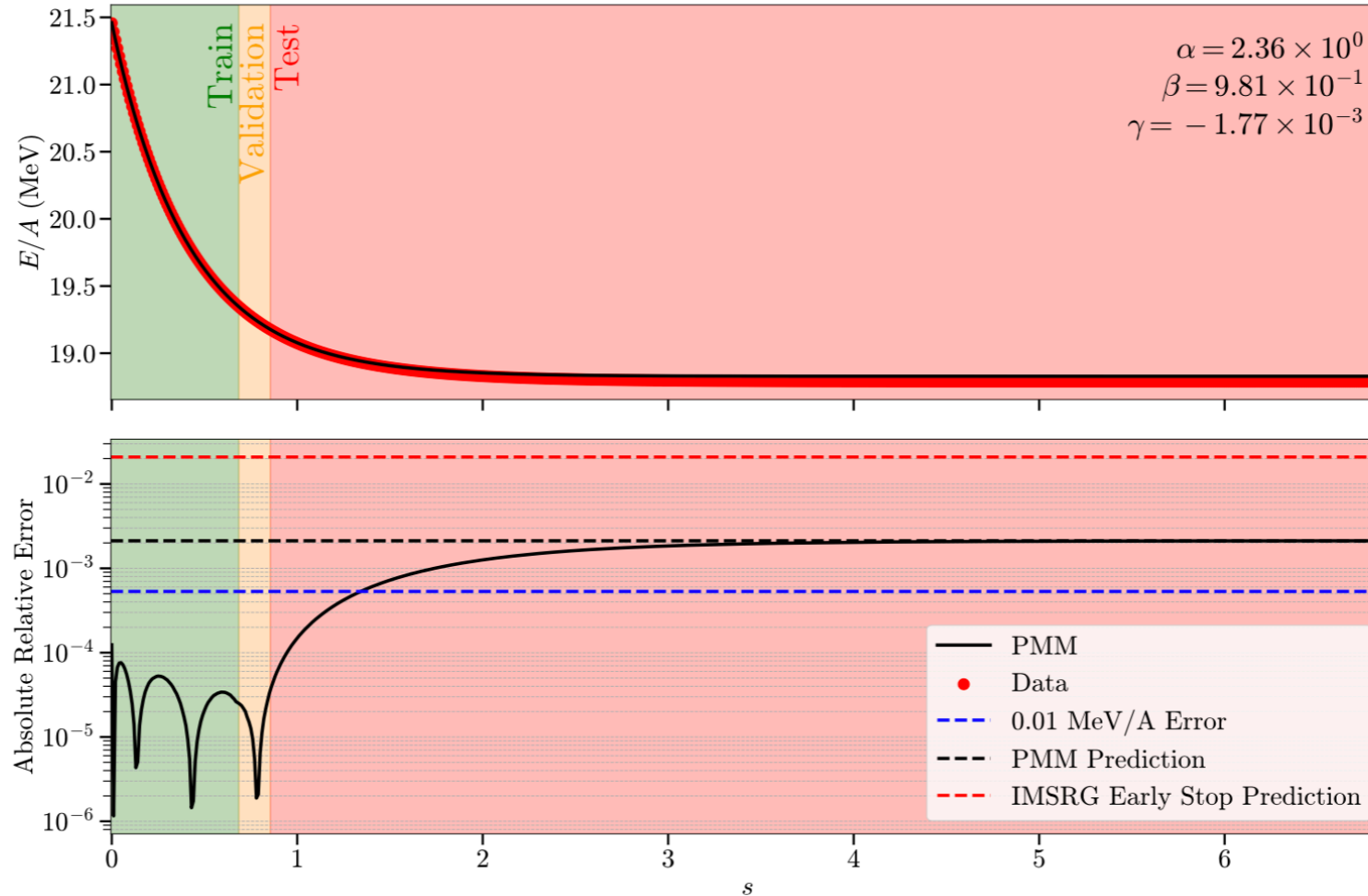


IMSRG flow and extrapolation error for $N = 66$, $Z = 66$, $\text{den} = 0.09$, $\text{NumShells} = 28$, N2LO_{op}



Numerical Techniques

Bayesian ML and Parametric Matrix Model (PMM)



Outlook - Astrophysical applications

■ Outlook

