



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



U.S. DEPARTMENT OF  
**ENERGY**

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Science

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# Outline

- Introduction
- IMSRG-EOS Framework
- EOS Results
- PMM Emulator
- Summary and Outlook

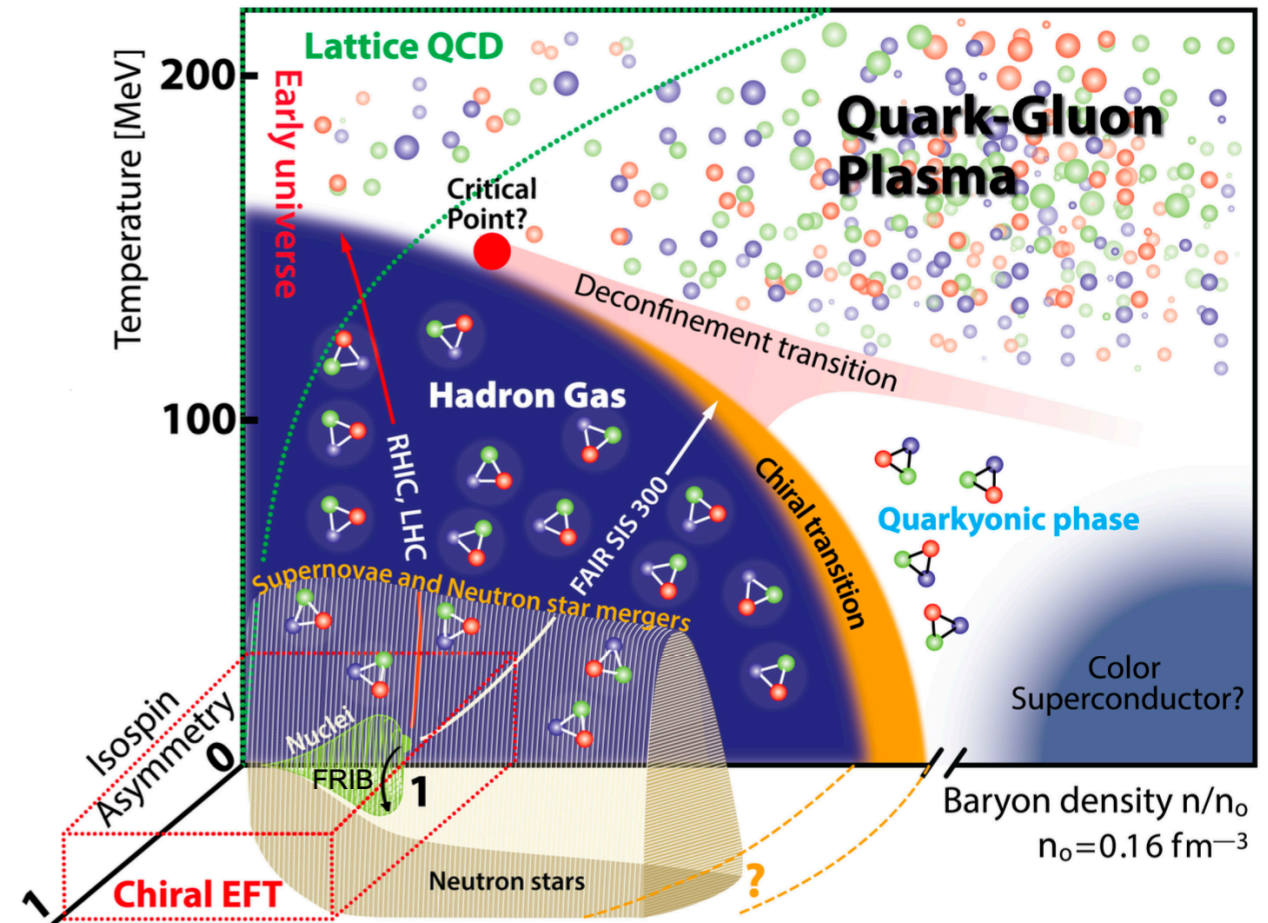


# Introduction - Nuclear Matter and Equation of State

- 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 & Many Body Methods

- Chiral effective field theory:
  - Consistent NN, NNN, ... interactions
  - Systematic low-momentum expansion
  - Link with underlying QCD
- Many Body Methods: QMC, CC, MBPT, **IMSRG...**

	NN forces	3N forces	4N forces
LO ( $Q^0$ )	 2		
NLO ( $Q^2$ )	 7		
N <sup>2</sup> LO ( $Q^3$ )	 0	 2	
N <sup>3</sup> LO ( $Q^4$ )	 12	 0	 0
N <sup>4</sup> 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 - In-Medium Similarity Renormalization Group

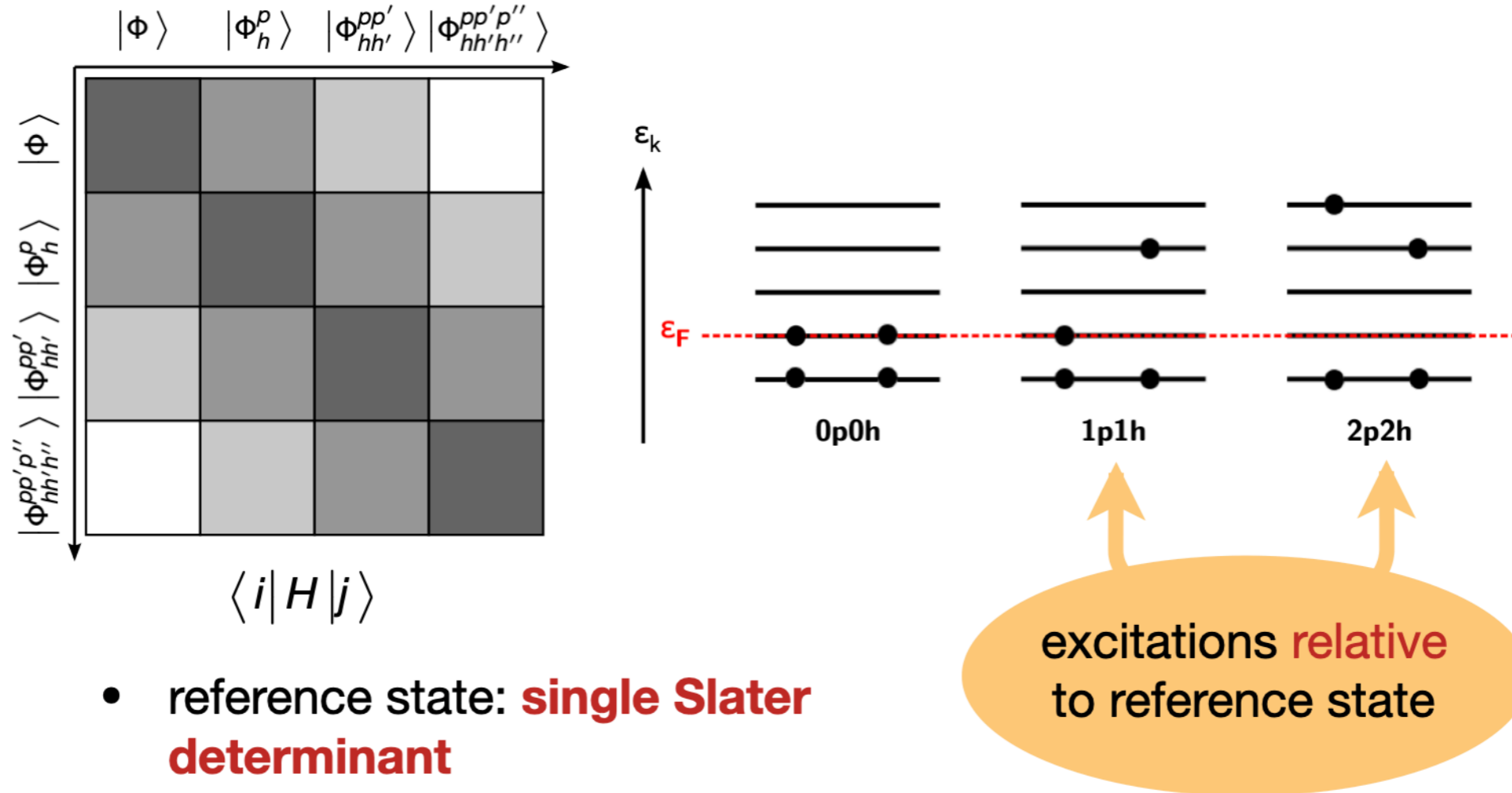
## Normal-Ordered Hamiltonian

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

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

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

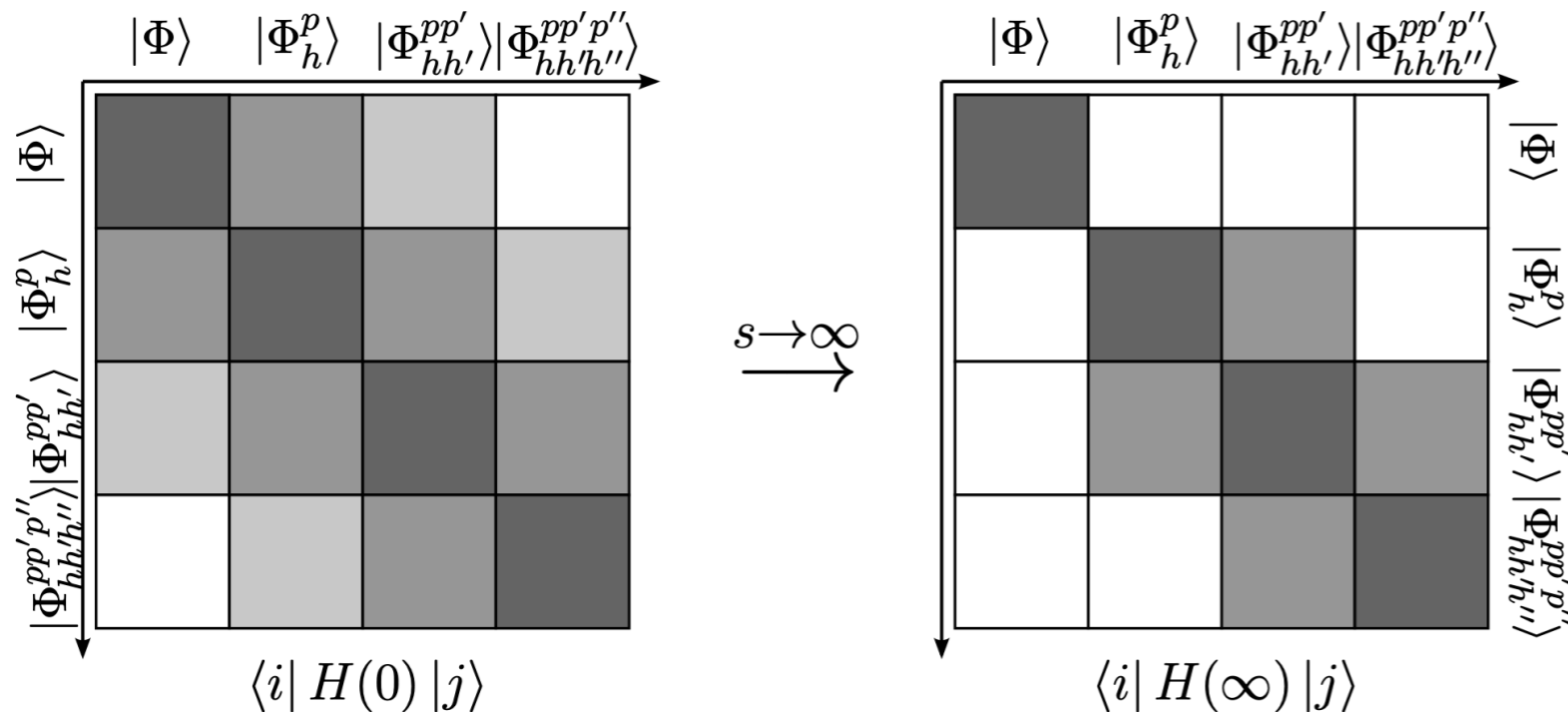
# Introduction - In-Medium Similarity Renormalization Group



# Introduction - In-Medium Similarity Renormalization Group

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

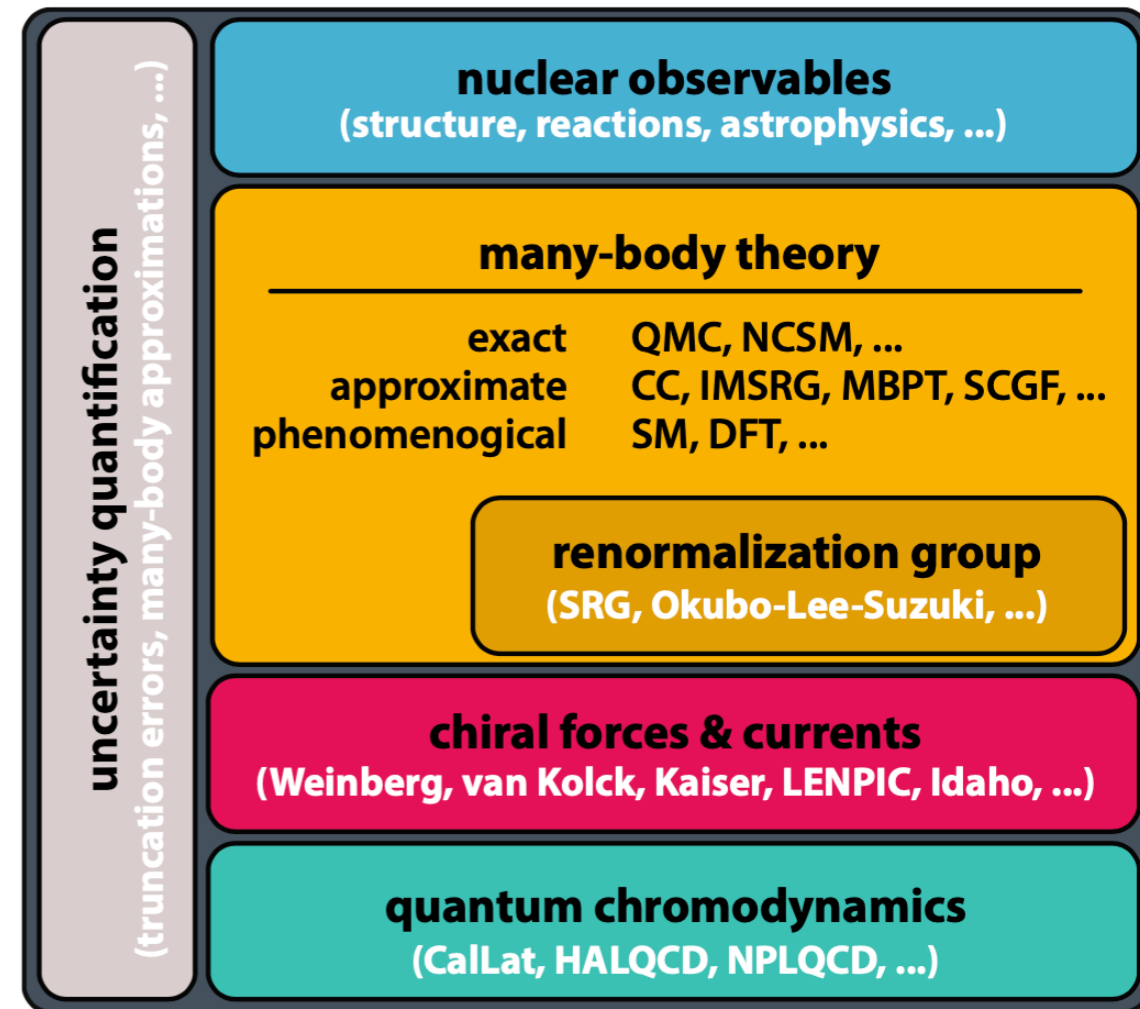
**IM-SRG(2):** Truncate  $H(s)$ ,  $\eta(s)$  to **normal ordered** 2-body terms



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

# 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



# Preliminary Results - Interactions

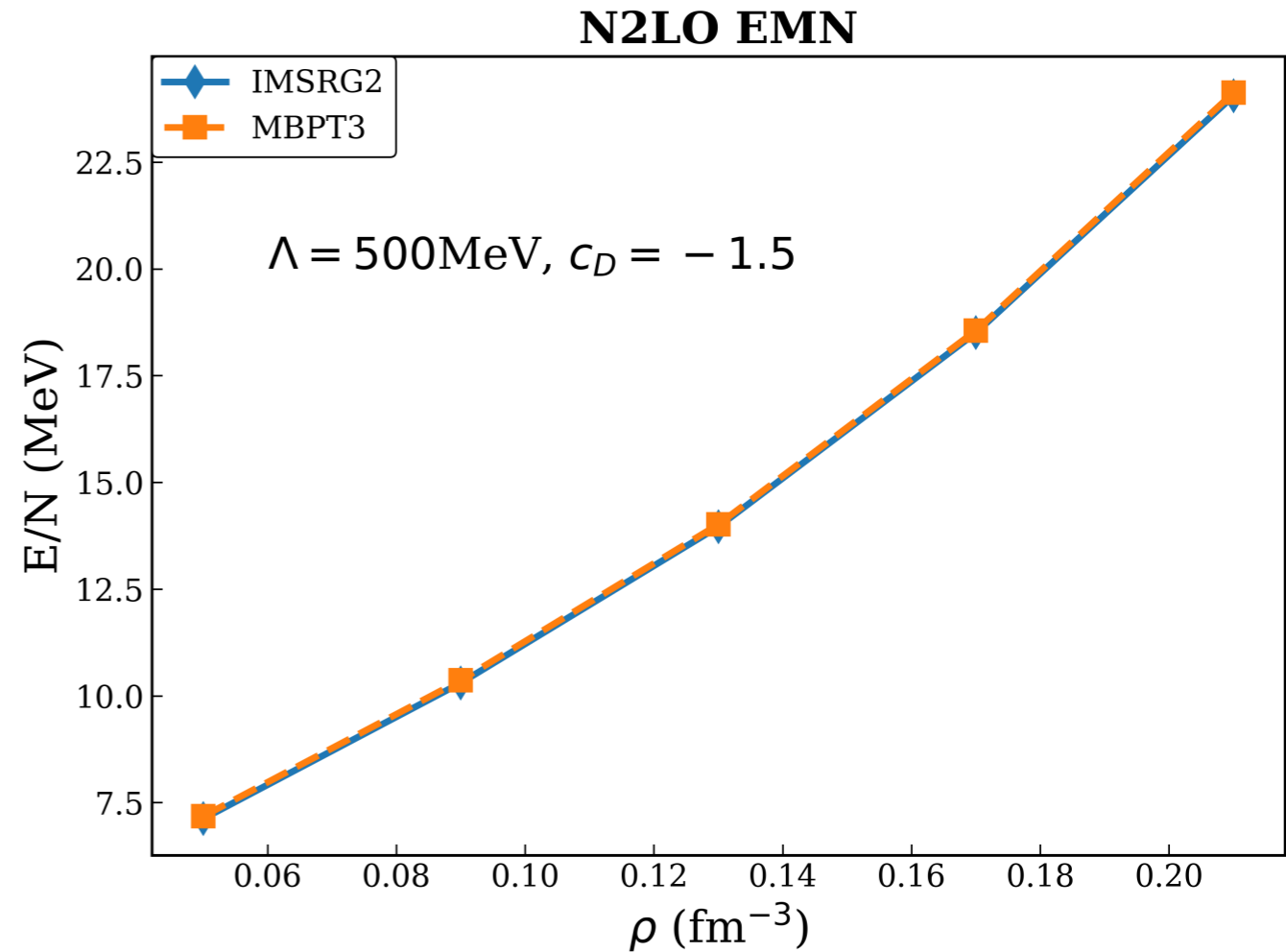
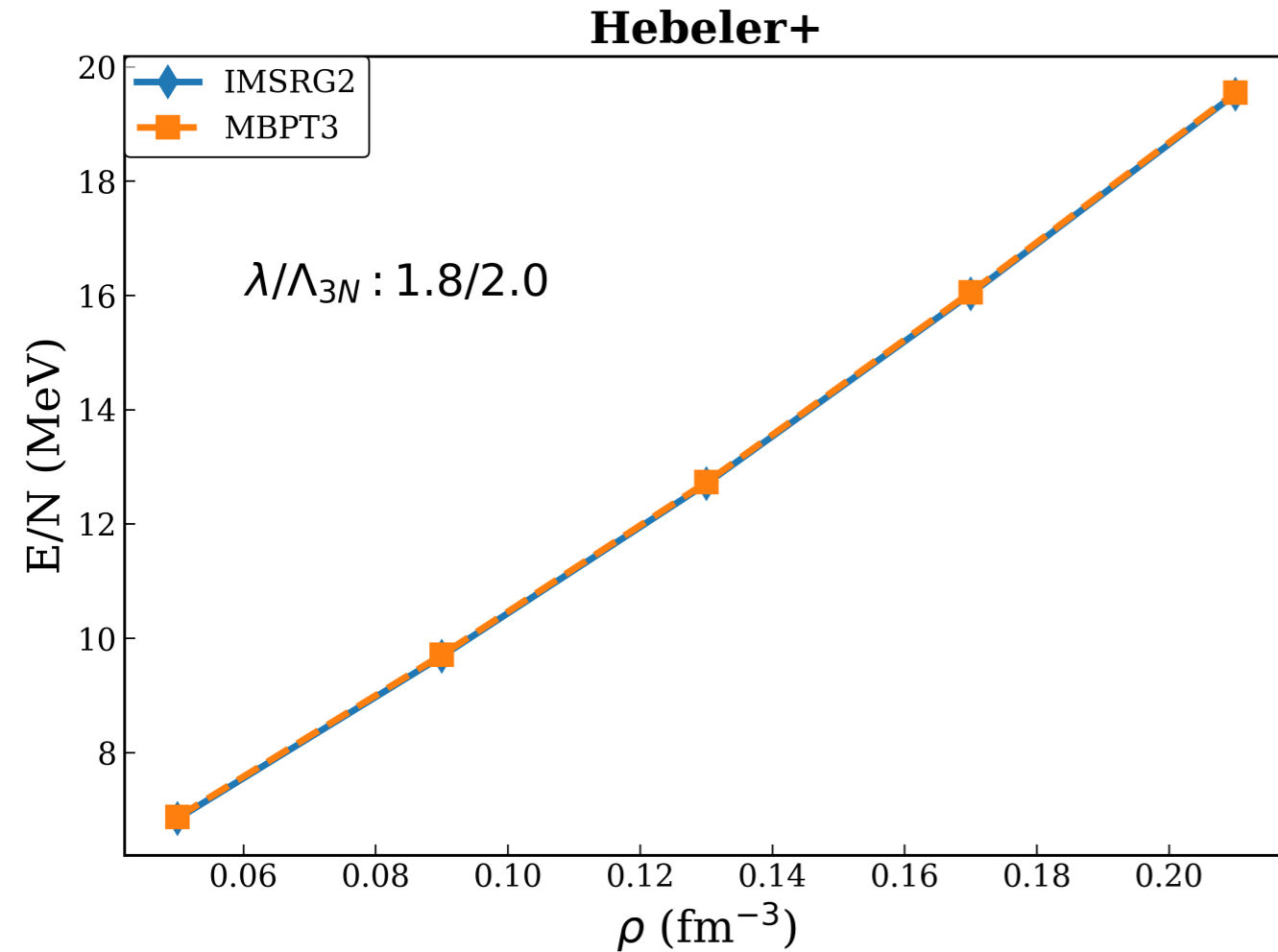
## ■ Hebeler Interactions:

- 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  $\lambda/\Lambda_{3N}$ , where  $\lambda$  is the SRG flow parameter,  $\Lambda_{3N}$  is the 3N cutoff

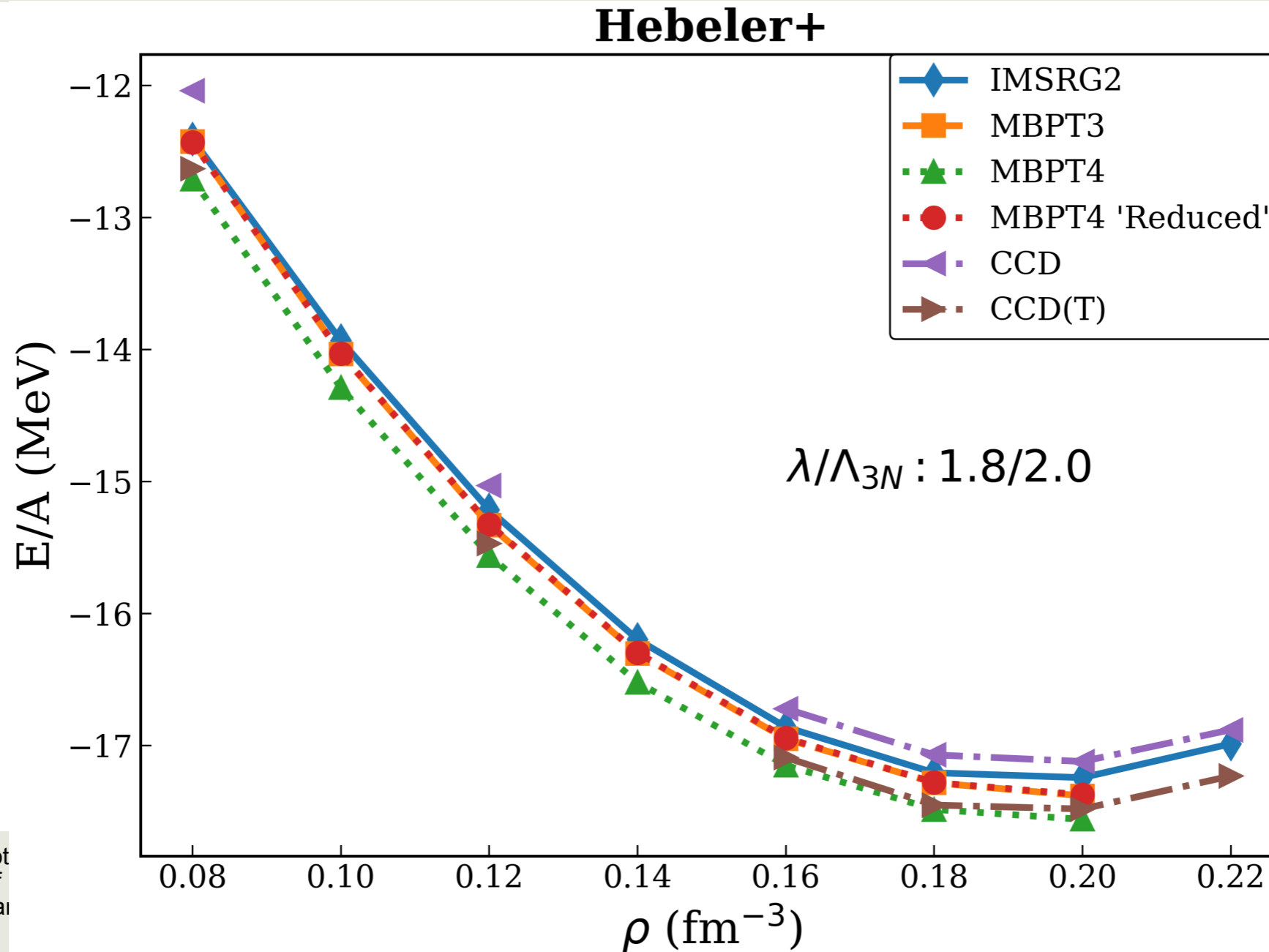
## ■ N2LO EMN Interactions:

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

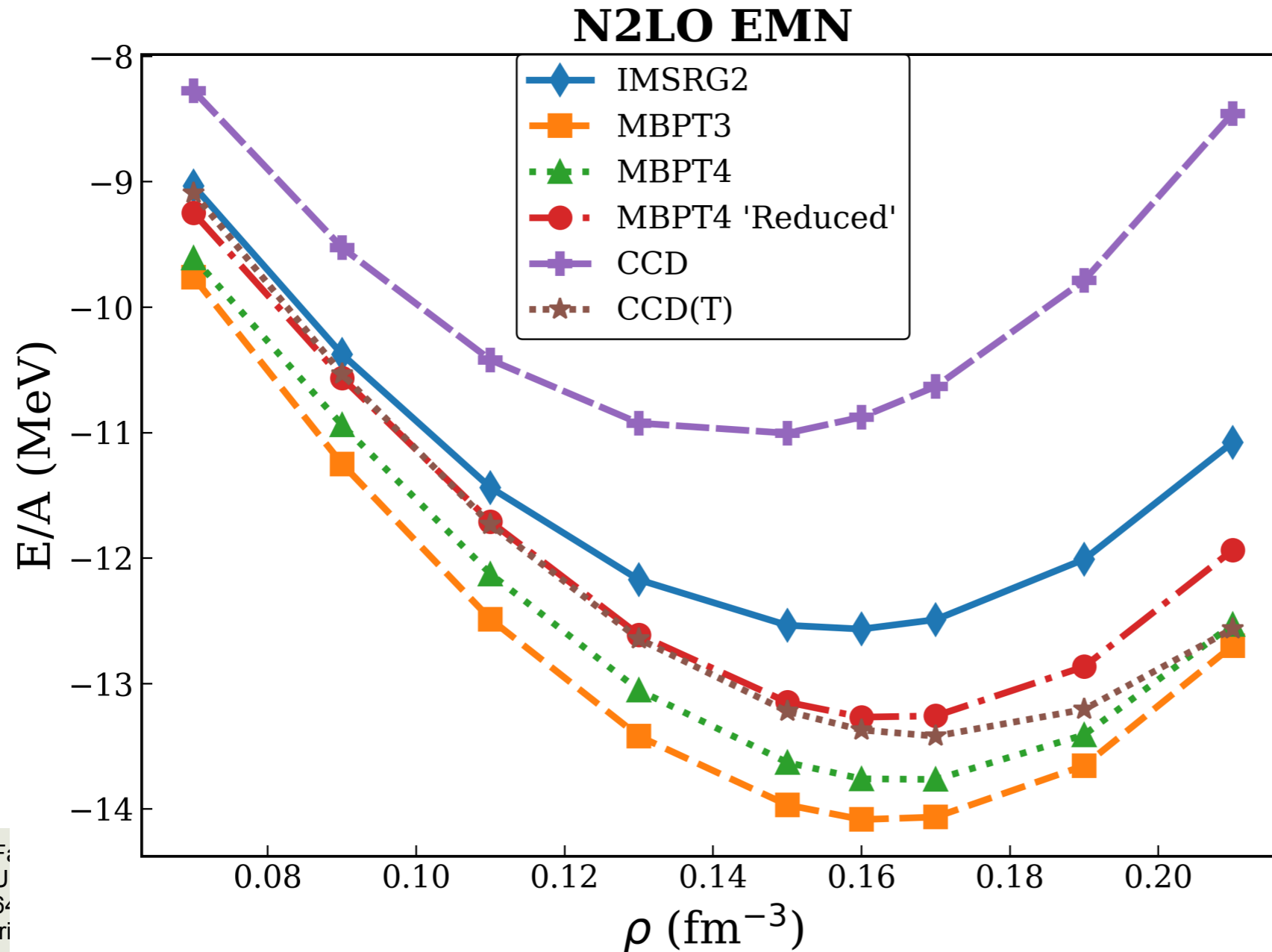
# Preliminary Results - PNM EOS



# Preliminary Results - SNM EOS with Hebeler Interaction

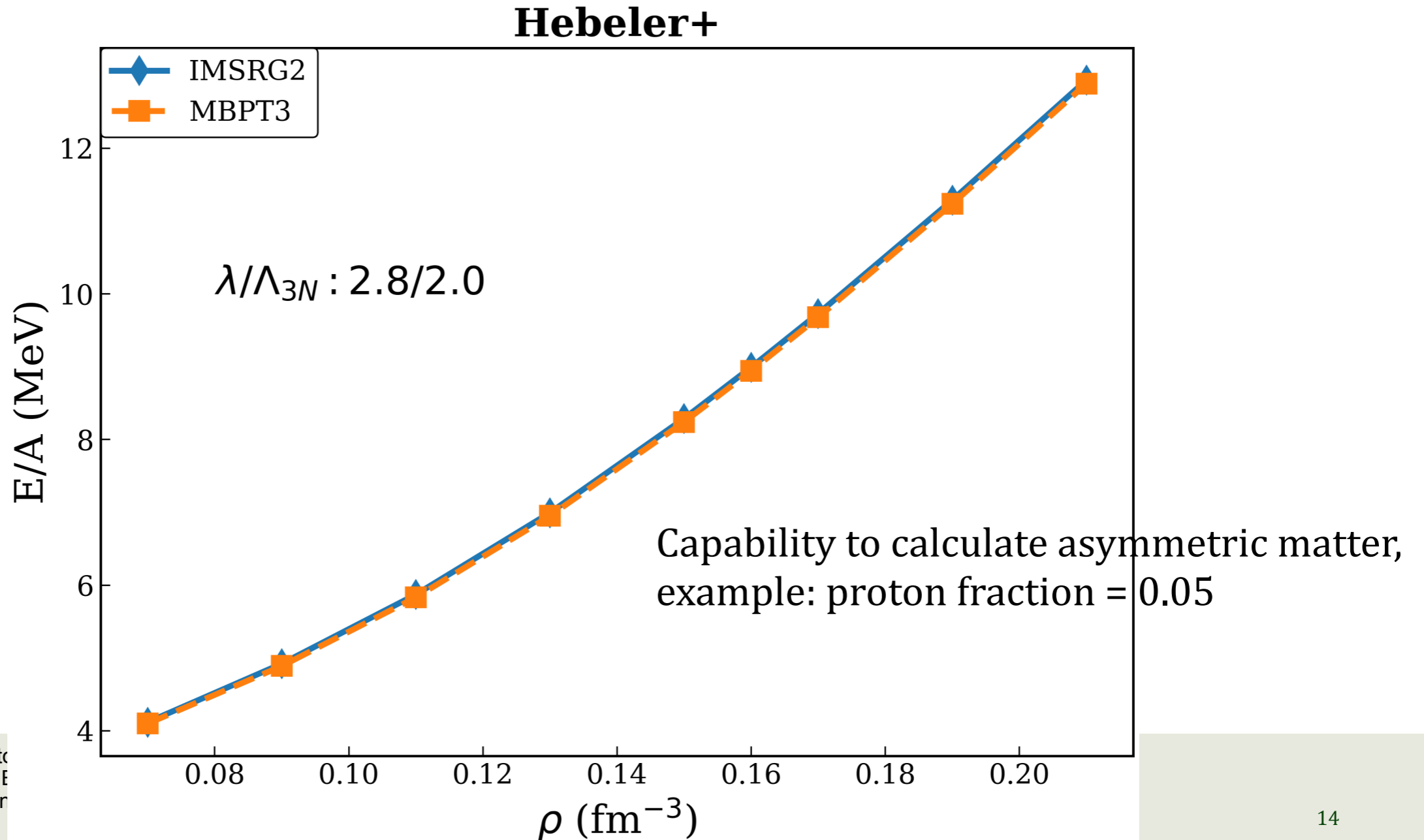


# Preliminary Results - SNM EOS with N2LO EMN Interaction

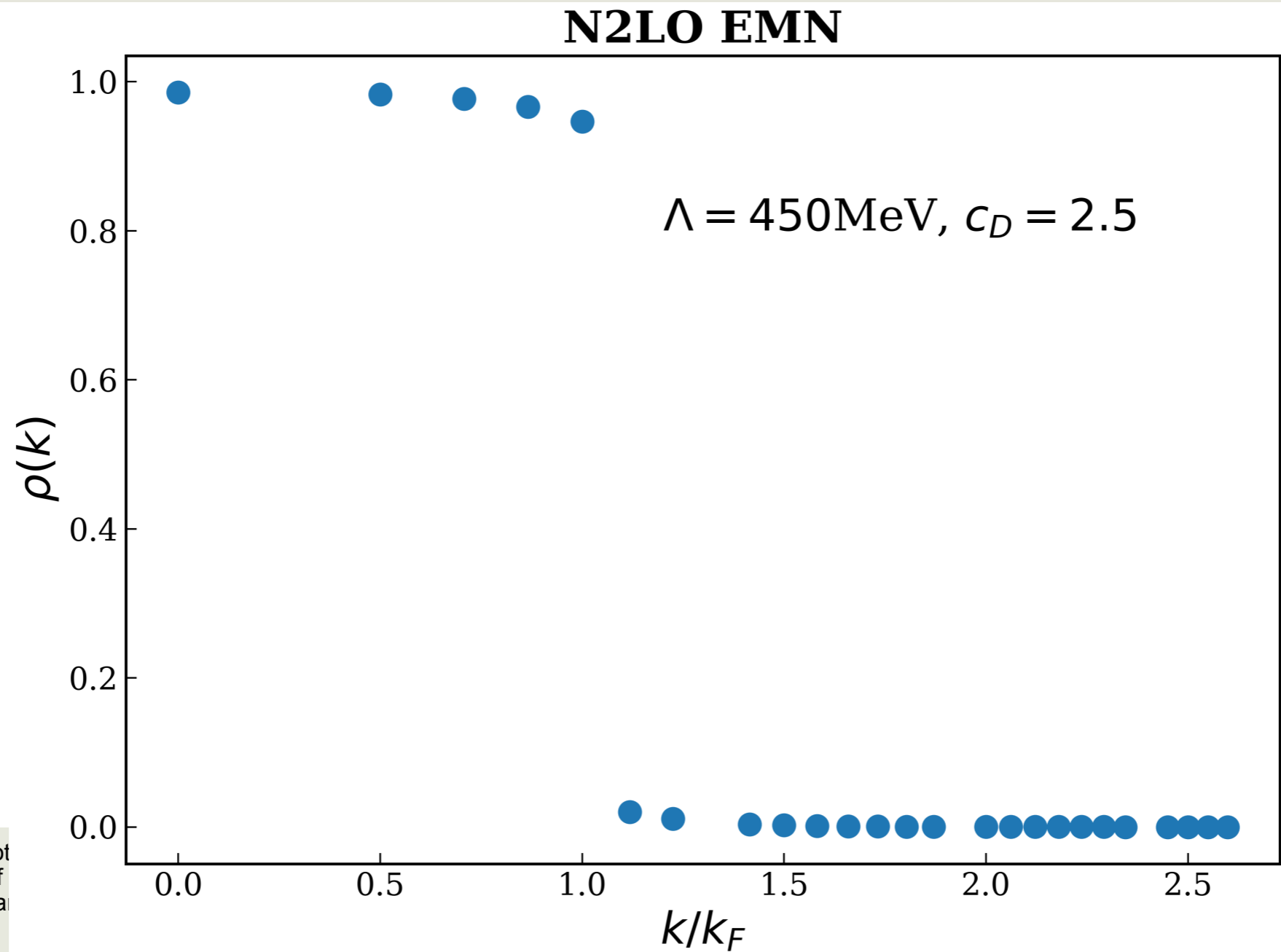


IMSRG(2) fall between  
CCD and CCD(T)

# Preliminary Results - ANM EOS with Hebeler Interactions

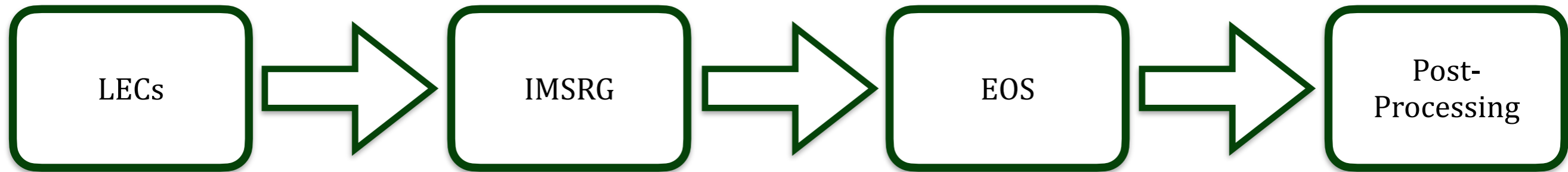


# Preliminary Results - Single Nucleus Momentum Distribution with N2LO EMN Interaction



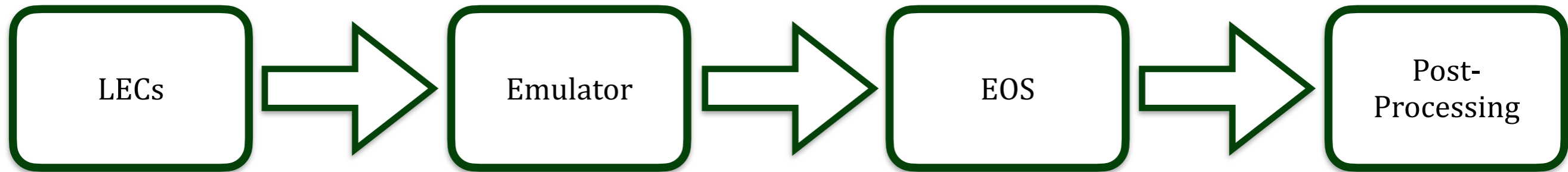
# Emulators - Why Do We Need Emulators?

- Full IMSRG calculations are accurate but expensive
- Uncertainty quantification, sensitivity studies and bayesian analysis need millions of samples
- Replace full IMSRG solver with accurate enough but much faster emulator that predicts EOS from LECs in order to propagate uncertainties in LEC to EOS



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# Emulators - Why Parametric Matrix Model (PMM)?

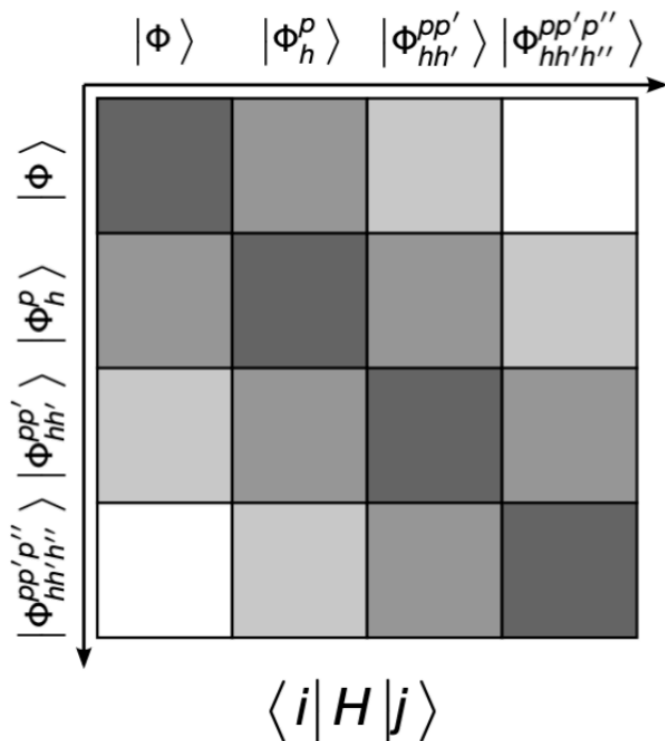
What is PMM?

- Physics (Equation) - Based Machine Learning Algorithm



# Emulators - Why Parametric Matrix Model (PMM)?

$$H(\mathbf{c}) = H_0 + \sum_i c_i H_i$$



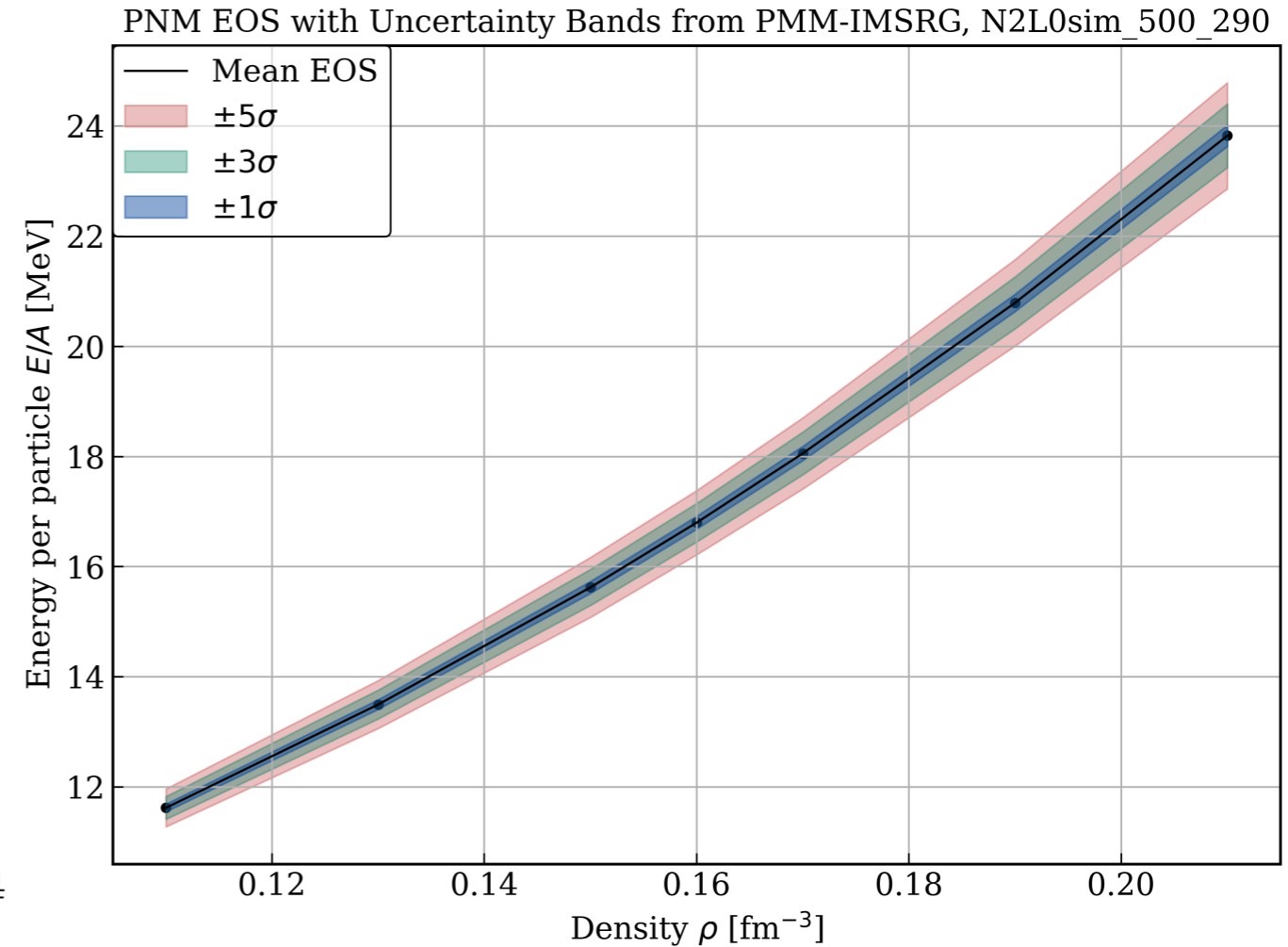
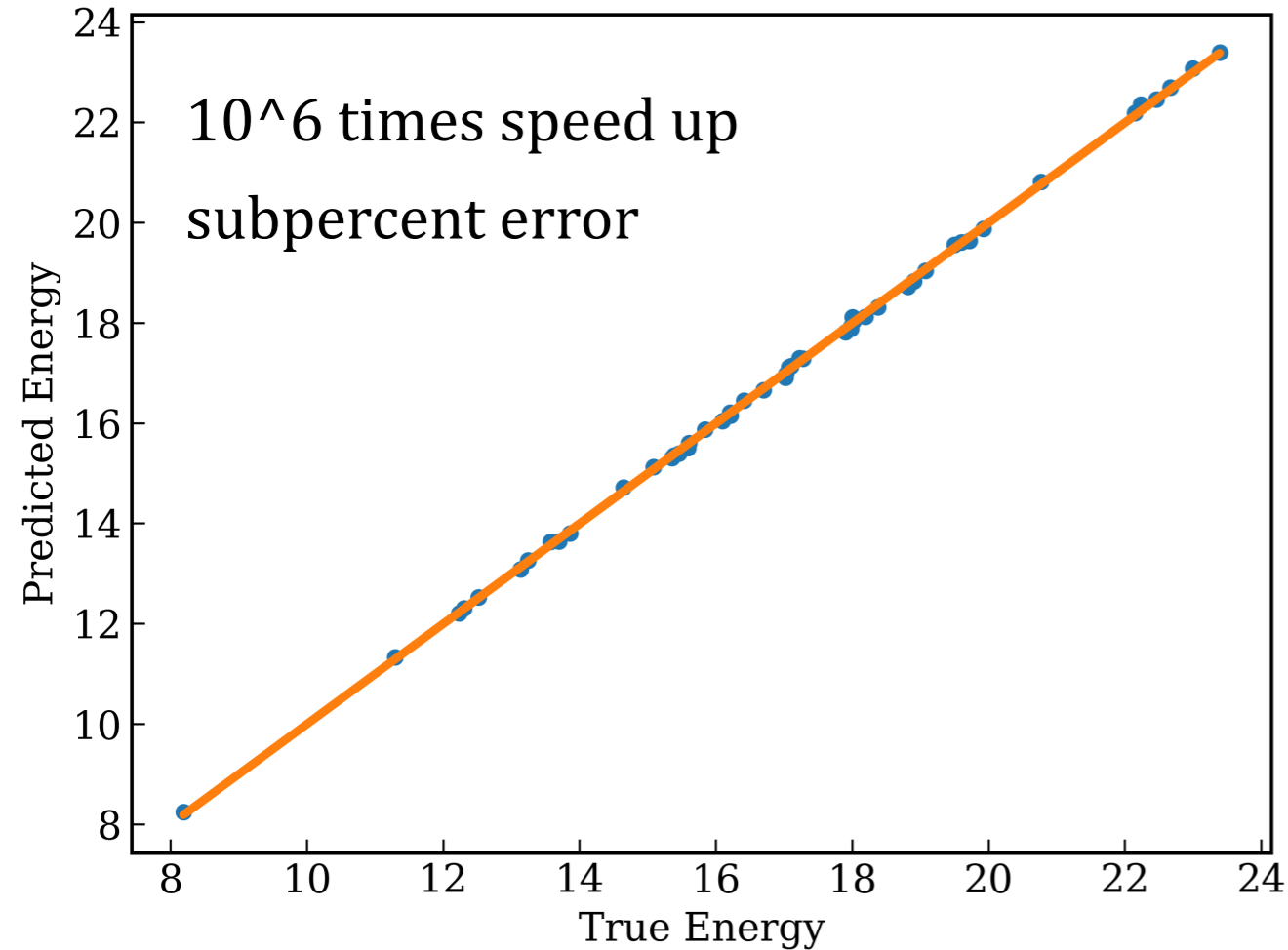
$$M(\{c_l\}) = \underline{M}_0 + \sum_{l=1}^p c_l \underline{M}_l$$

$$\begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{n1} & m_{n2} & \cdots & m_{nn} \end{bmatrix}$$

Infinite Dimensions in Many-Body Hilbert Space

Finite Dimensions in Learned Subspace

# Emulators - Preliminary Results



# 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)

We've constructed a fast and accurate emulator for the IMSRG framework based on a machine learning technique called parametric matrix model (PMM), which enables systematic propagation of nuclear interaction uncertainties to our EOS.

# Outlook

- More detailed uncertainty quantification at  $T = 0$  for different chiral EFT interactions with the PMM emulator
  - Bayesian analysis of EFT truncation errors (BUQEYE)
  - Comparison of different many body methods
- Provide astrophysical available ab initio EOS with tunable LECs using PMM emulator and reliable interpolators in both density and proton fraction
- 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



# Thank you for your attention!



# Introduction - Similarity Renormalization Group

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

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

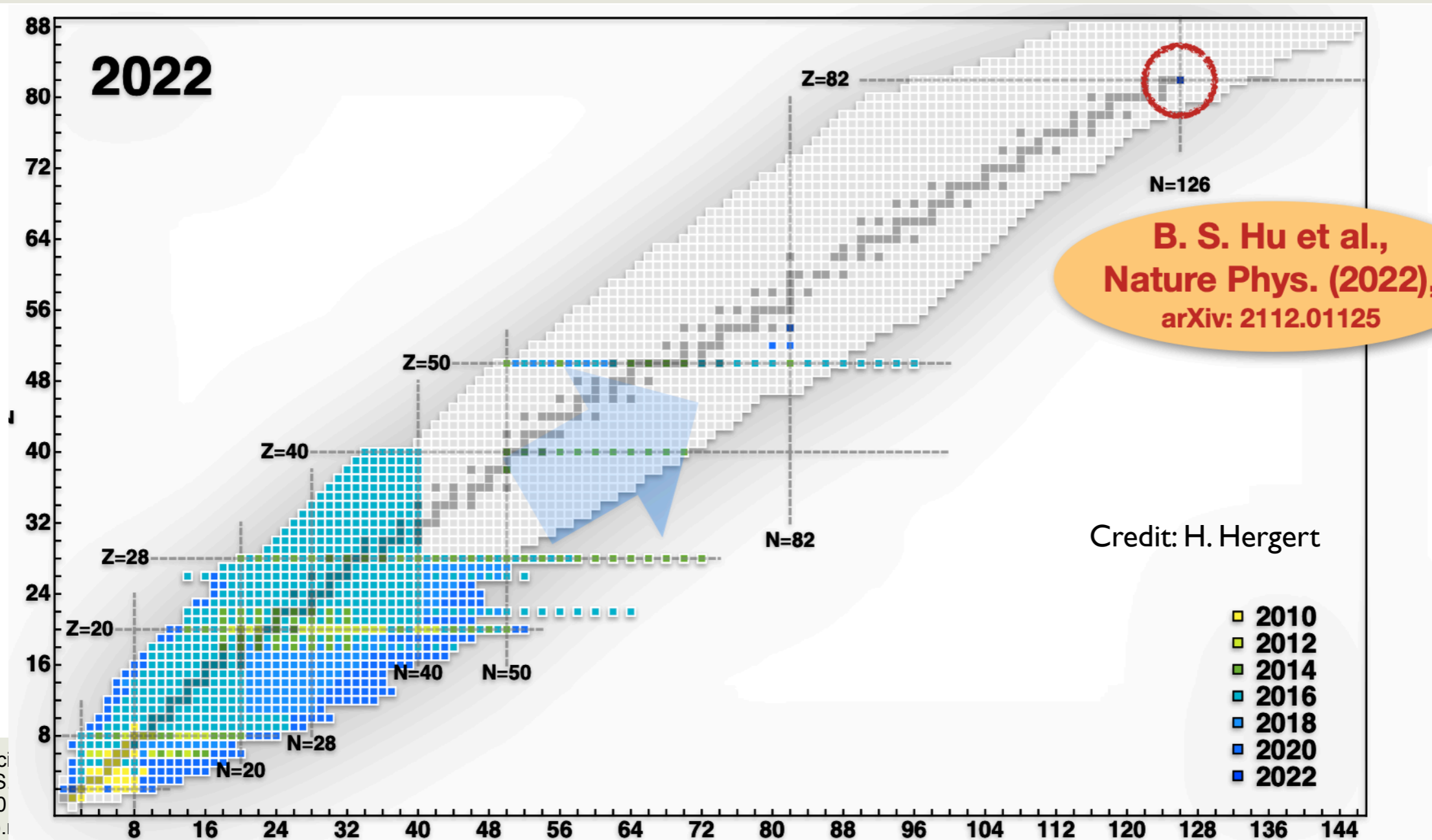
- choose  $\eta(s)$  to achieve desired behavior, e.g.,

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

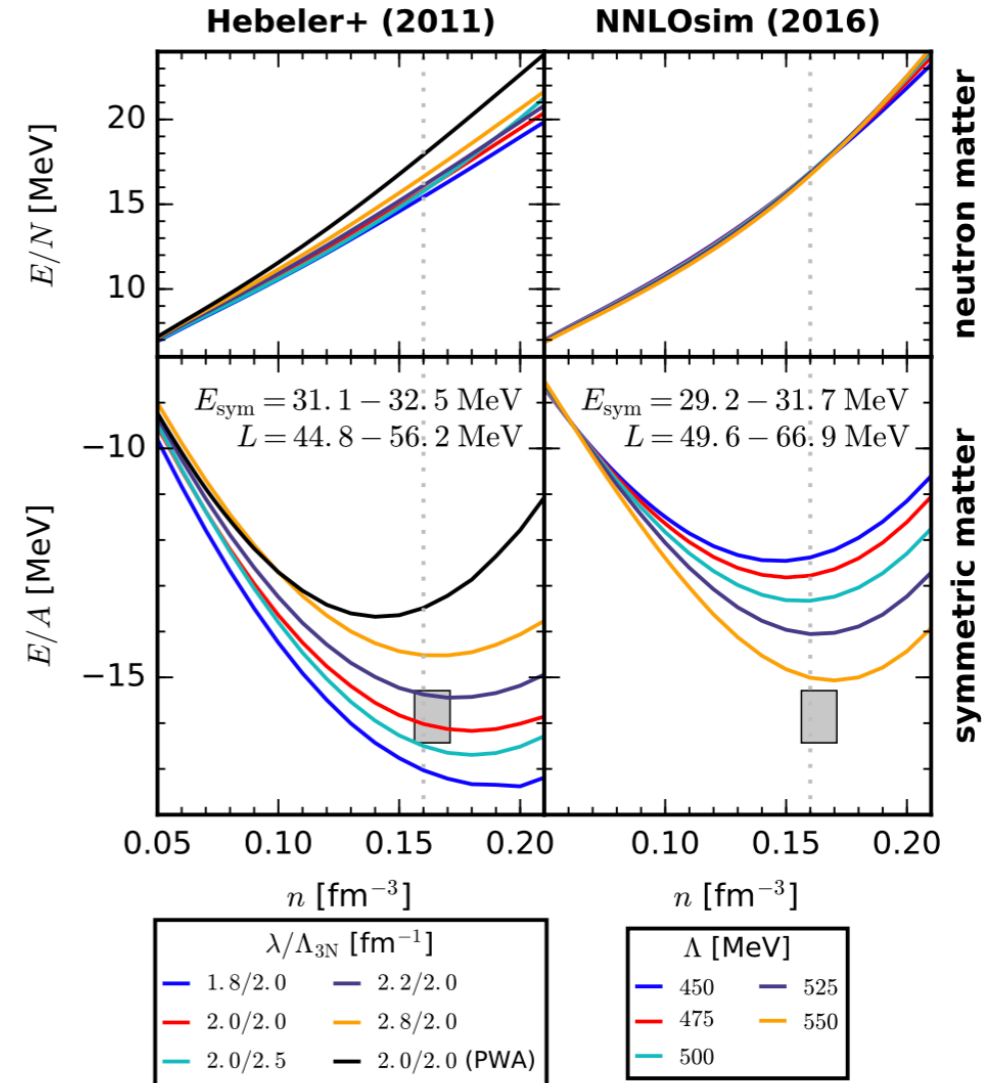
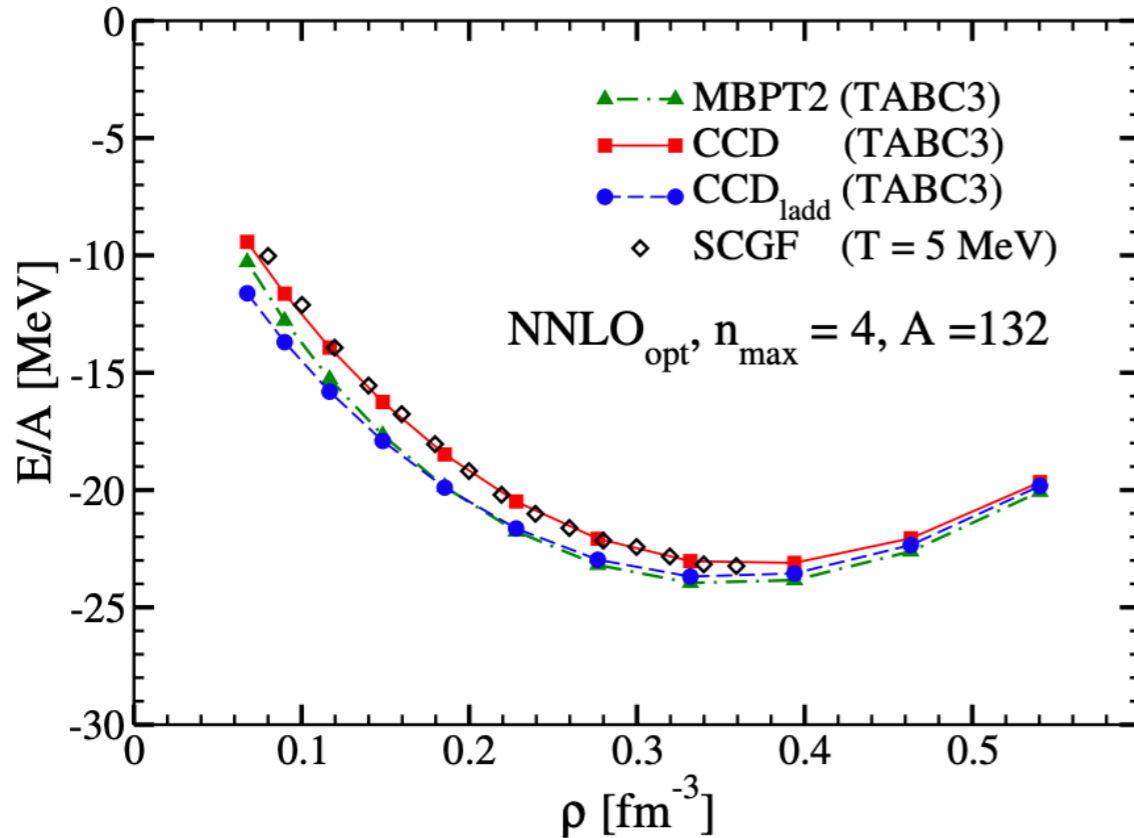
to **suppress** (suitably defined) **off-diagonal Hamiltonian**

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

# Introduction - Application of Ab Initio Methods in Nuclear Structure



# Introduction - Application of Other Ab Initio Methods in NM EOS



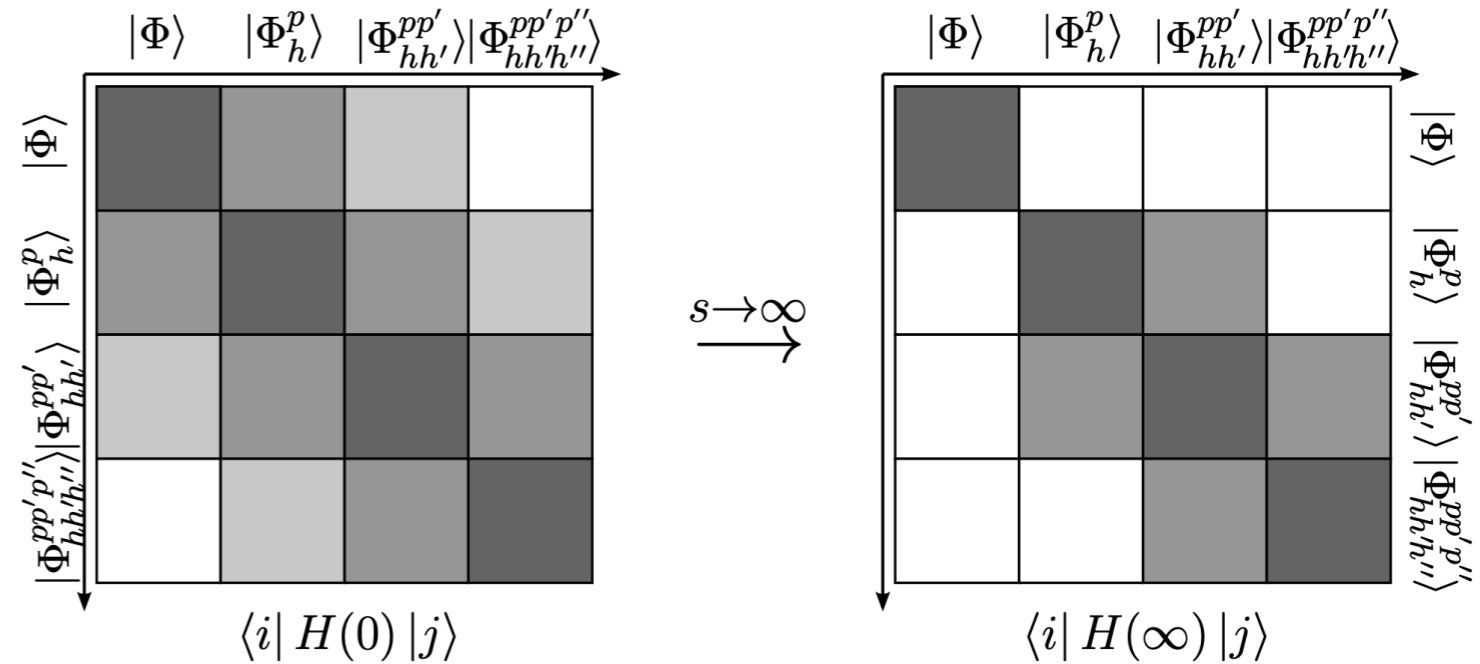
# Introduction - In-Medium Similarity Renormalization Group

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

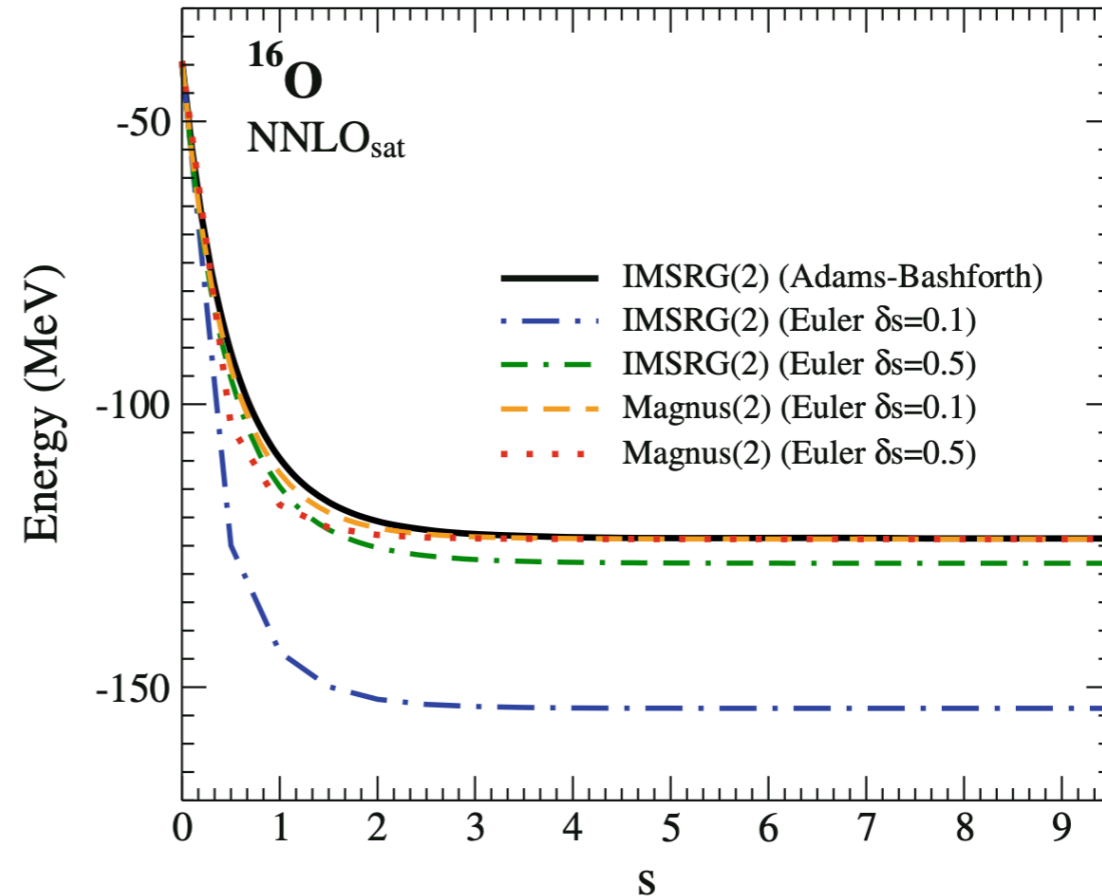
$$\hat{U}(s) \equiv e^{\hat{\Omega}(s)}$$

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

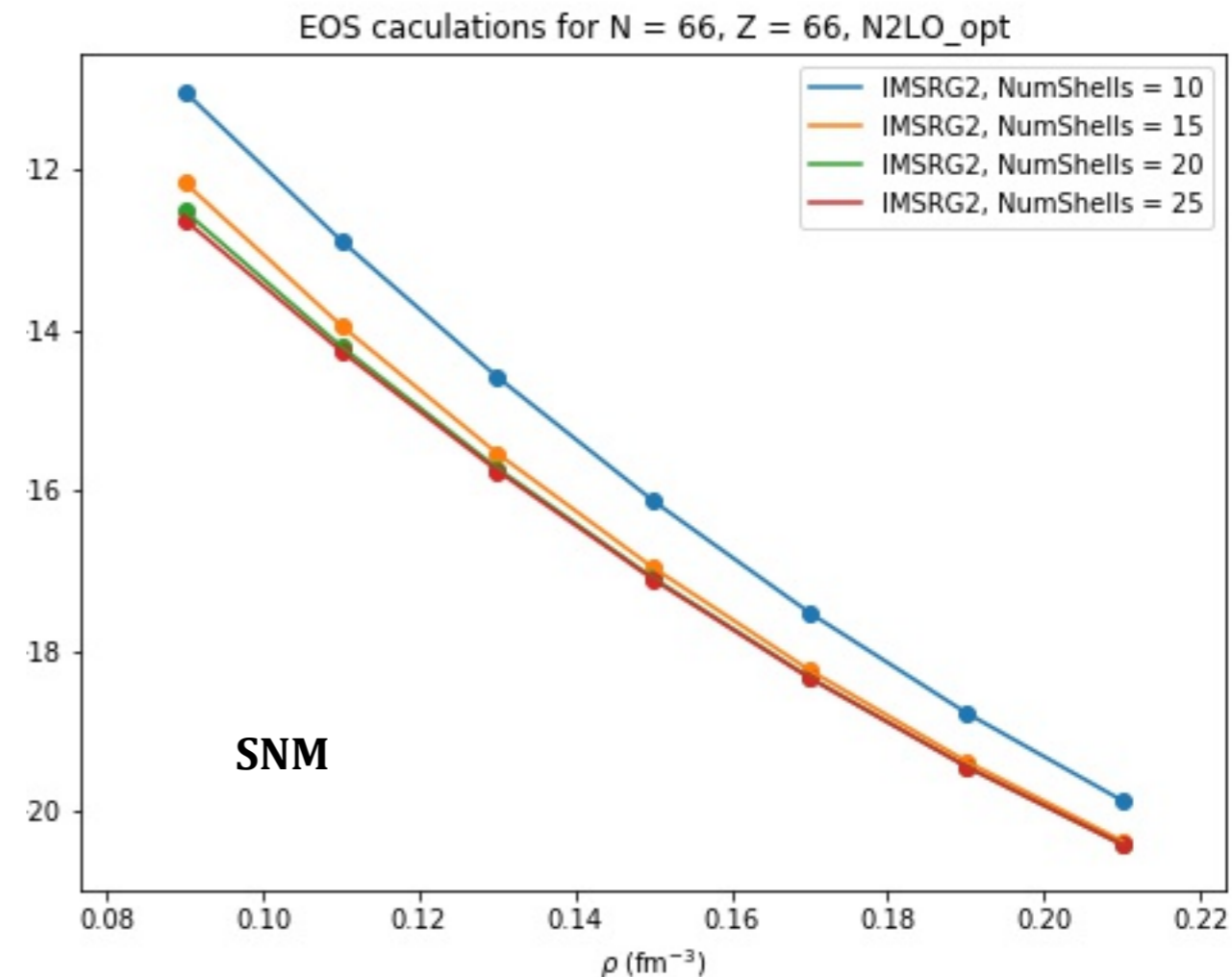
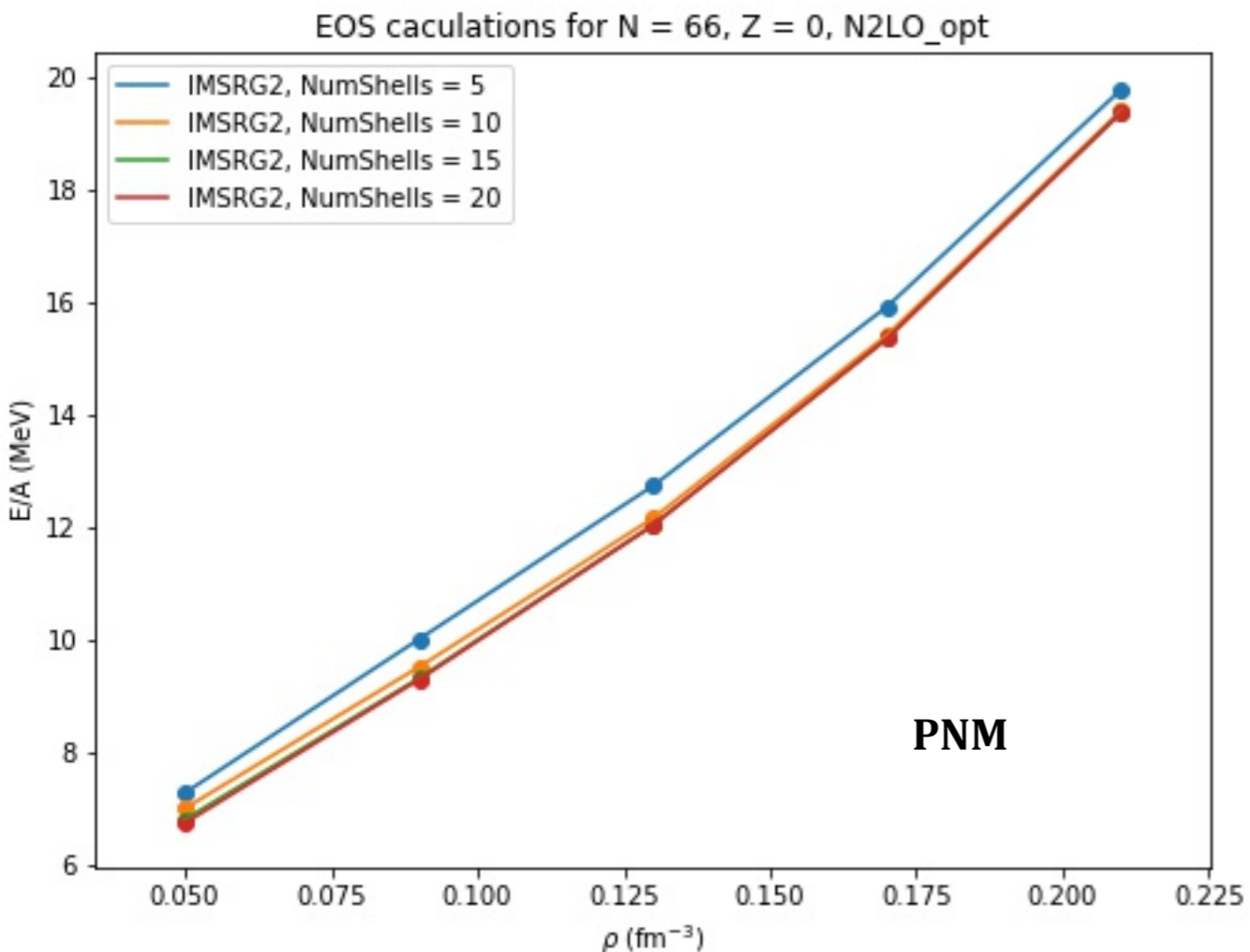
$$\text{ad}_{\hat{\Omega}}^0(\hat{\eta}) = \hat{\eta}$$

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

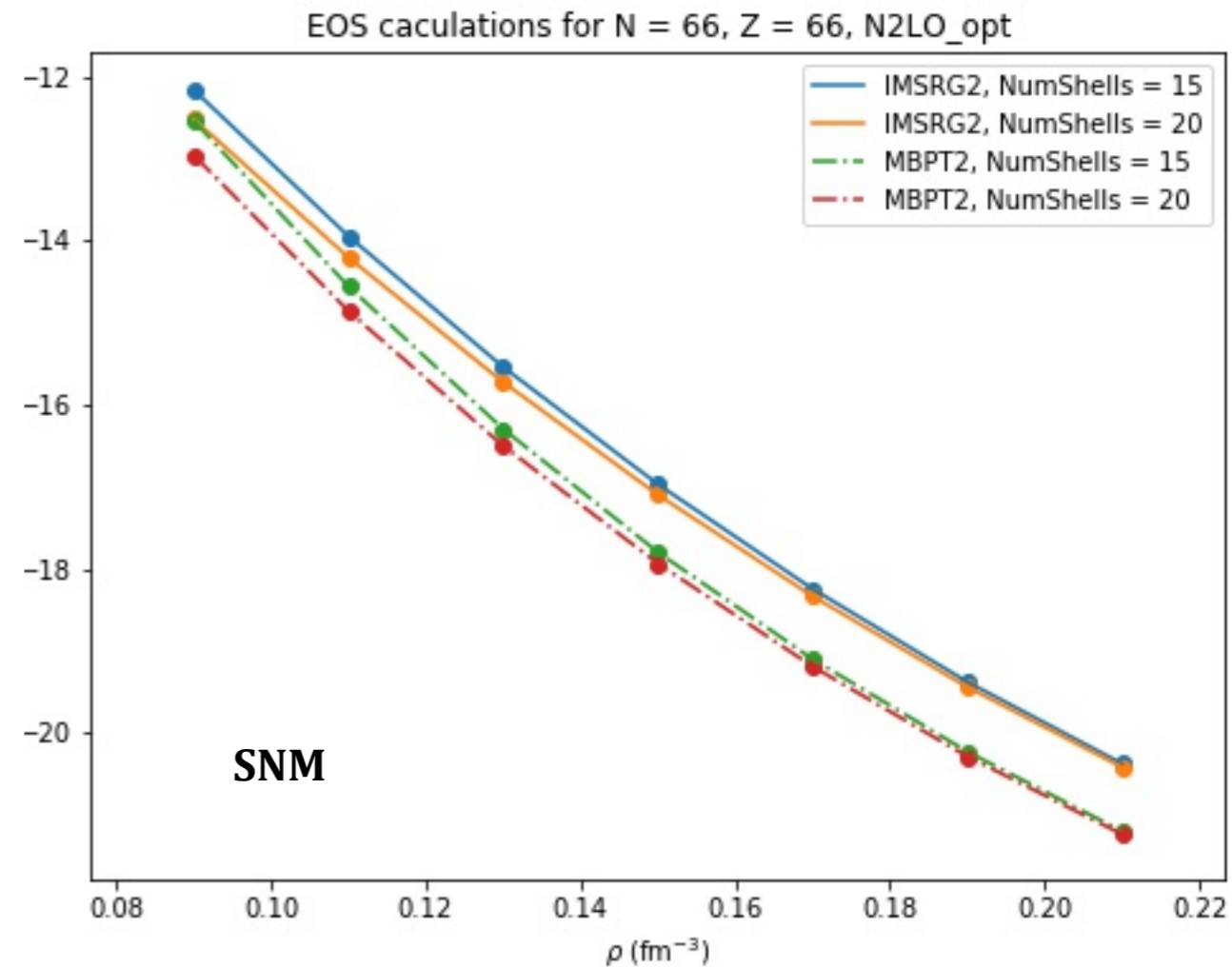
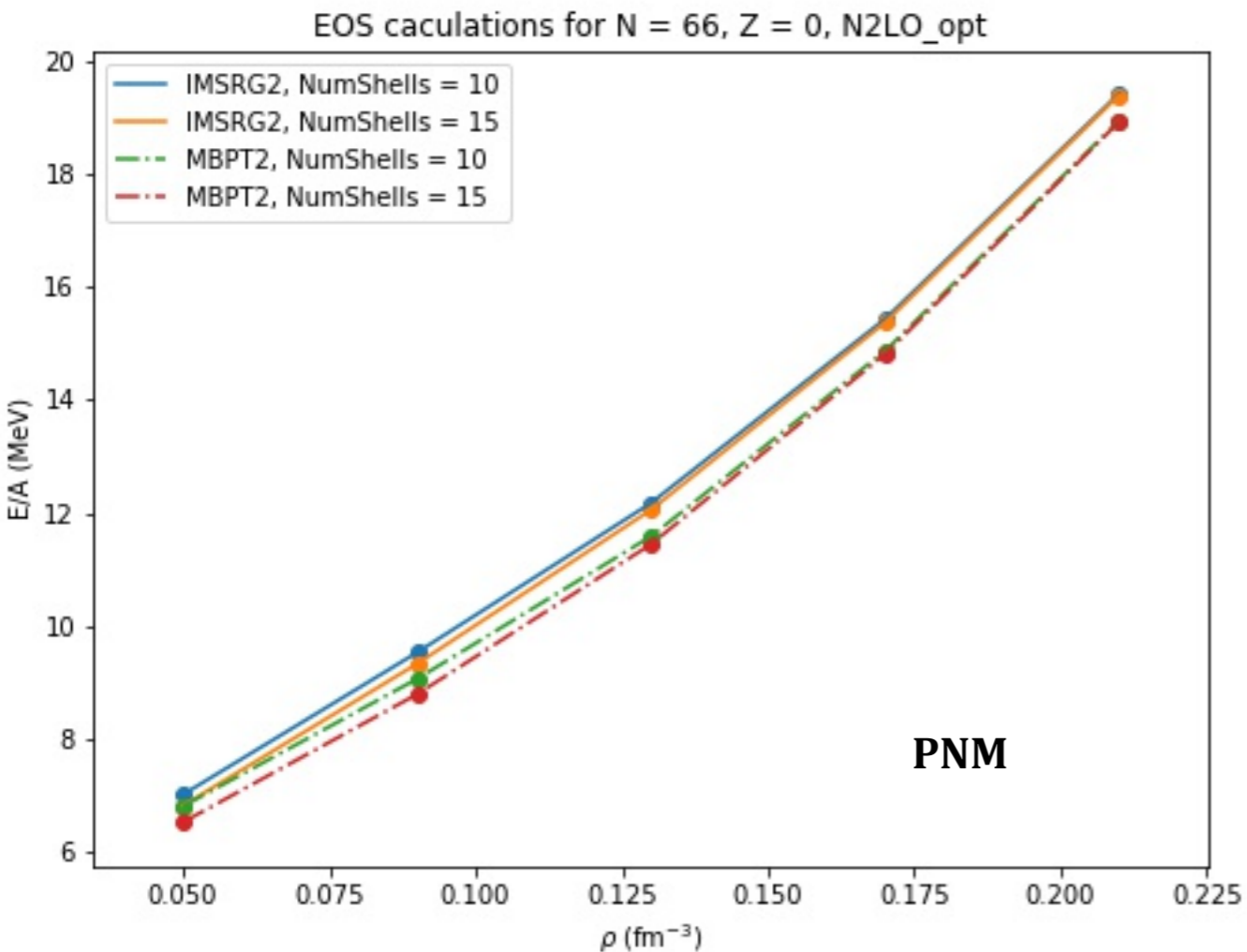
$$\hat{H}(s) \equiv e^{\hat{\Omega}(s)} \hat{H}(0) e^{-\hat{\Omega}(s)} = \sum_{k=0}^{\infty} \frac{1}{k!} \text{ad}_{\hat{\Omega}(s)}^k(\hat{H}(0))$$



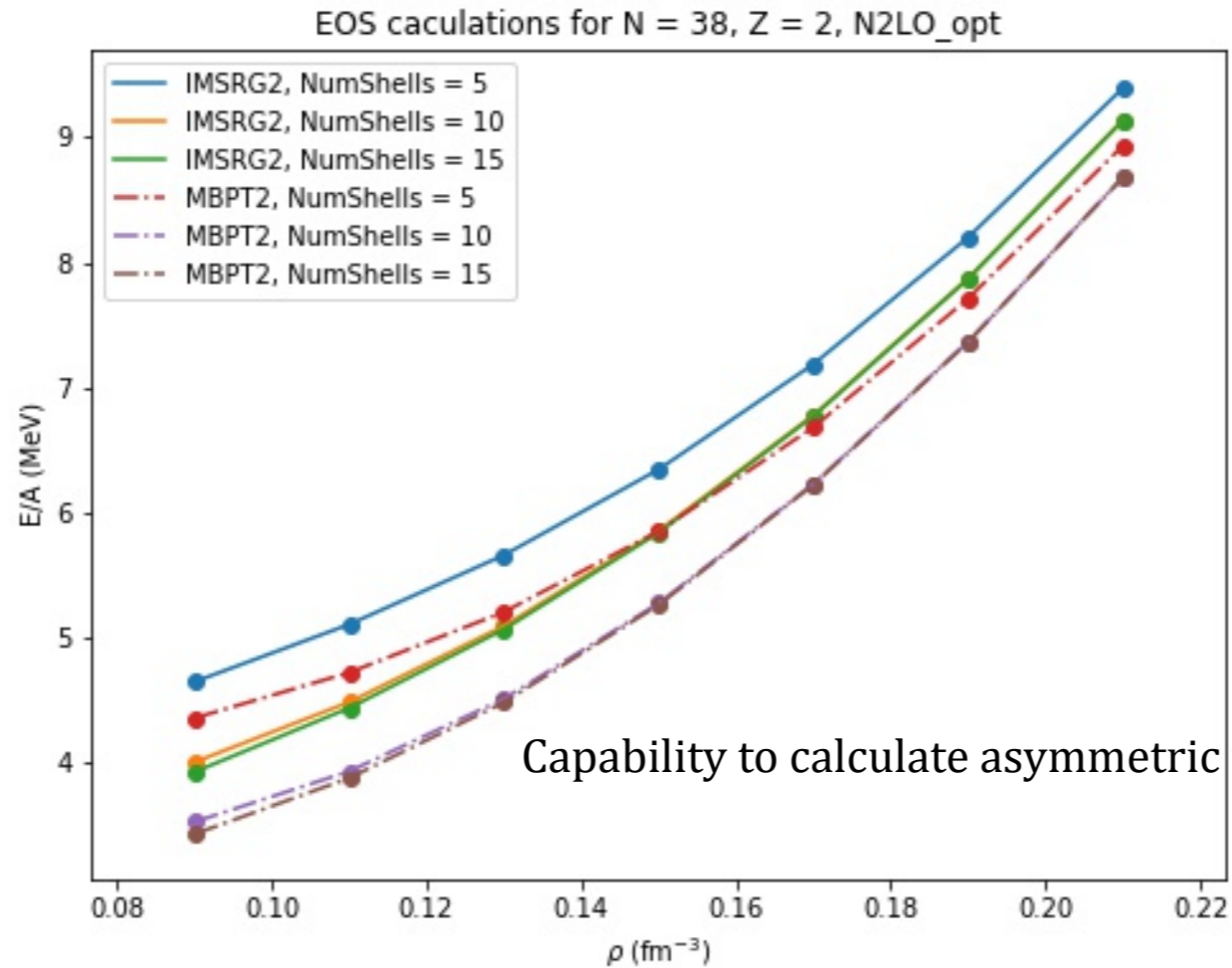
# Results - Basis Convergence



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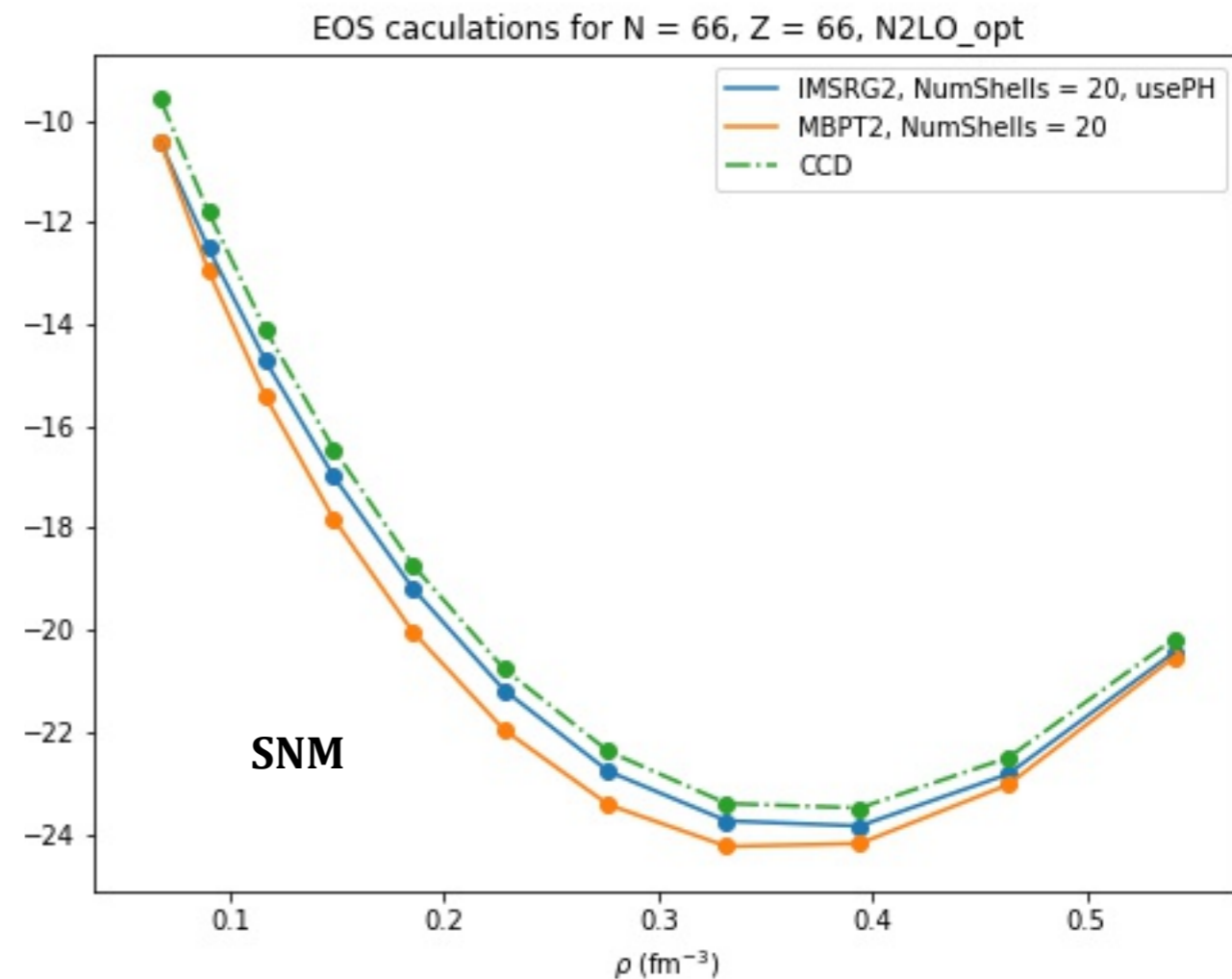
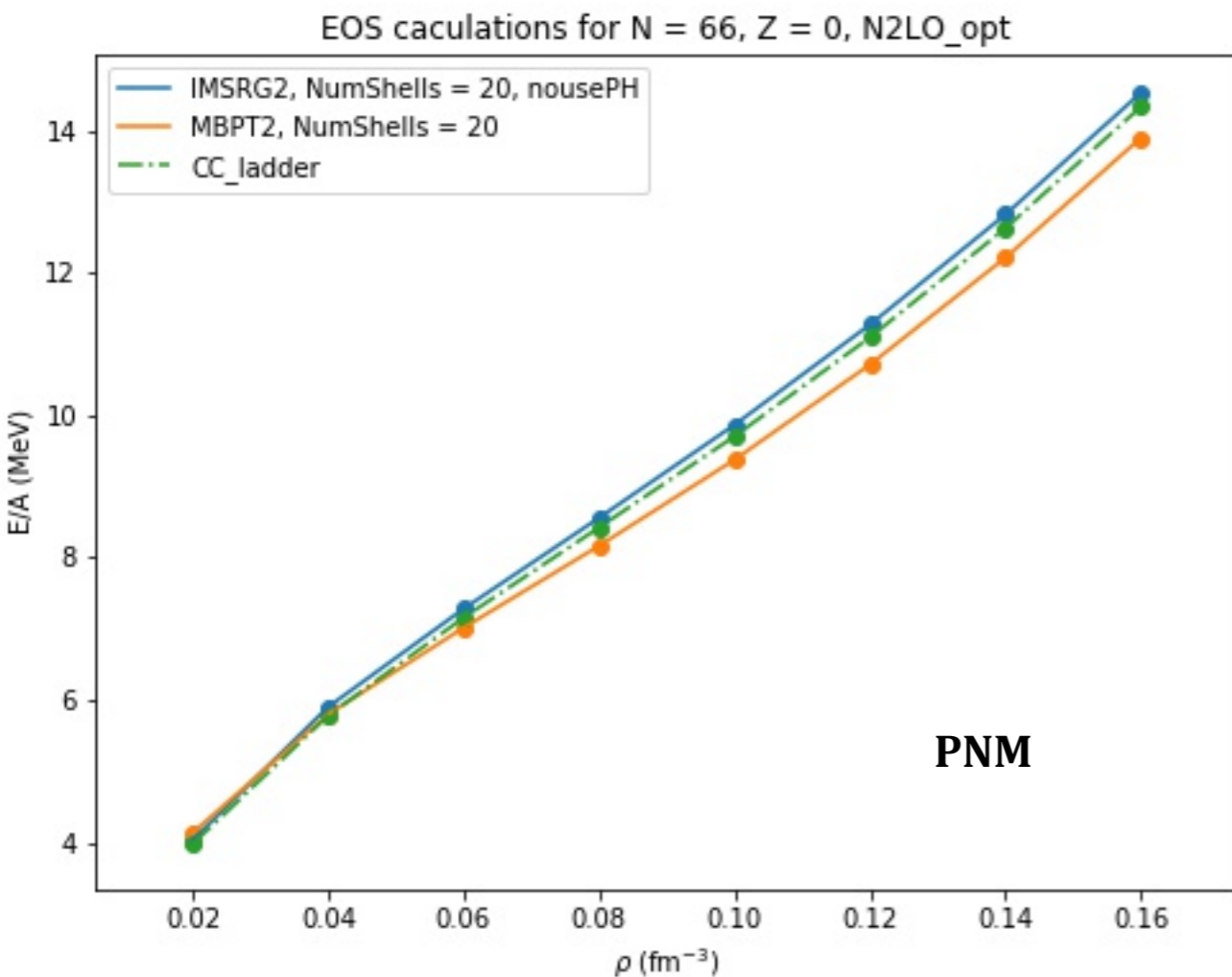


# Results - Basis Convergence

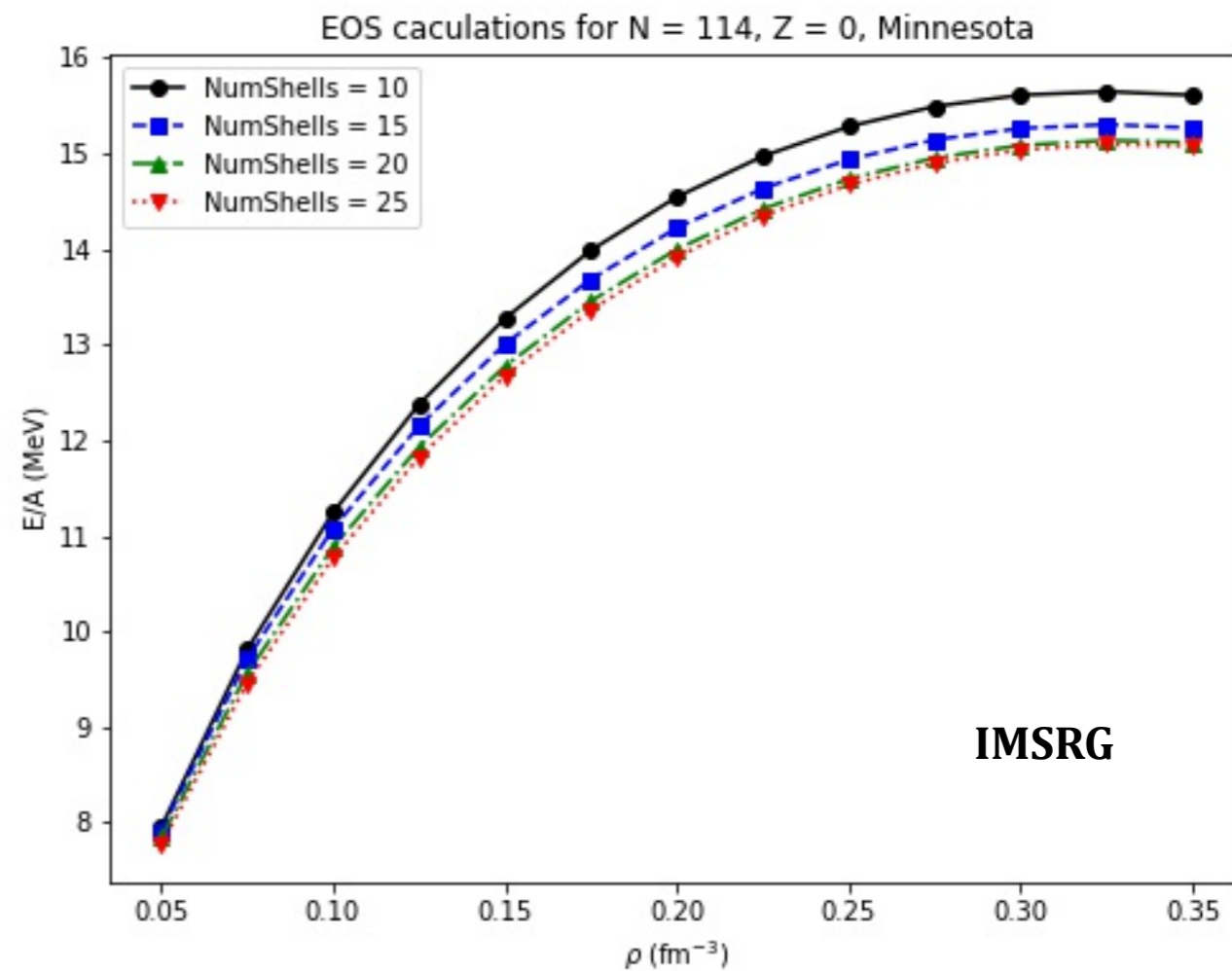
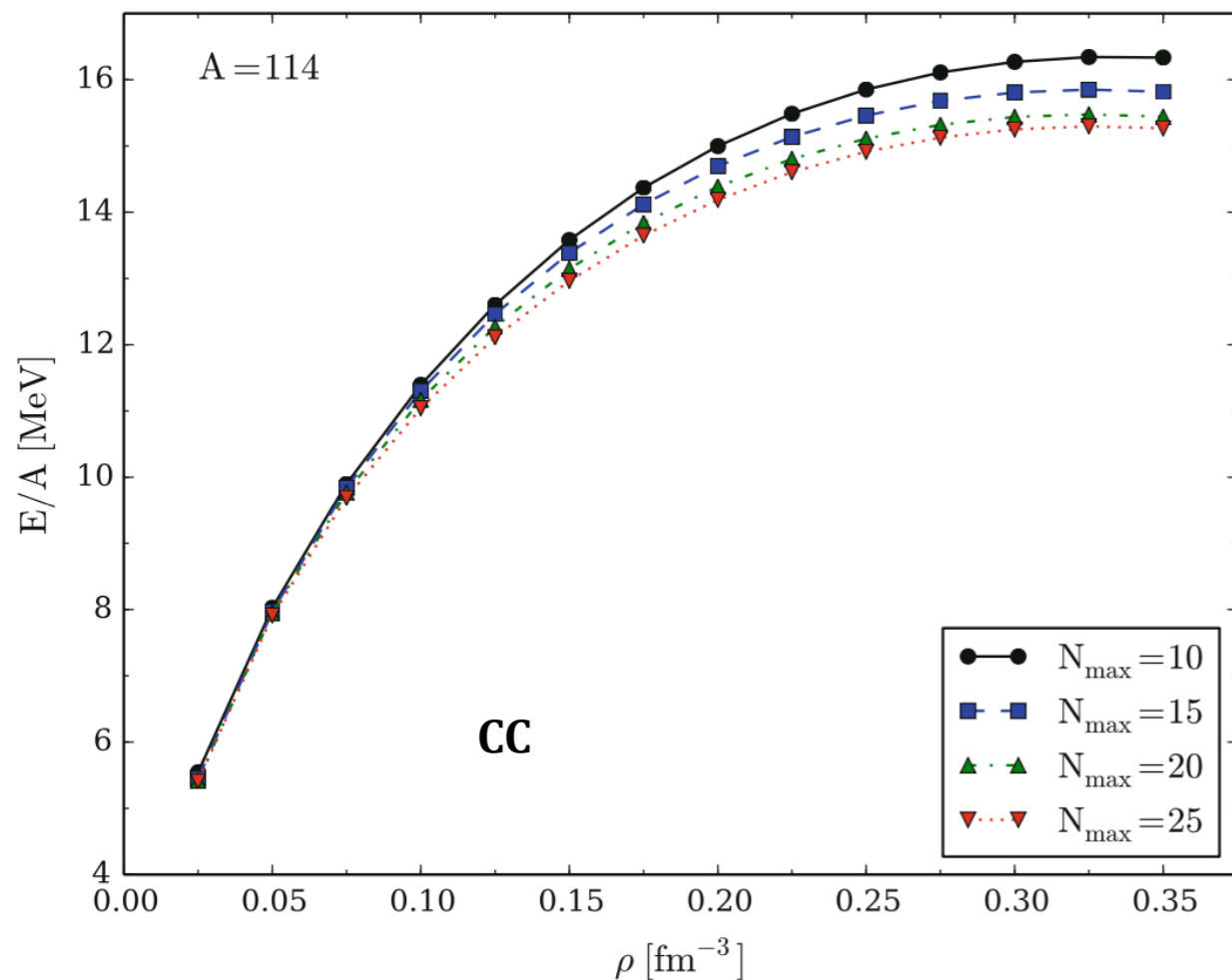


Capability to calculate asymmetric matter, proton fraction = 0.05

# Results - Benchmark

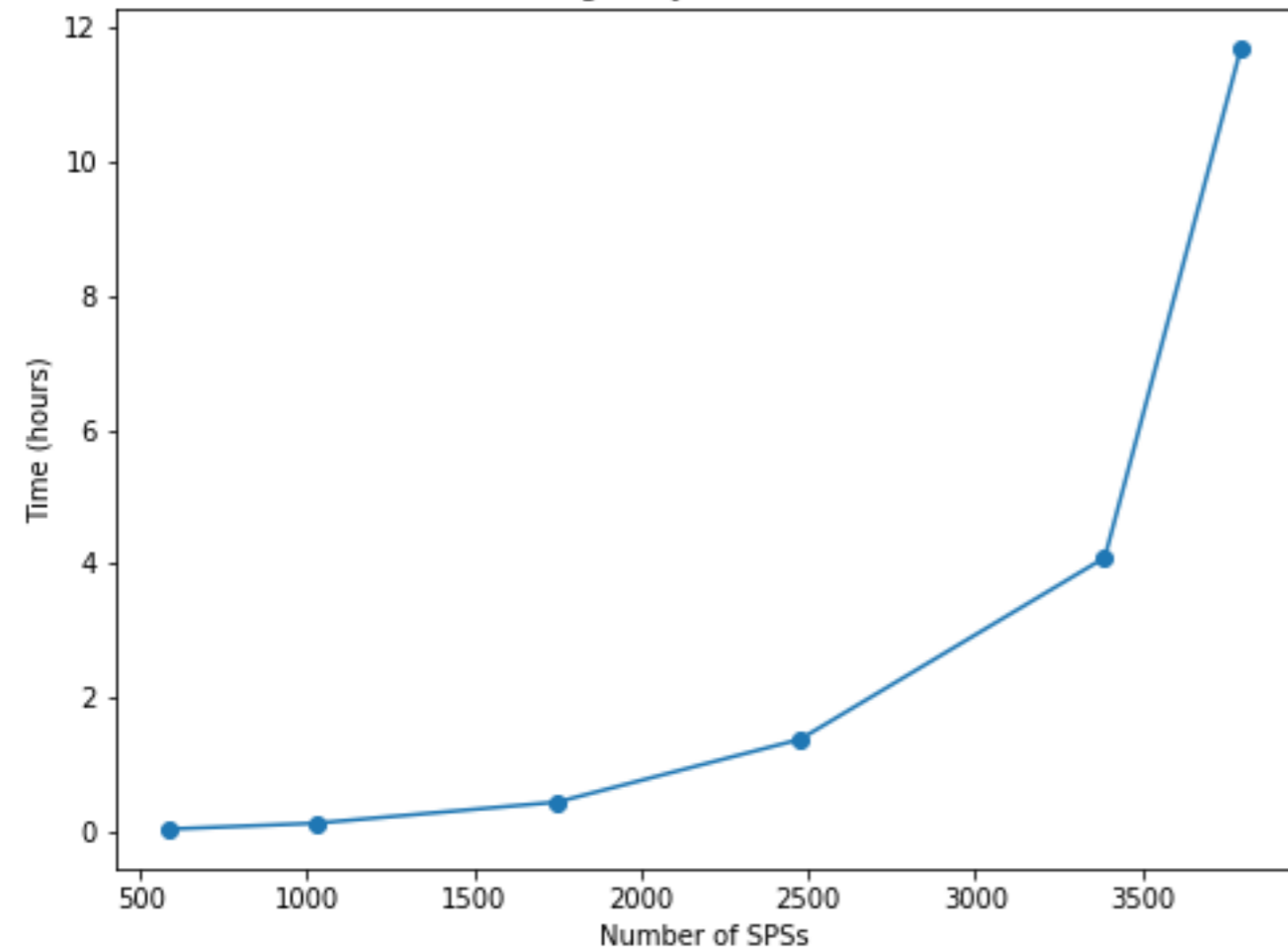


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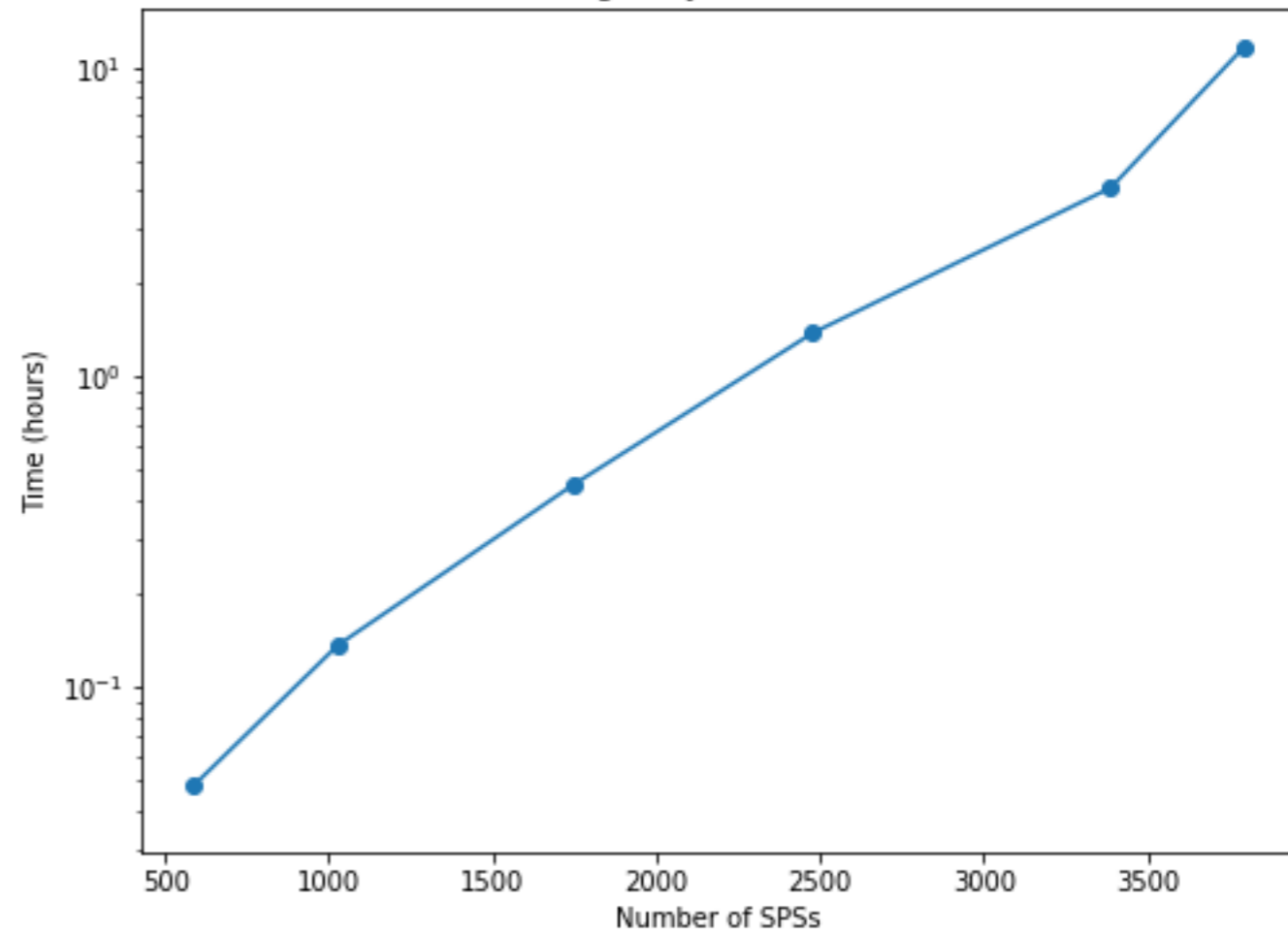


# Results - Scaling

Runtime Scaling of Symmetric Nuclear Matter

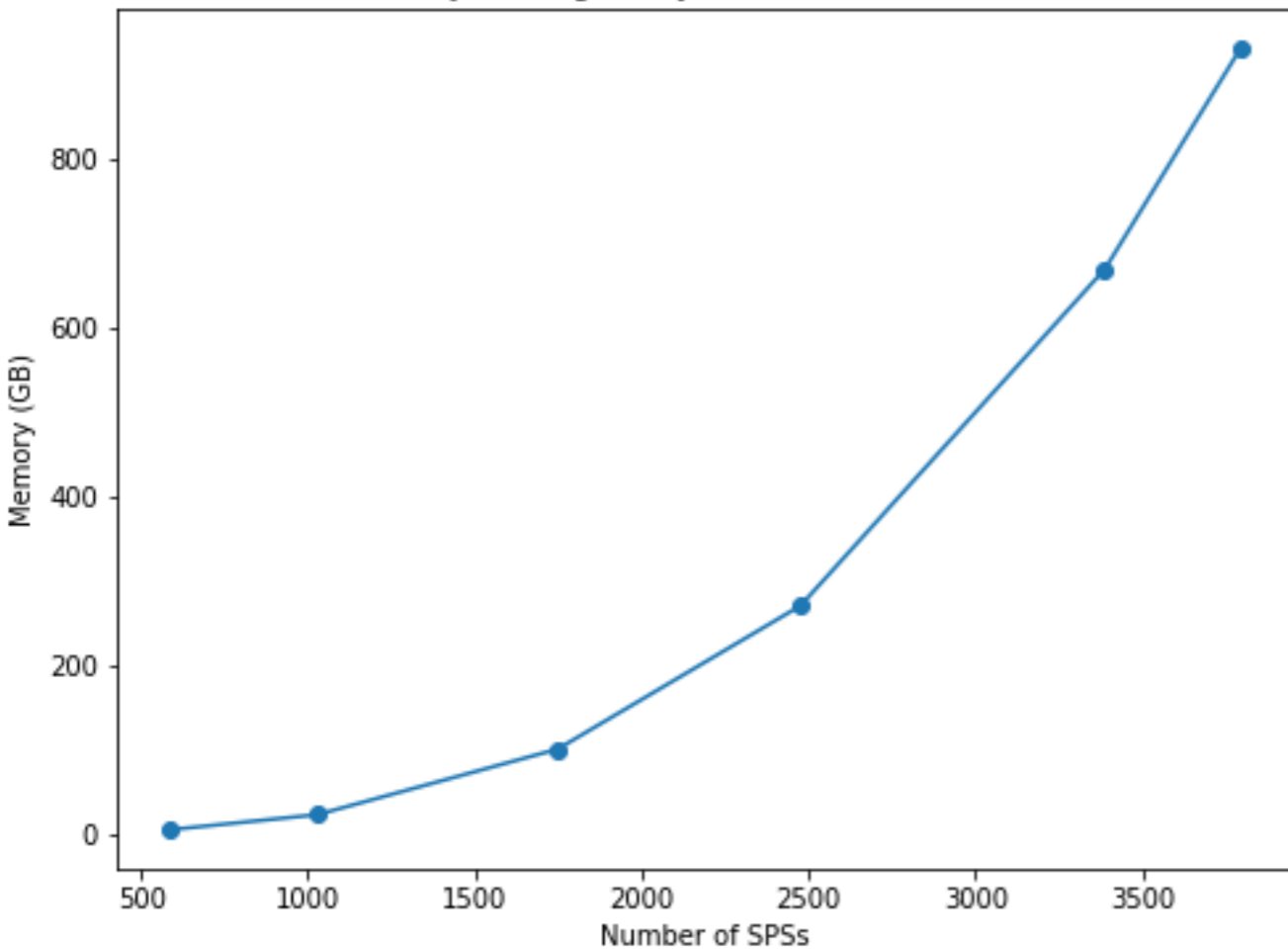


Runtime Scaling of Symmetric Nuclear Matter

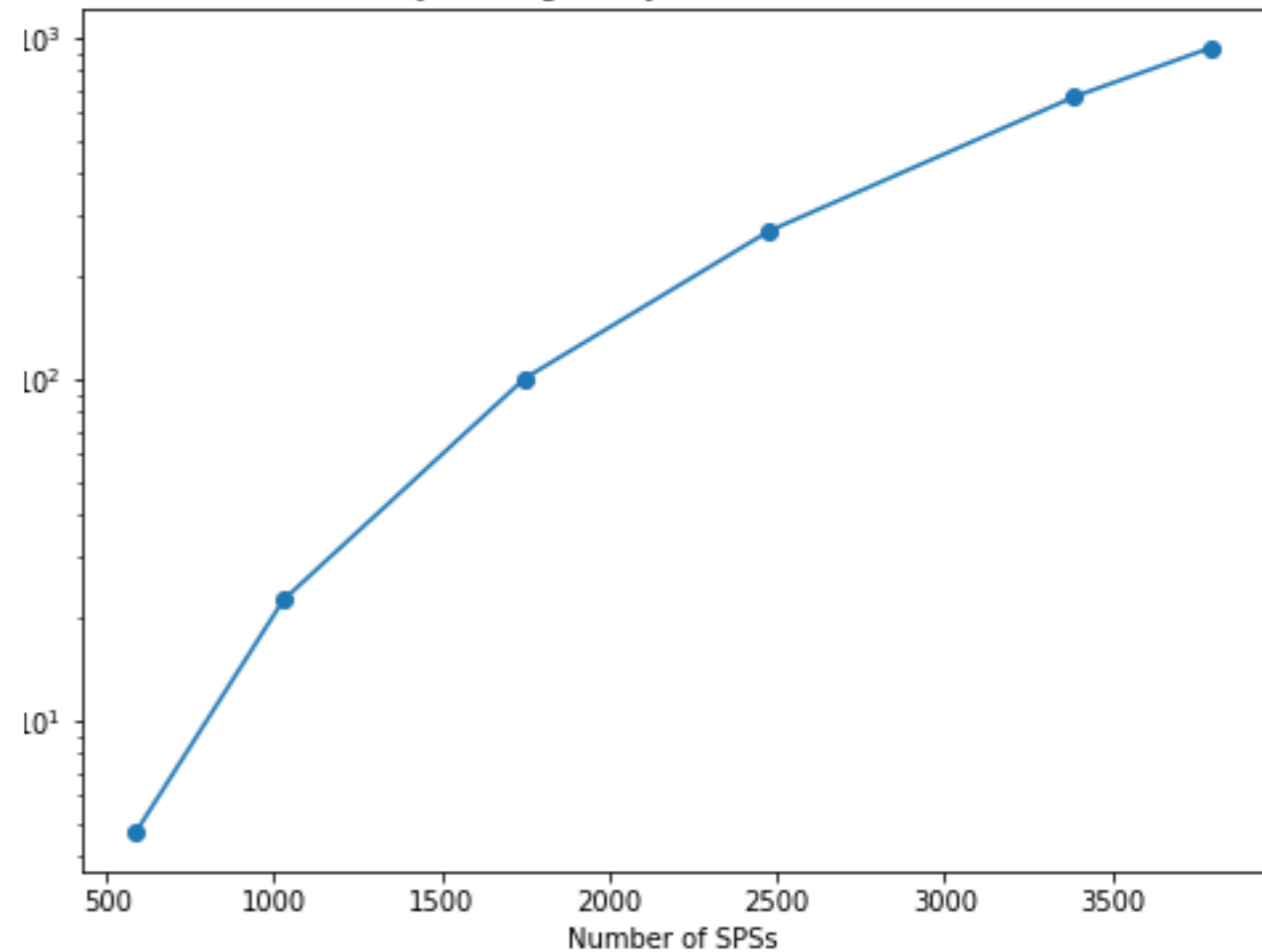


# Results - Scaling

Memory Scaling for Symmetric Nuclear Matter



Memory Scaling for Symmetric Nuclear Matter



# Results - Finite Size Effect

