Analyzing the nuclear interactions: challenges and new opportunities

Maria Piarulli—Washington University, St. Louis

August 9-10, 2022

Ab initio calculations of nuclear systems

Goal: develop a predictive understanding of nuclei and nucleonic matter in terms of the interactions between individual nucleons and external probes

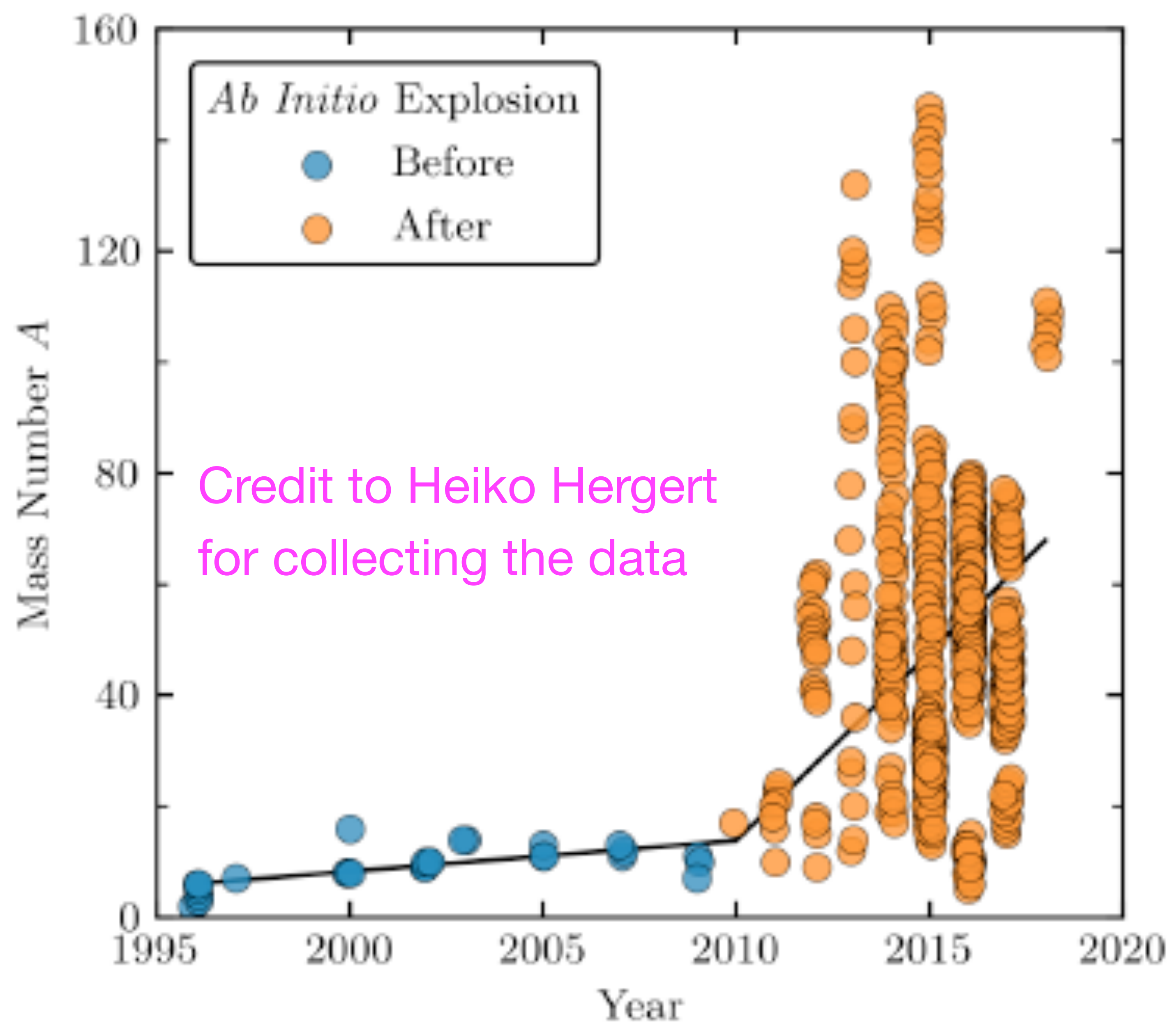
Two and many-body interactions:

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j=1}^{A} v_{ij} + \sum_{i<j<k=1}^{A} V_{ijk} + ...$$

Electroweak current operators:

$$j^{\mathrm{EW}} = \sum_{i=1}^{A} j_i + \sum_{i<j=1}^{A} j_{ij} + \sum_{i<j<k=1}^{A} j_{ijk} + ...$$

Ab-initio methods: solve the nuclear many-body problem:



- Improved and novel many-body frameworks
- Increased computational resources
- Nuclear interactions and currents based on EFTs
- Theoretical uncertainty quantification

Nuclear Interactions, Nuclei, and Infinite Matter

Challenge: consistent description of BEs, radii, saturation properties of NM, EoS of PNM, EW properties….

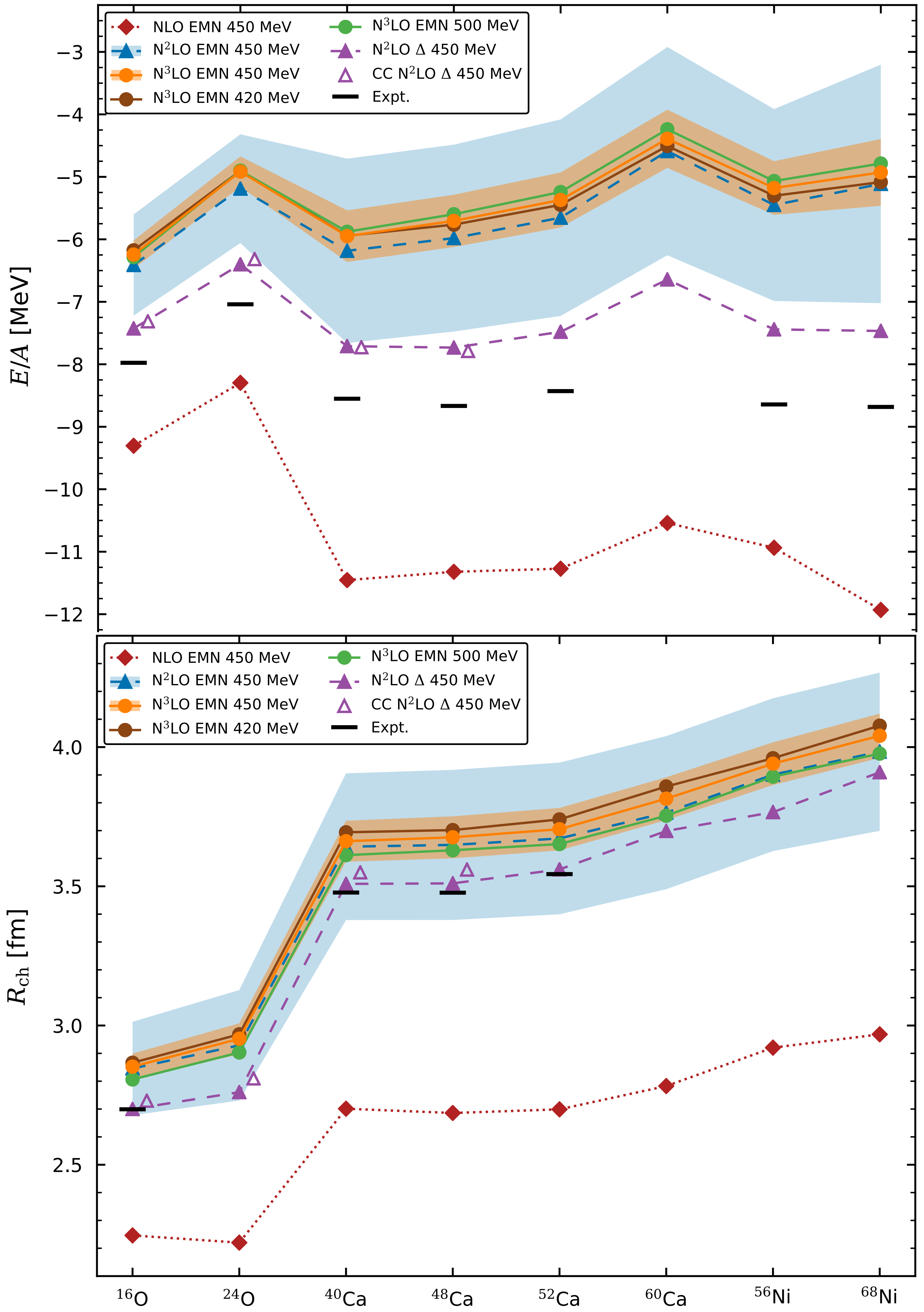


Fig.1

Fig.1

- IM-SRG calculations**
- NN (N3LO)**+3N (N3LO)**
- 3N fitted to 3H b.e. + saturation region NM at Λ=420**, 450**, 500** MeV
- Underbound g.s. energies and radii too large

Entem *et al.*, PRC **96, 024004 (2017)
Hoppe et al., PRC **100, 024318 (2019)

Fig.2

- IM-SRG calculations**
- NN (N3LO)**+3N (N3LO)**
- 3N fitted to 3H and 16O g.s. energies at Λ=450, 500, and 550** MeV
- Unable to satisfy NM saturation**

Huther *et al.*, PLB **808, 135651 (2020)
Sammarruca et al., PRC **102, 034313 (2020)

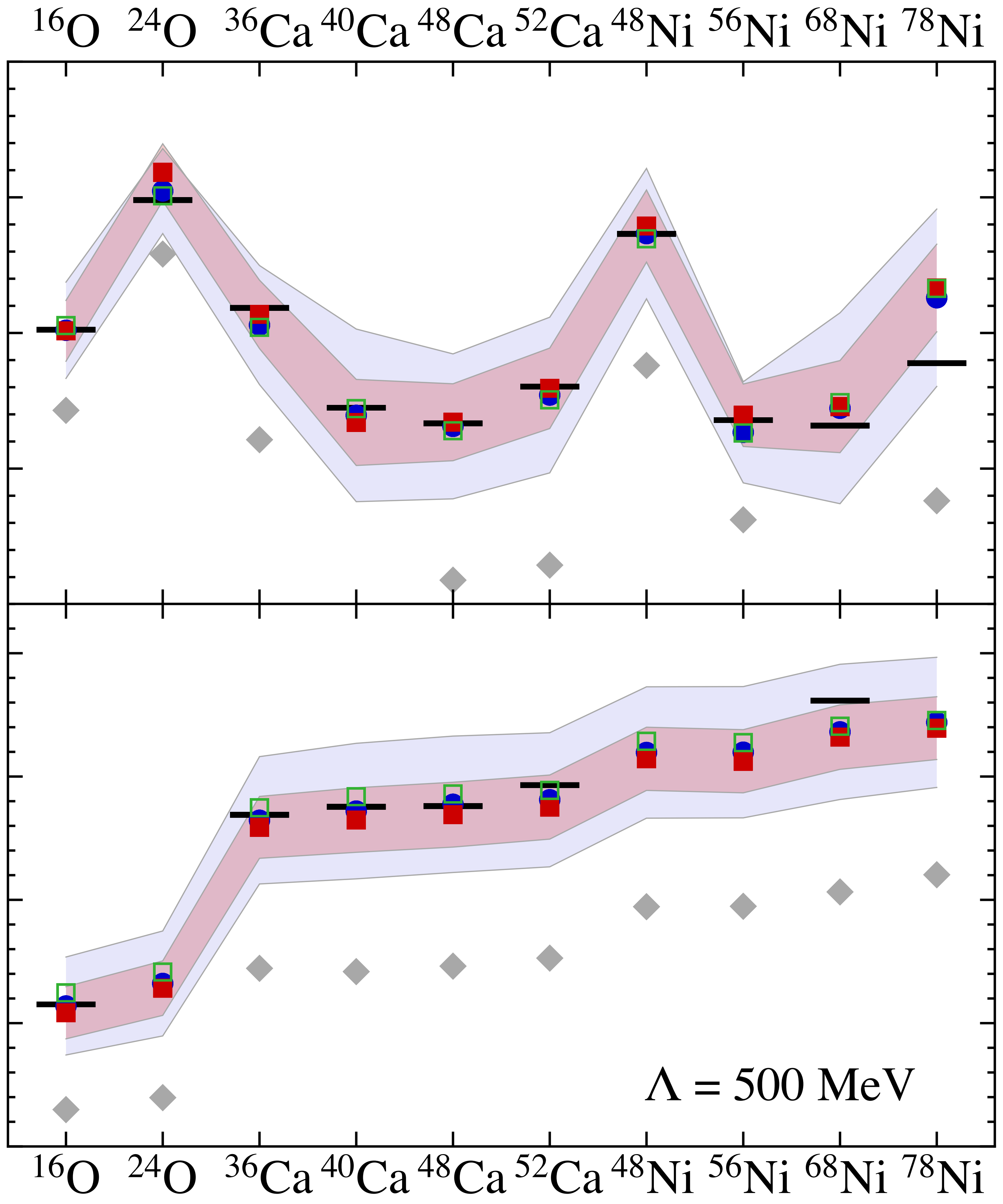


Fig.2

Success: increased many-body capability, algorithms under control

Issue: largest uncertainty from input Hamiltonian; a deeper and more quantitative understanding of the connection between properties of matter and finite nuclei is still lacking

How we are contributing to this grand-challenge….

- **Theoretical formulation and optimization of models for nuclear interactions (and corresponding electroweak currents—S. Pastore) using effective field theories**
  - Inclusion of Bayesian methods to develop and improve order-by-order NN minimally non-local/local pion-less, delta-less, delta-full models
  - Inclusion of subleading 3N contributions with emphasis on 3N contact interactions—relevant for 3N scattering observable
- **Implementation of chiral models in Quantum Monte Carlo methods for:**
  - Calculations of binding energies, radii, electroweak transitions, muon captures, EM form factors,…, in light nuclei up to A=12—validation of the models
  - Calculations of spacial densities/momentum distributions/spectroscopic overlaps—relevant to understand short range correlations, generate better spectral functions for neutrino-nucleus scattering,..
  - Studies of neutrino scattering and neutrinoless double beta decay (S. Pastore)—where data are scarce or not available
  - Calculations of the EoS of nucleonic matter with focus on different aspects of the 3N force
- **Extension of QMC methods to larger nuclei: major new wave function advances extended to A=11, 13 – 14 nuclei**
- **QMC ab initio calculations provide an important benchmark to test other computational methods that can be extended to the heavy nuclei**

NN interactions: MCMC Implementation and its application

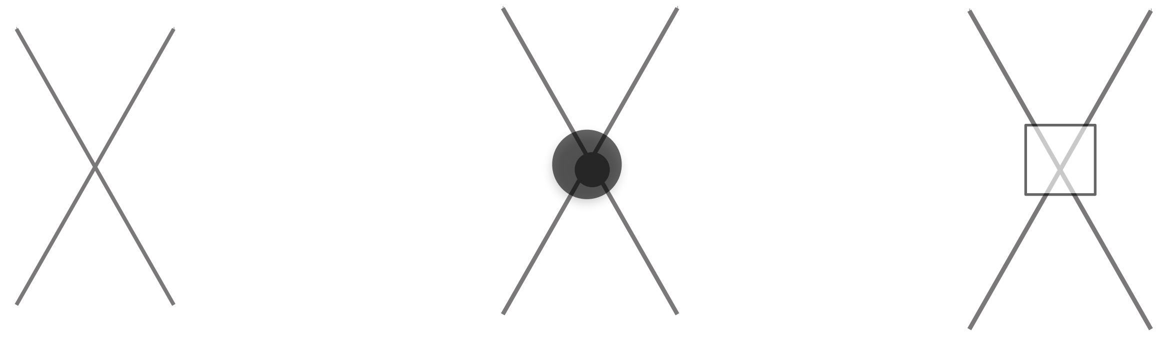
Jason Bub

Summer 2022
BAND Fellowship

- Implementing Bayesian statistics, we can efficiently sample the parameter space to extract the posterior distribution: $\mathrm{pr}(\mathbf{a}|\mathrm{Data}, I) \propto \mathrm{pr}(\mathrm{Data}|\mathbf{a}, I) \times \mathrm{pr}(\mathbf{a}|I)$

  posterior — likelihood $\propto e^{-\chi^2(\mathrm{a})/2}$ — prior

- We are working (for now) with a “simpler case”: only local short-range interactions



CI: 2 LECs 7 LECs 15 LECs

$$v_{\mathrm{LO}} = v_{\mathrm{LO}}^{\mathrm{CI}} + v^{\mathrm{EM}}$$
$$v_{\mathrm{NLO}} = v_{\mathrm{LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CD}} + v^{\mathrm{EM}}$$
$$v_{\mathrm{N3LO}} = v_{\mathrm{LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CI}} + v_{\mathrm{N3LO}}^{\mathrm{CI}} + v_{\mathrm{NLO}}^{\mathrm{CD}} + v_{\mathrm{N3LO}}^{\mathrm{CD}} + v^{\mathrm{EM}}$$

- To do so, we:
  - are using our existing codes written in Fortran to calculate the likelihood from NN scattering data (thousands of data available)
  - are using a MCMC package for the fitting: emcee package in Python (zeus to be tried!), schwimmbad for distributed computation (MPI)
  - are using f2py to convert Fortran into a Python module

Emulation of observable calculations

Jason Bub

Summer 2022
BAND Fellowship

Challenge:

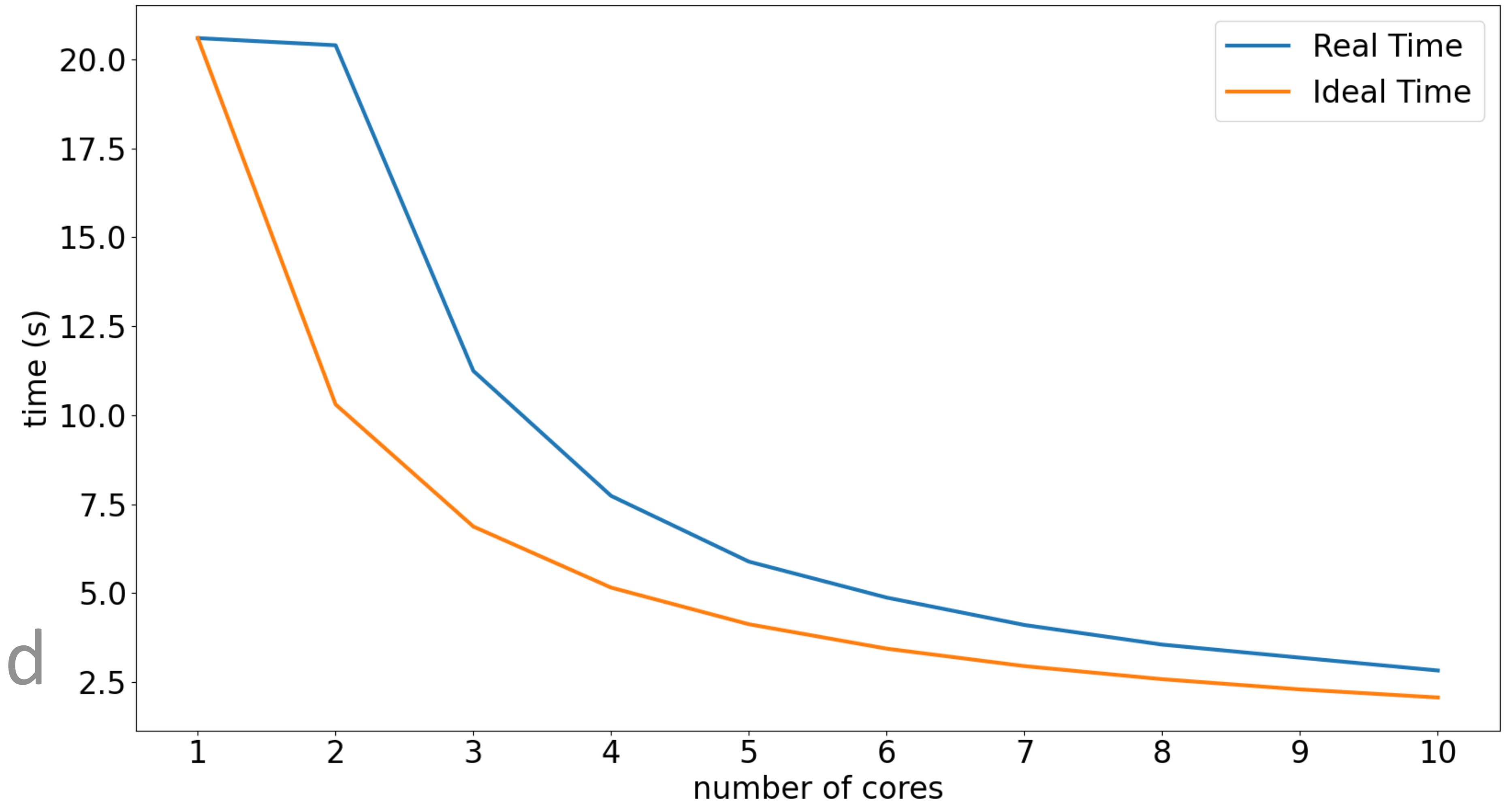
- A full Bayesian treatment requires millions of samples:
  - Likelihood calculation respect to NN data relatively expensive

    Serial likelihood calculation -> slow propagation

  - Improvement route: Parallel likelihood calculation

    Upsides:
    ✓ Quicker propagation
    ✓ Ability to leverage more resources

    Downsides:
    ✤ Inefficiencies due to MPI overhead and need for non-computing master processes



Opportunity:

- Solution: Emulation
  - Use surmise from BAND Collaboration
  - Easier to emulate residuals than observables

Bayesian Analysis of Nuclear Dynamics

Ozge Surer

Stefan Wild

Matt Plumlee

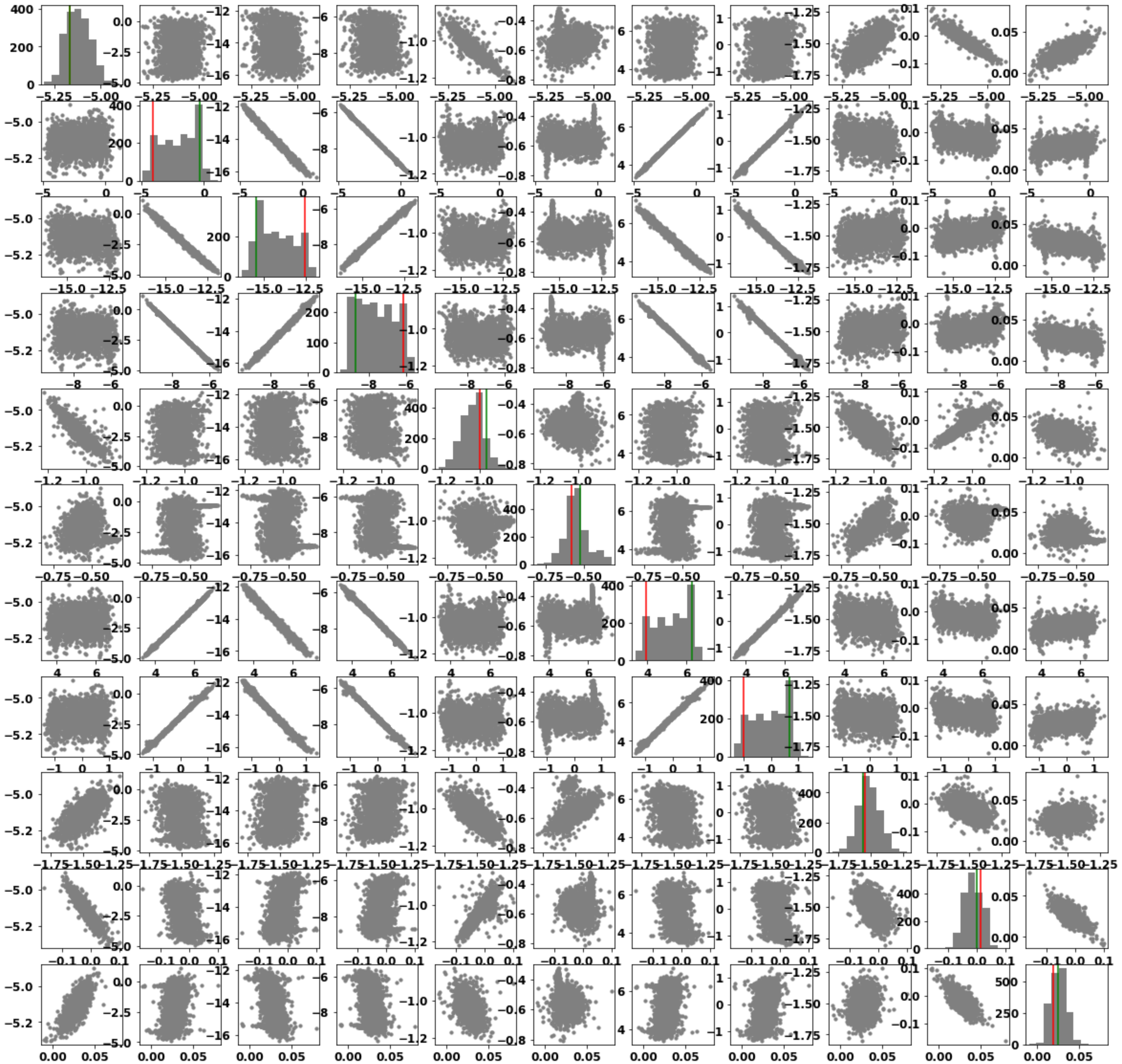
Emulator results

Steps for emulation:

- Generate training dataset
  - Start with POUNDerS optimization
- Train Gaussian Process emulator
- Validate emulator

Promising steps at NLO

Preliminary!!!



Emulation: How To

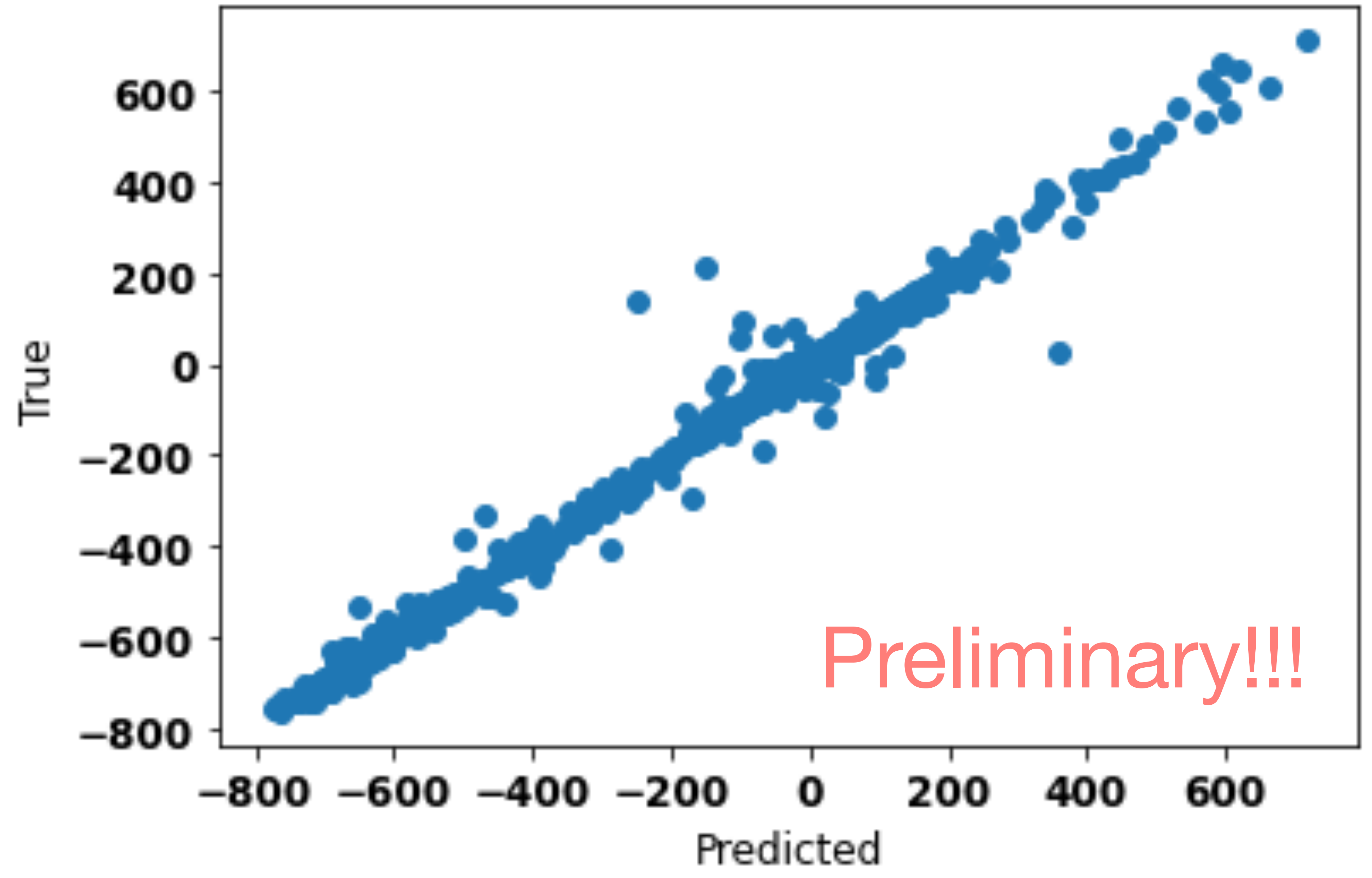
We can validate the emulator by comparing emulated value to simulated value.

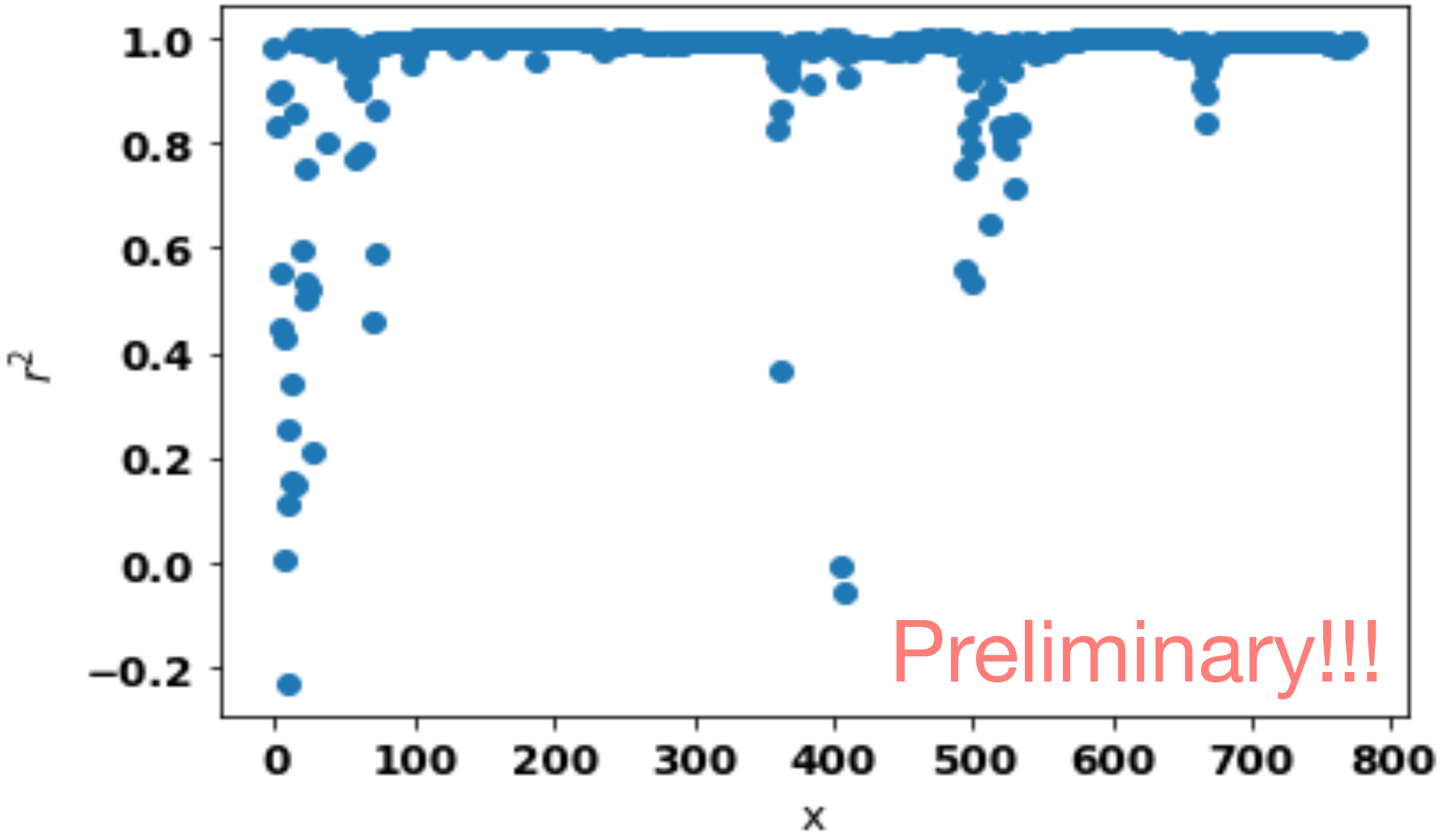
At NLO, emulator performs quite well.

Challenge:
For N3LO, the parameter space is larger, requiring more thought in training point generation.

- Multiple POUNDerS trajectories?
- …..???

Work in progress!!!





Full Bayesian truncation error

Jason Bub
Summer 2022
BAND Fellowship

- To move to a full Bayesian approach, we include (uncorrelated) theoretical errors, see arXiv:2104.04441

$$\chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\exp,i}} \to \chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\exp,i} + \sigma^2_{\mathrm{ther},i}}$$

where

$$\sigma^2_{\mathrm{ther},i} = \frac{(y_{\mathrm{ref},i}\, \bar{c}\, Q_i^{n+1})^2}{1 - Q_i^2}, \quad Q_i = \frac{p_i}{\Lambda_b \sim m_\pi}$$

and $y_{\mathrm{ref},i}$ sets the scale of the correction for observable y_i, and $\bar{c}$ sets the magnitude of the correction.

The Ohio State University

Ohio University

Dick Furnstahl

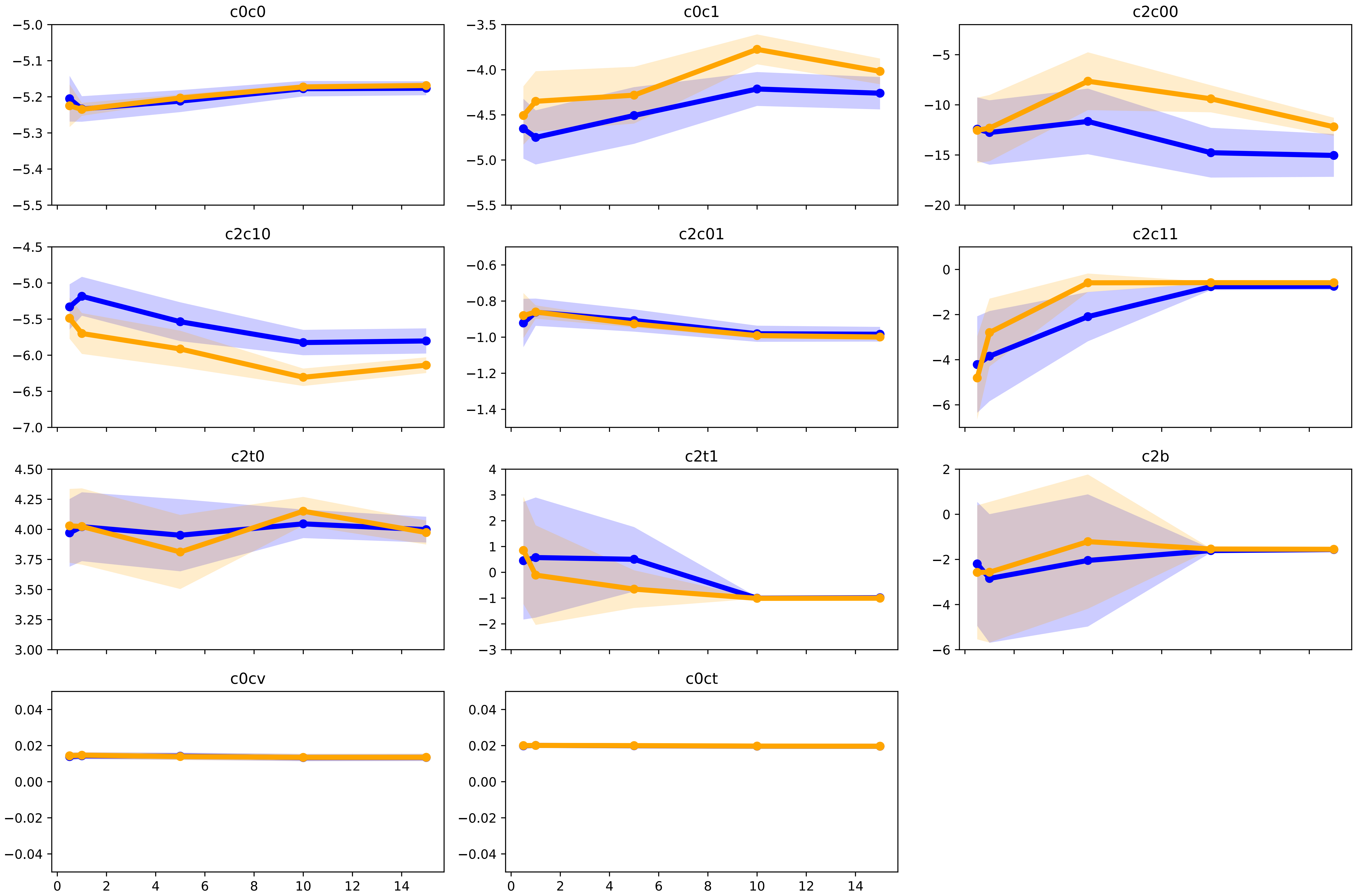
Daniel Phillips

BAND Bayesian Analysis of Nuclear Dynamics

LEC dependance on max fitting energy

First step: Investigate how LECs change depending on max fitting energy at NLO

- No theory errors and uncorrelated theory errors have some differing dependance.
- Dependence should be resolved by correlations.



Preliminary!!!

Correlated theory errors

In a correlated model, we use

$$\sigma^2_{\text{ther},i} = \frac{(y_{\text{ref},i}\, \bar{c}\, Q_i^{n+1})^2}{1 - Q_i^2} \to \sigma^2_{\text{ther},ij} = \frac{y_{\text{ref},i}\, y_{\text{ref},j}\, \bar{c}^2\, Q_i^{n+1} Q_j^{n+1}}{1 - Q_i\, Q_j}$$

with the goodness of fit determined by the Mahalanobis distance (i.e. “modified” χ^2)

$$d_M(\vec{a}) = \chi^2 = \left(\vec{y} - \vec{t}(\vec{a})\right)^T (\sigma^2_{\text{exp}} + \sigma^2_{\text{ther},ij})^{-1} \left(\vec{y} - \vec{t}(\vec{a})\right)$$

Correlations on data introduces strong degeneracies in the covariance matrix.
Work in progress to overcome them!

Local chiral Hamiltonian with Δ's

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

Norfolk NV2: $v_{ij} = v_{ij}^{\rm EM} + v_{ij}^{\pi} + v_{ij}^{2\pi} + v_{ij}^{\rm CT} = \sum_{p=1}^{16} v^p(r_{ij}) O_{ij}^p$

- derived in chiral effective field theory with *Δ*-intermediate states
- 16 spin, tensor, spin-orbit, isospin, etc., operators
- full EM and strong CD and CSB terms included
- predominantly local operator structure suitable for quantum Monte Carlo
- multiple models with different regularization fit to Granada PWA2013 data: models a (b) cutoff ~500 MeV (600 MeV) in p-space

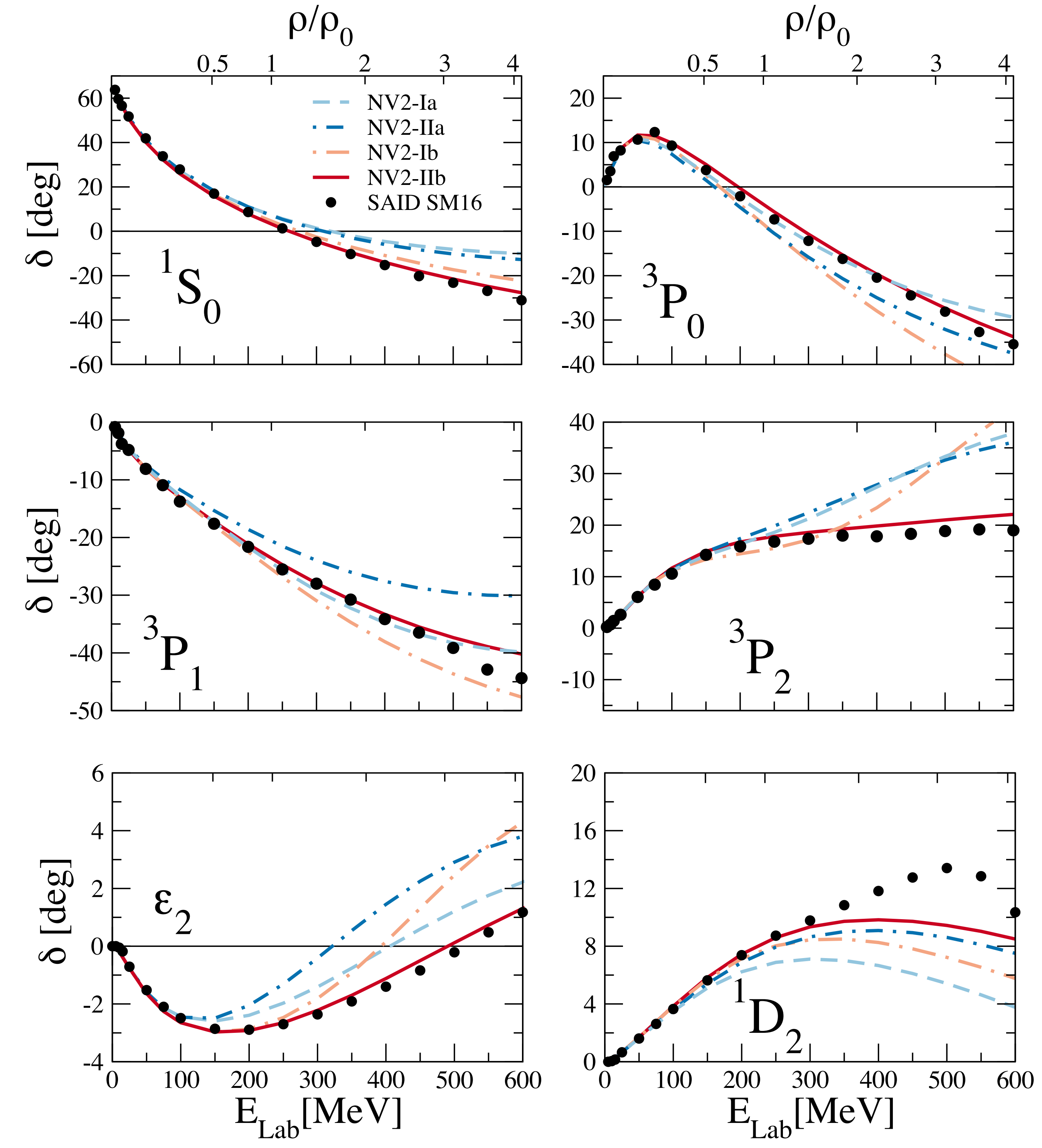
model	order	$E_{\rm Lab}$ (MeV)	N_{pp+np}	χ^2/datum
Ia	N3LO	0–125	2668	1.05
Ib	N3LO	0–125	2665	1.07
IIa	N3LO	0–200	3698	1.37
IIb	N3LO	0–200	3695	1.37

MP et al. PRC **91**, 024003 (2015); PRC **94**, 054007 (2016)

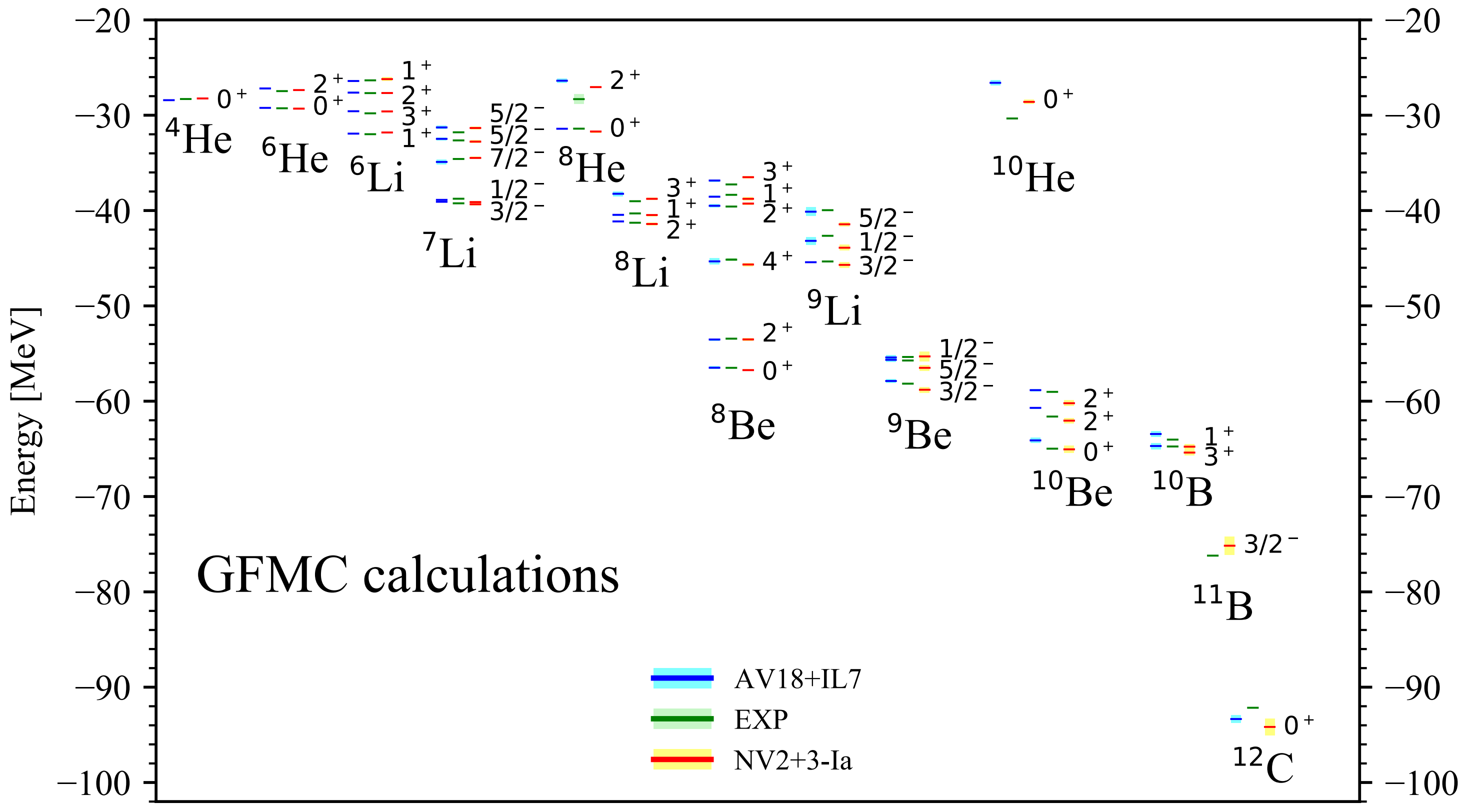
Norfolk NV3: $V_{ijk} = V_{ijk}^{2\pi} + V_{c_{\rm D}} + V_{c_{\rm E}}$

- standard 2π S-wave and 2π P-wave terms consistent with chiral NN potential
- contact terms of cD (π-short range) and cE (short-short range τi.τk) type
- fit to 3H binding and nd scattering length (NV3) MP *et al.* PRL **120**, 052503 (2018)
- or 3H binding and β− decay (NV3*) Baroni *et al.* PRC **98**, 044003 (2018)

MP et al. PRC **101**, 045801 (2020)

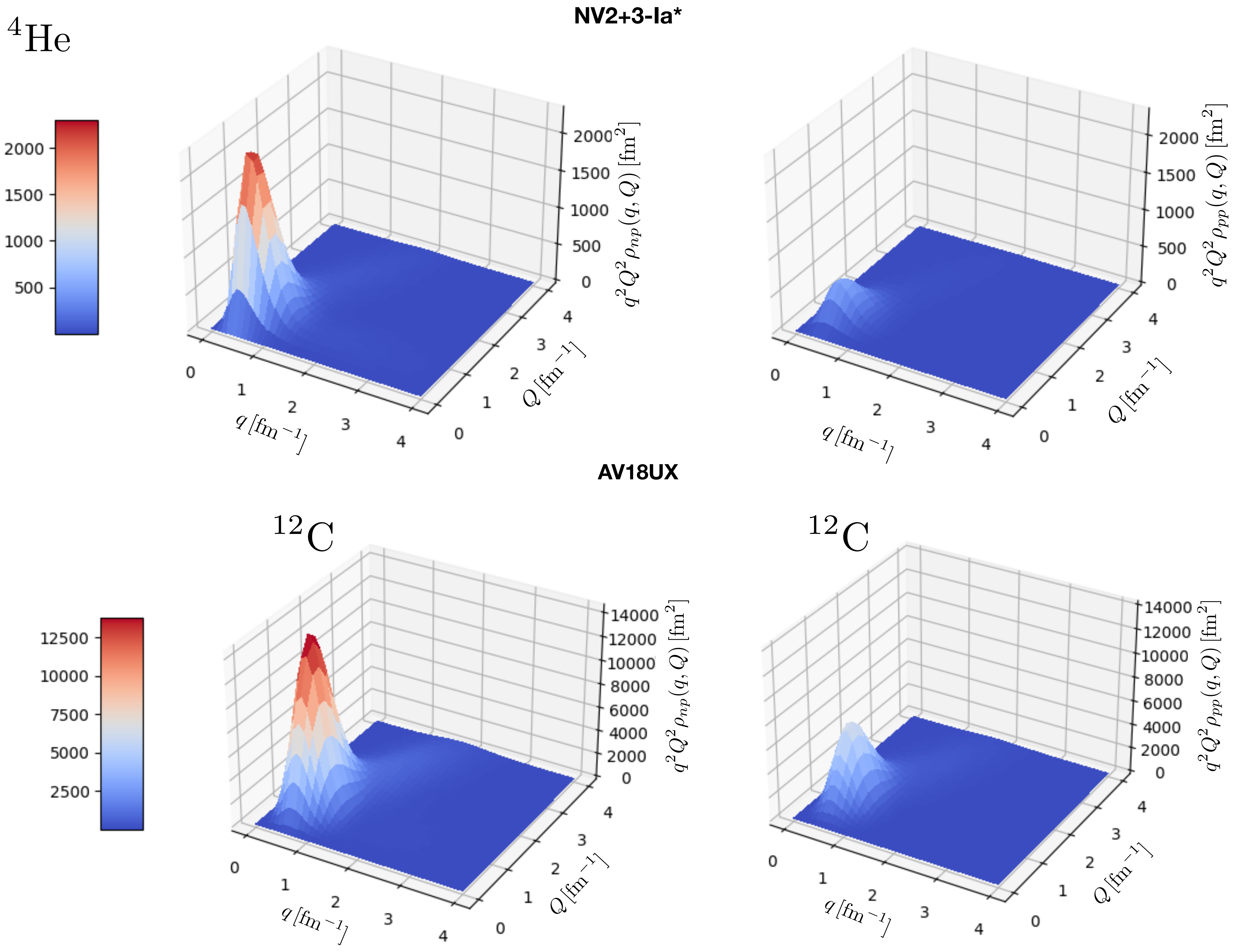


MP *et al.* PRL **120**, 052503 (2018)



Nuclear structure: two-nucleon momentum distribution

- The probability of finding two nucleons in a nucleus with relative momentum **q** and total-center-of-mass momentum **Q**: $\rho_{NN}(\mathbf{q}, \mathbf{Q})$

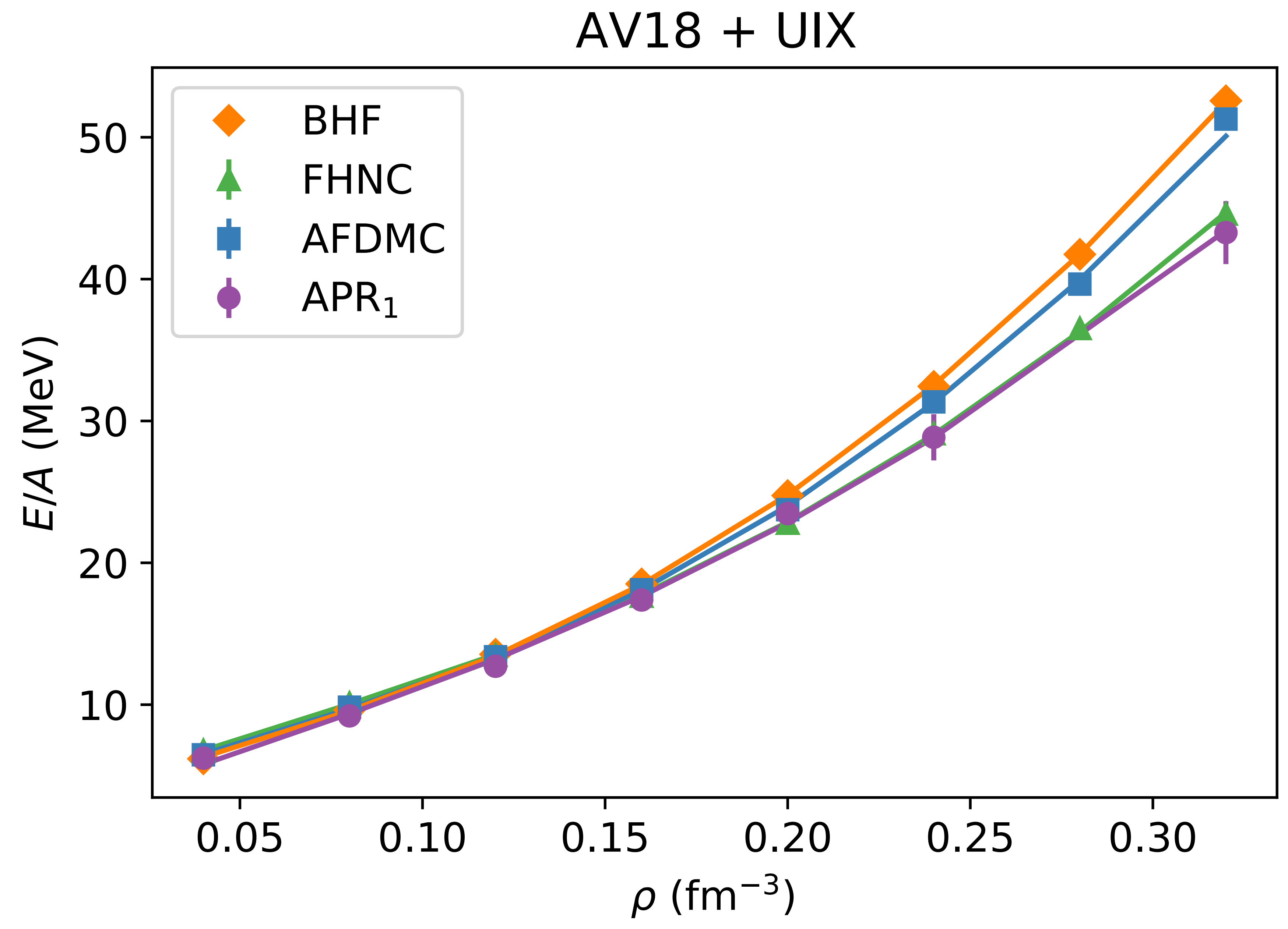


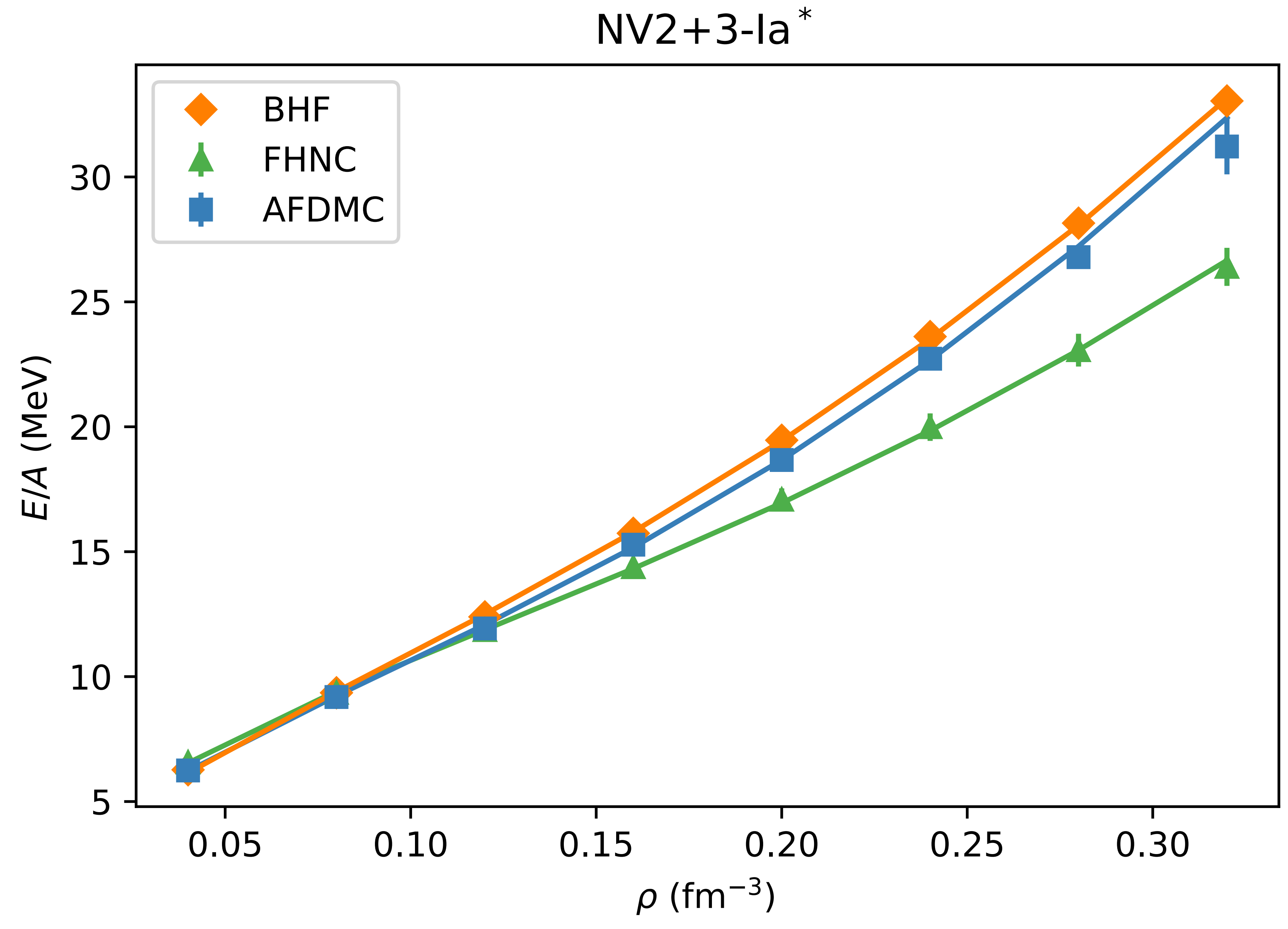
- Tables and figures that tabulate the single-nucleon momentum distribution (including proton and neutron spin momentum distribution) and two-nucleon momentum distribution (including pair distributions in different combinations of ST) will be available online
- A new capability in the VMC code: constraint in the momentum distribution according to pair separation distance

Neutron Matter with realistic NN+3N potentials

Benchmark calculations between BHF, FHNC/SOC, AFDMC-UP for both the AV18 and chiral-EFT interactions only (MP *et al.* *PRC*101 (2020) 045801) and with the inclusion of the corresponding 3N interactions (Lovato, MP *et al*. *PRC*105 (2022) 055808)

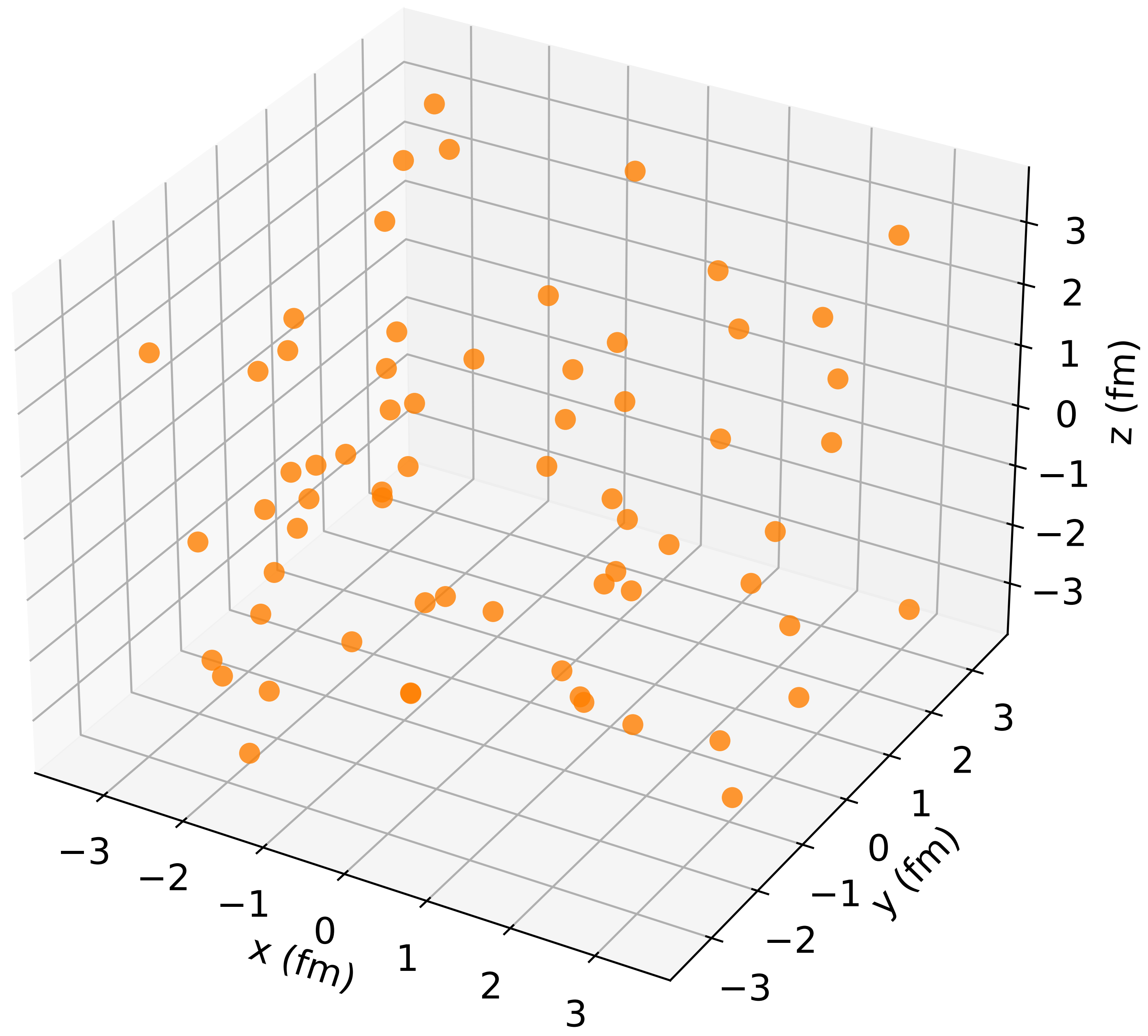
- AFDMC-UC, BHF, FHNC/SOC are very close to each other up to $\rho \leq \rho_0$. They differ at most by ~2 MeV per particle at $\rho = \rho_0$.
- AFDMC-UC and BHF are remarkably close up to $\rho = 2\,\rho_0$ with the maximum difference remaining within ~2.7 MeV per particle.
- FHNC/SOC is below AFDMC and BHF at higher density: limited three-body terms into the cluster expansion and enhancement tensor correlation. They differ at most by ~6 MeV per particle at $\rho = 2\rho_0$.



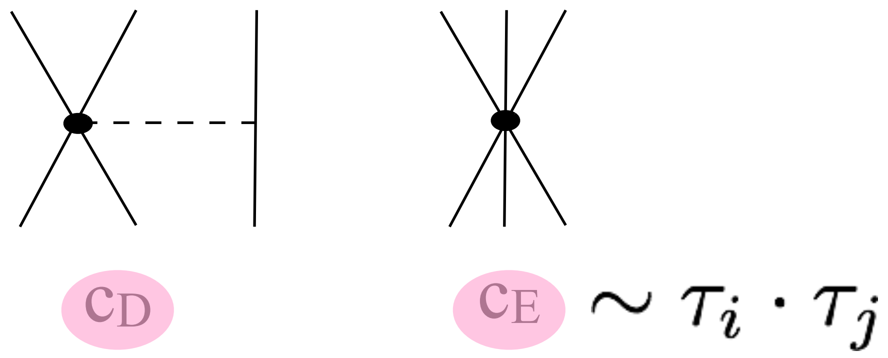


Neutron Matter with realistic NN+3N potentials

First generation NV2+3s are characterized by relatively large and negative values of c_E: "collapse" of PNM, whose energy per particles became large ($\sim$ several GeV per particle).

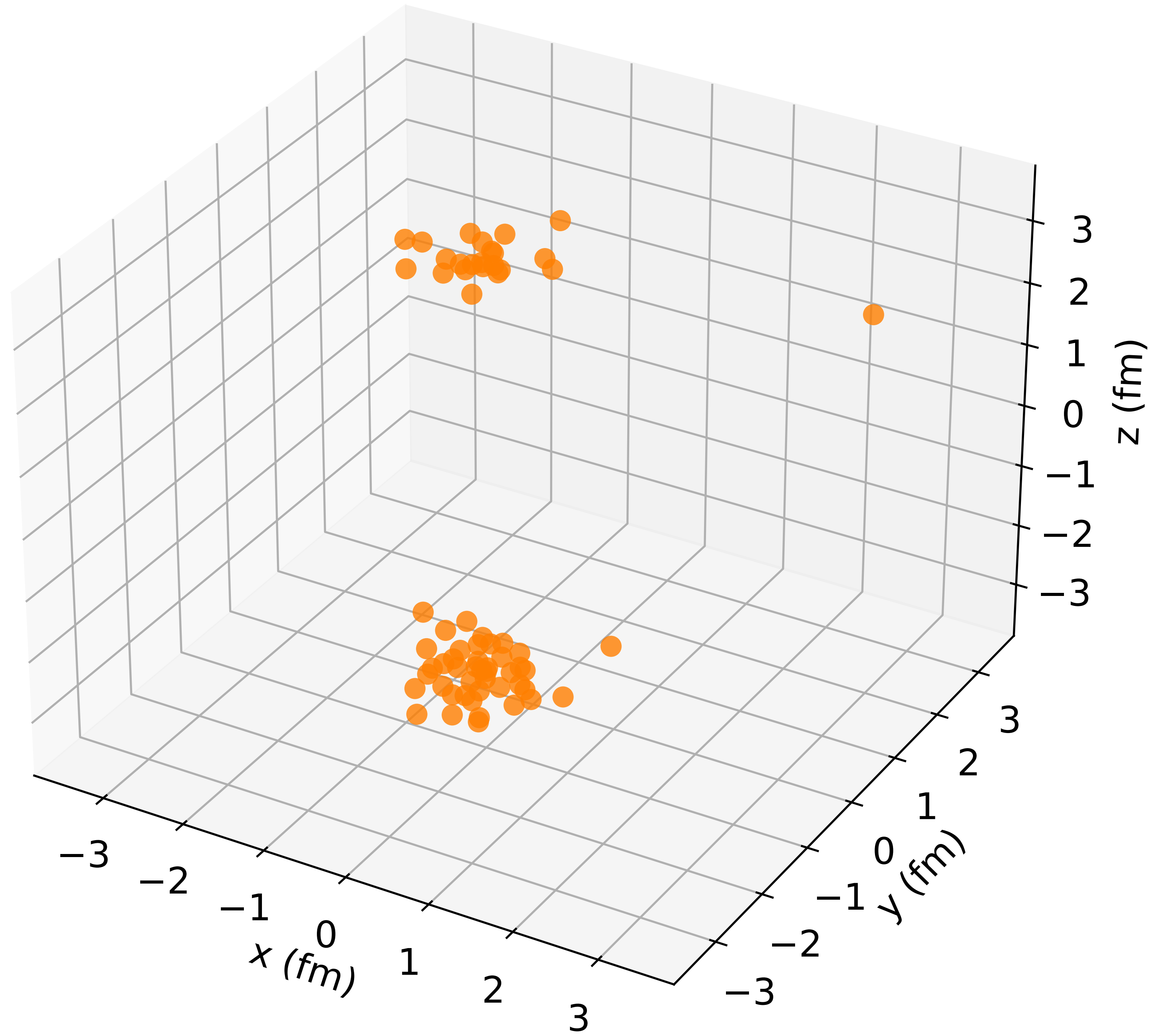


✳ Positions of 66 neutrons with PBC obtained from a single Metropolis random walk of a VMC calculation. The 3N force is turned off and the neutrons are distributed uniformly in the box



NV2+3s:

Model	c_D	c_E
Ia	3.666	−1.638
Ib	−2.061	−0.982
IIa	1.278	−1.029
IIb	−4.480	−0.412

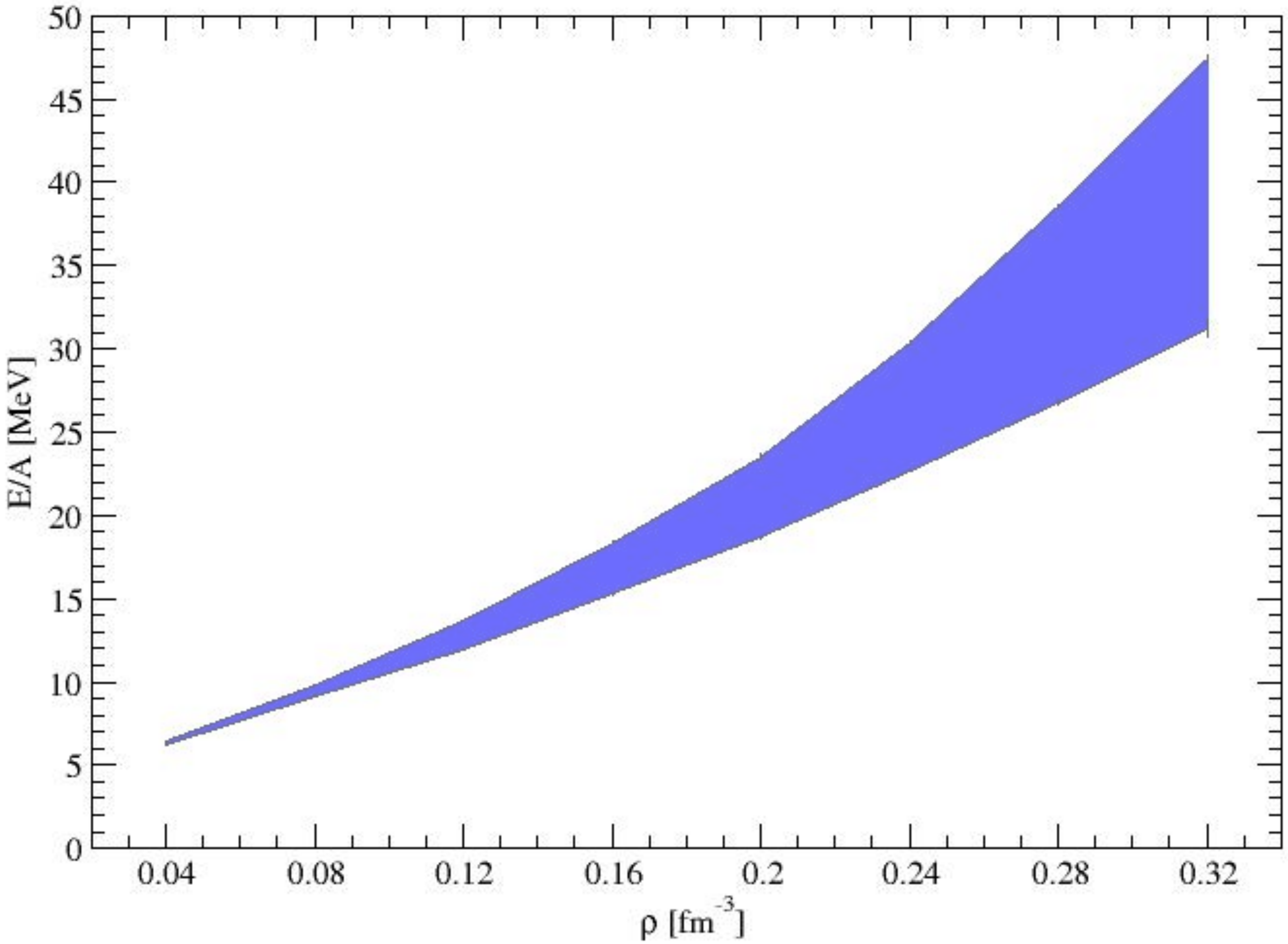


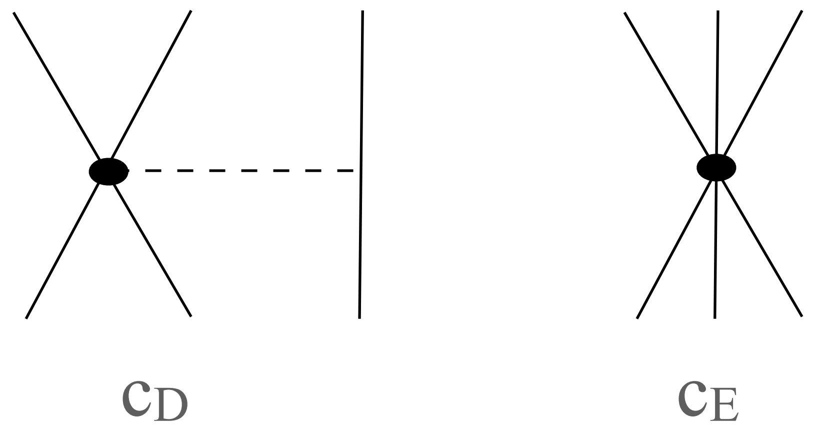
✳ The inclusion of 3N in the Hamiltonian changes dramatically the variational wave function, making the neutrons form closely-packed droplets.

✳ Requiring the energy per particle of PNM to be positive at $\rho = \rho_0$ yields lower bounds on c_E: $c_E \gtrsim -0.1$ (conservative estimate)

Lovato, MP *et al*. *PRC*105 (2022) 055808

Neutron Matter with realistic NN+3N potentials





$\sim \tau_i \cdot \tau_j$

NV2+3s*:

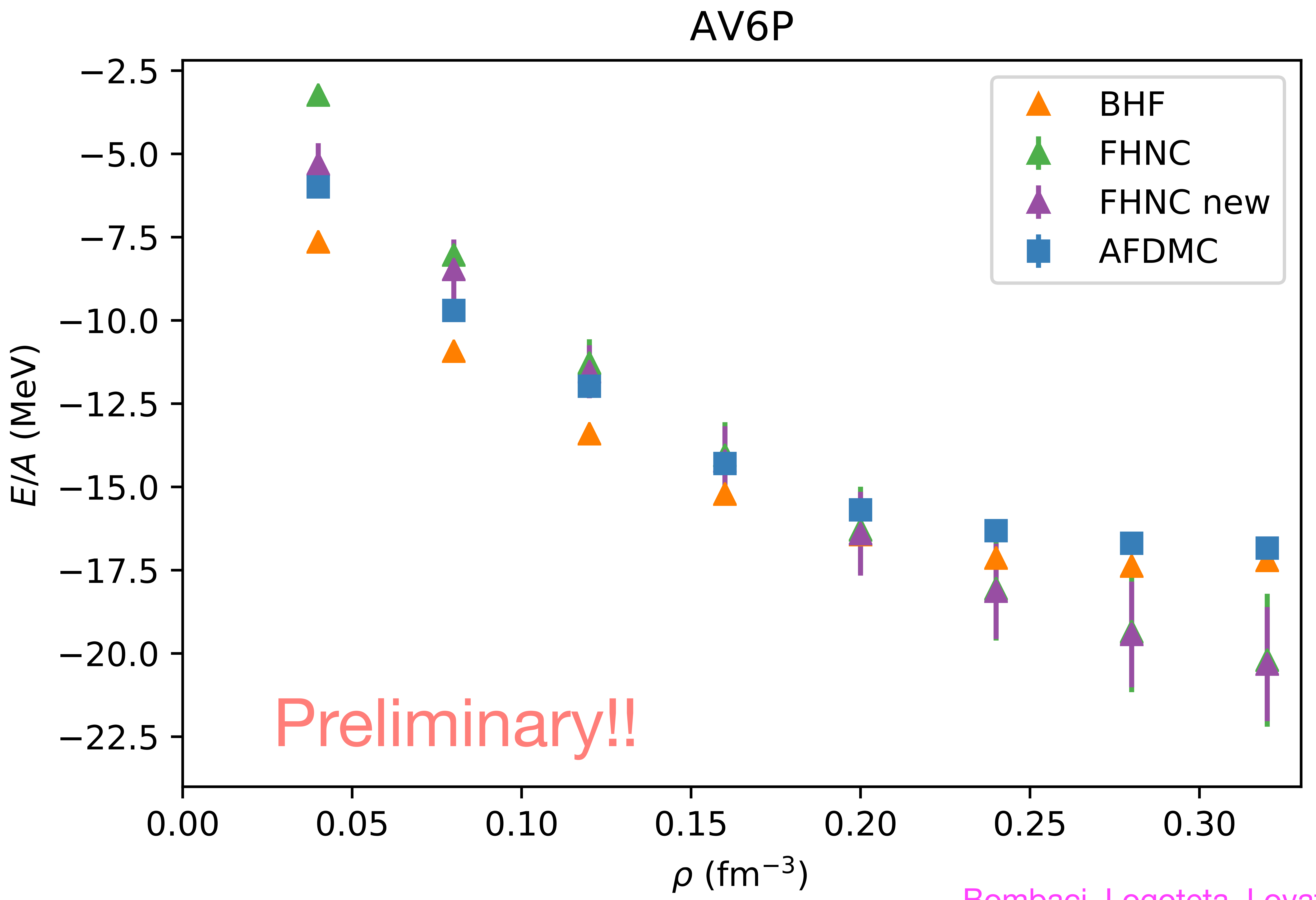
Model	c_D	c_E
Ia*	−0.635(255)	−0.09(8)
Ib*	−4.705(285)	0.550(150)
IIa*	−0.610(280)	−0.350(100)
IIb*	−5.250(310)	0.05(180)

- Model dependence of the EOS at three-body level $\rho = 2\rho_0$ (~16 MeV)
- The exp error on the 3H beta decays in the NV2+3s* (numbers in parenthesis) is not propagated yet

Lovato, MP *et al*. *PRC*105 (2022) 055808

Nuclear matter with realistic NN potentials

Benchmark calculations SNM between BHF, FHNC/SOC, AFDMC-UP for the AV6P



Bombaci, Logoteta, Lovato, Piarulli, Wiringa work in progress!!!

Studying B(GT) in nuclei with A=11

Schmitt, King *et al*. submitted to PRC

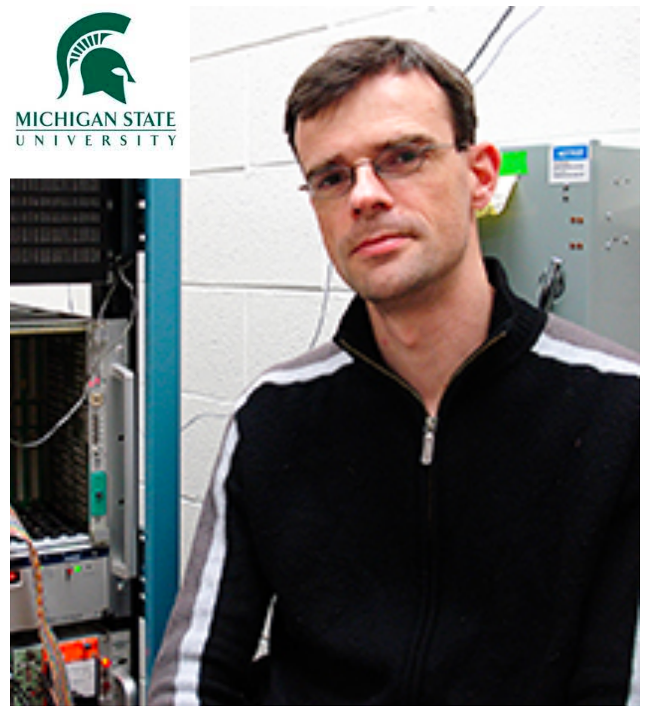
Garrett King

Reduced matrix element from QMC can be used to obtain transition strengths to exclusive final states

$$\mathrm{GT} = \frac{\sqrt{2J_f+1}}{g_A}\frac{\langle J_F M | j^z_{\pm,5}(\mathbf{q}\to 0) | J_i M\rangle}{\langle J_i M, 10 | J_f M\rangle}$$

$$B(GT) = \frac{|\mathrm{GT}|^2}{2J_i+1}$$

Recently B(GT) from charge exchange (CE) reactions has been extracted for ${}^{11}\mathrm{C[gs]} \to {}^{11}\mathrm{N}^*[1/2^-,3/2^-]$ and compared the results with previously measured B(GT) values from mirror ${}^{11}\mathrm{B[gs]} \to {}^{11}\mathrm{Be}^*[1/2^-,3/2^-]$ transitions



Jaclyn Schmitt Remco Zegers Alex Brown

B(GT) values can be extracted from the CE cross section via a well-established proportionality relationship with the CE differential cross sections at small momentum transfer

Comparing theoretical and experimental B(GT) in neutron and proton rich nuclei can provide information about the quality of ab initio wave functions and many-body methods

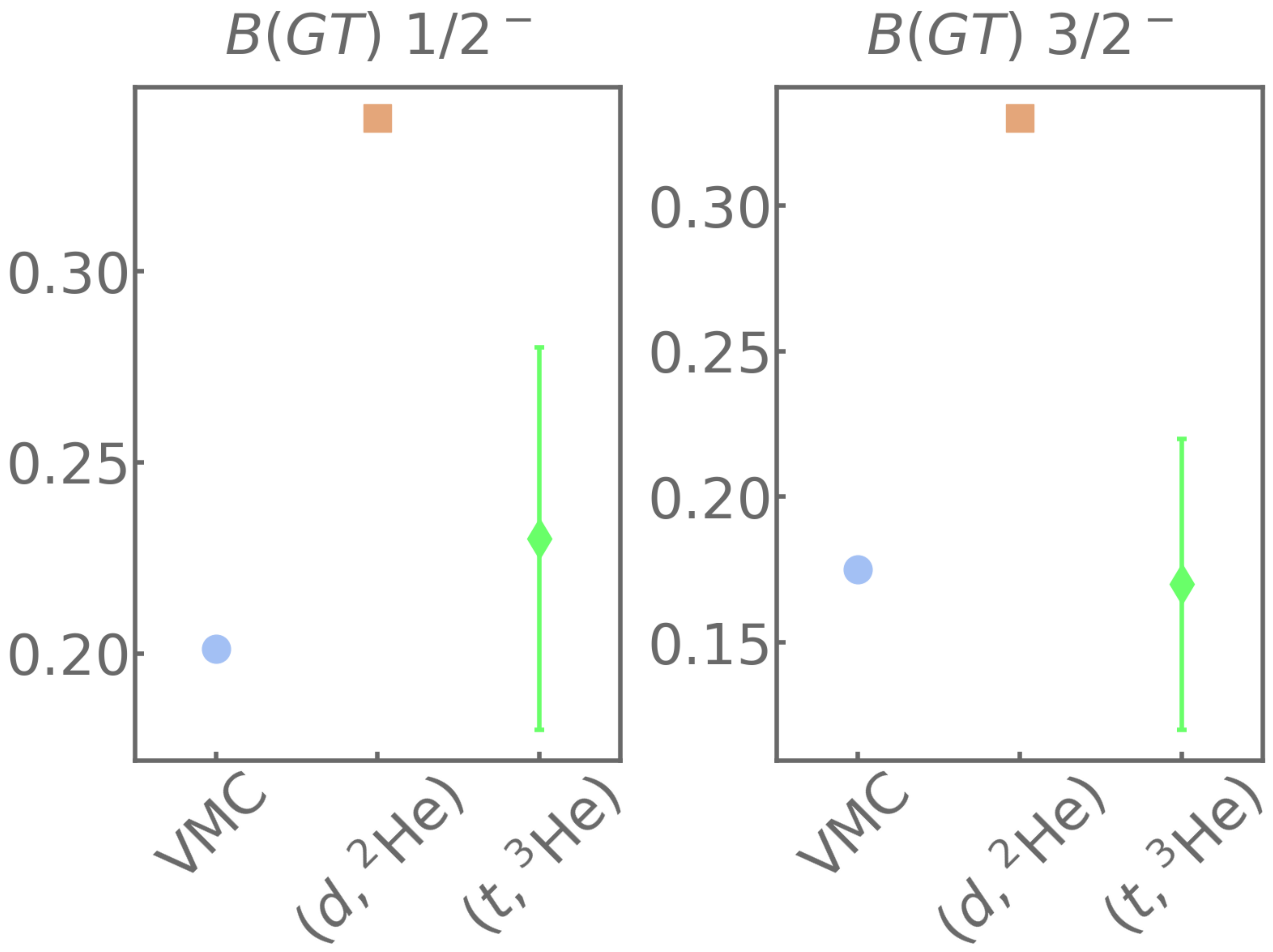
Studying B(GT) in nuclei with A=11

$^{11}B(g.s.) \rightarrow {}^{11}Be^{*}$

VMC agrees well with the value extracted from *(t,^{3}He)*

(d,^{2}He) data consistent with unquenched shell model calculation

Two-body effects ~2%-3% and subtractive



(d,^{2}He) – Ohnishi et al., Nucl. Phys. A 687 (2001)
(t,^{3}He) – Daito et al., Phys. Lett. B (1998)

Schmitt, King *et al*. submitted to PRC

Studying B(GT) in nuclei with A=11

$^{11}C(g.s.) \rightarrow {}^{11}N^*$

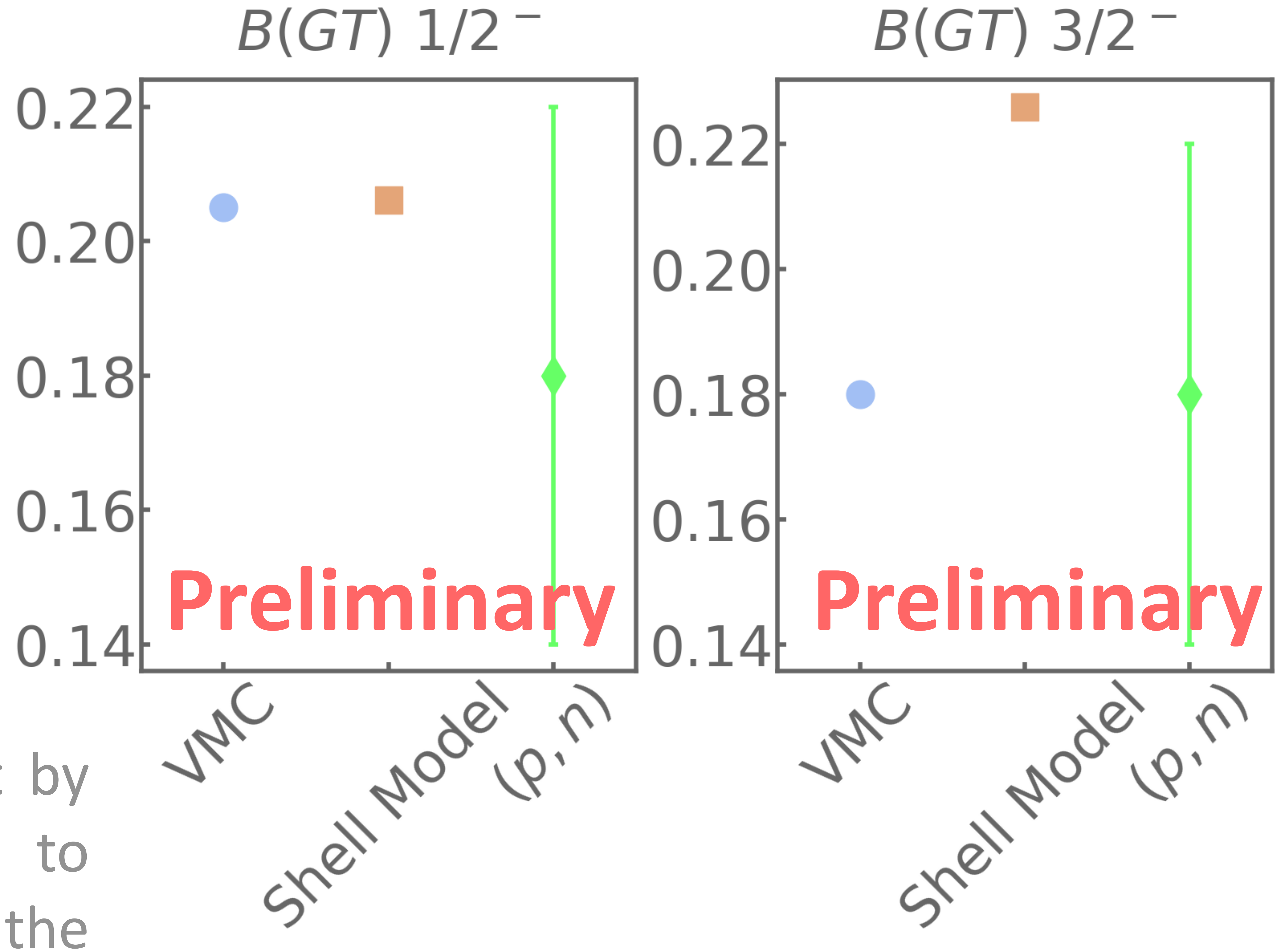
VMC result consistent under isospin symmetry when studying mirror transition

Good agreement between central value of VMC and experimental error bars

Two-body effects ~2%-4% and subtractive

GFMC typically quench the GT matrix element by 2% to 3% from the VMC, which would lead to results that are still in good agreement with the data

Sensitivity to nuclear models to be performed



Shell Model – courtesy of B. A. Brown (MSU)
(p,n) – courtesy of J. Schmitt (MSU)

Schmitt, King *et al*. submitted to PRC

Summary:

- *(Progress):* Tremendous progress in ab-initio theory: algorithms and interactions
  - increased algorithm efficiency,
  - new algorithms (hybrid),
  - successful algorithm benchmarks,
  - advent of EFTs and UQ
- *(Progress):* Possibility to perform consistent calculations for nuclei and infinite matter, connecting nuclei observables to astrophysical quantities and observations

- *(Needs):* New protocols to build realistic nuclear interactions:
  - which observables to use? In which mass range?
  - Bayesian tools and UQ
  - improvements in the formulation of the 3NFs

- *(Needs):* A deeper and more quantitative understanding of the connection between properties of matter and finite nuclei is needed

- *(Needs):* light and medium-mass n-and p-rich phenomenology: input for Hamiltonian constraints, theory validation

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Thank you for your attention!

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BAND Bayesian Analysis of Nuclear Dynamics