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

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

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

Two and many-body interactions:

\[ H = \sum_{i=1}^{A} \frac{p_i^2}{2m_i} + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \ldots \]

Electroweak current operators:

\[ j^{\text{EW}} = \sum_{i=1}^{A} j_i + \sum_{i<j}^{A} j_{ij} + \sum_{i<j<k}^{A} j_{ijk} + \ldots \]

Credit to Heiko Hergert for collecting the data
Nuclear Interactions, Nuclei, and Infinite Matter

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

**Fig. 1**
- IM-SRG calculations**
- NN (N3LO)**+3N (N3LO)**
- 3N fitted to 3H b.e. + saturation region NM at \( \Lambda = 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 \( \Lambda = 450, 500, \) and 550** MeV
- Unable to satisfy NM saturation**
  - **Huther et al., PLB 808, 135651 (2020)
  - **Sammarruca et al., PRC 102, 034313 (2020)

**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

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

\[
\frac{\text{pr}(a|\text{Data}, I)}{\text{pr}(\text{Data}|a, I) \times \text{pr}(a|I)} \propto e^{-\chi^2(a)/2}
\]

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

\[
\begin{align*}
\nu_{\text{LO}} &= \nu_{\text{LO}}^{\text{CI}} + \nu_{\text{EM}} \\
\nu_{\text{NLO}} &= \nu_{\text{LO}}^{\text{CI}} + \nu_{\text{NLO}}^{\text{CI}} + \nu_{\text{NLO}}^{\text{CD}} + \nu_{\text{EM}} \\
\nu_{\text{N3LO}} &= \nu_{\text{LO}}^{\text{CI}} + \nu_{\text{NLO}}^{\text{CI}} + \nu_{\text{N3LO}}^{\text{CI}} + \nu_{\text{NLO}}^{\text{CD}} + \nu_{\text{N3LO}}^{\text{CD}} + \nu_{\text{EM}}
\end{align*}
\]

- 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

**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
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!!!

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

\[ \chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma_{\text{exp},i}^2} \rightarrow \chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma_{\text{exp},i}^2 + \sigma_{\text{ther},i}^2} \]

where

\[ \sigma_{\text{ther},i}^2 = \frac{(y_{\text{ref},i} \bar{c} Q_i^{n+1})^2}{1 - Q_i^2}, \quad Q_i = \frac{p_i}{\Lambda_b \sim m_\pi} \]

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

\[ \sigma_{\text{ther},i}^2 = \frac{(y_{\text{ref},i} \bar{c} Q_i^{n+1})^2}{1 - Q_i^2} \rightarrow \sigma_{\text{ther},ij}^2 = \frac{y_{\text{ref},i} y_{\text{ref},j} \bar{c}^2 Q_i^{n+1} Q_j^{n+1}}{1 - Q_i Q_j} \]

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

\[ d_M(\vec{a}) = \chi^2 = (\bar{y} - \bar{t}(\vec{a}))^T (\sigma_{\text{exp}}^2 + \sigma_{\text{ther},ij}^2)^{-1} (\bar{y} - \bar{t}(\vec{a})) \]

Correlations on data introduces strong degeneracies in the covariance matrix. Work in progress to overcome them!
Local chiral Hamiltonian with $\Delta$’s

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

Norfolk NV2: $v_{ij} = v^{\text{EM}}_{ij} + v^\pi_{ij} + v^{2\pi}_{ij} + v^{\text{CT}}_{ij} = \sum_{p=1}^{16} v^p (r_{ij}) O^p_{ij}$

- derived in chiral effective field theory with $\Delta$-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 $\sim$500 MeV (600 MeV) in p-space

<table>
<thead>
<tr>
<th>model</th>
<th>order</th>
<th>$E_{\text{Lab}}$ (MeV)</th>
<th>$N_{p+p}$</th>
<th>$\chi^2$/datum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ia</td>
<td>N3LO</td>
<td>0–125</td>
<td>2668</td>
<td>1.05</td>
</tr>
<tr>
<td>Ib</td>
<td>N3LO</td>
<td>0–125</td>
<td>2665</td>
<td>1.07</td>
</tr>
<tr>
<td>IIa</td>
<td>N3LO</td>
<td>0–200</td>
<td>3698</td>
<td>1.37</td>
</tr>
<tr>
<td>IIb</td>
<td>N3LO</td>
<td>0–200</td>
<td>3695</td>
<td>1.37</td>
</tr>
</tbody>
</table>

Norfolk NV3: $V_{ijk} = V^{2\pi}_{ijk} + V^\text{CD} + V^\text{CE}$

- standard 2\pi S-wave and 2\pi P-wave terms consistent with chiral NN potential
- contact terms of cD (π-short range) and cE (short-short range τi.tk) type
- fit to 3H binding and nd scattering length (NV3) \cite{MP_PRL_120_052503_2018}
- or 3H binding and β− decay (NV3*) \cite{Baroni_PRC_98_044003_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 $Q$: $\rho_{NN}(q, Q)$

- 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. PRC101 (2020) 045801) and with the inclusion of the corresponding 3N interactions (Lovato, MP et al. PRC105 (2022) 055808)

- AFDMC-UC, BHF, FHNC/SOC are very close to each other up to $\rho \leq \rho_0$. They differ at most by $\sim 2$ 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 $\sim 2.7$ 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 $\sim 6$ 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

- 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)

\[
\begin{array}{c|cc}
\text{Model} & c_D & c_E \\
\hline
\text{Ia} & 3.666 & -1.638 \\
\text{Ib} & -2.061 & -0.982 \\
\text{IIa} & 1.278 & -1.029 \\
\text{IIb} & -4.480 & -0.412 \\
\end{array}
\]
Neutron Matter with realistic NN+3N potentials

- 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

<table>
<thead>
<tr>
<th>Model</th>
<th>$c_D$</th>
<th>$c_E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ia*</td>
<td>-0.635(255)</td>
<td>-0.09(8)</td>
</tr>
<tr>
<td>Ib*</td>
<td>-4.705(285)</td>
<td>0.550(150)</td>
</tr>
<tr>
<td>IIa*</td>
<td>-0.610(280)</td>
<td>-0.350(100)</td>
</tr>
<tr>
<td>IIb*</td>
<td>-5.250(310)</td>
<td>0.05(180)</td>
</tr>
</tbody>
</table>

Lovato, MP et al. PRC105 (2022) 055808
Nuclear matter with realistic NN potentials

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

Preliminary!!

Bombaci, Logoteta, Lovato, Piarulli, Wiringa work in progress!!
Studying $B(GT)$ in nuclei with $A=11$

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

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

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

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

$B(GT)$ 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 $ab\ ini\o$ wave functions and many-body methods
$^{11}\text{B}(\text{g.s.}) \rightarrow ^{11}\text{Be}^*$

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

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

Two-body effects $\sim$2%-3% and subtractive

Schmitt, King et al. submitted to PRC
Studying $B(GT)$ in nuclei with $A=11$

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

VMC result consistent under isospin symmetry when studying mirror transition

Good agreement between central value of VMC and experimental error bars

Two-body effects $\sim 2\%-4\%$ 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
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
Quantum Monte Carlo Group for Nuclear Physics

Dr. Andreoli: Universities Research Association's Visiting Scholars Program (2022)
J. Bub: Summer BAND Fellowship (2022)
G. King: DOE/NNSA Stewardship Science Graduate Fellowship (2021)
Dr. Anna McCoy: FRIB Theory Fellow (Sep 2022)

- DOE DE-SC0021027 (PI: Pastore), DOE ECA DE-SC0022002 (PI: Piarulli)
- FRIB Theory Alliance DE-SC0013617, Neutrino Theory Network
- Computational resources awarded by the DOE: 2019 (PI: Pastore), 2020 (PI: Piarulli), 2021 (PI: Lovato), 2022 (PI: Rocco) ALCC and INCITE (PI: Hagen) programs
Thank you for your attention!

Collaborators:
Alessandro Baroni — Postdoc LANL
Josh Barrow — Postdoc MIT
Vincenzo Cirigliano, LANL
Wouter Dekens, UCSD/UW
Alex Gnech — Postdoc JLab
Joe Carlson, LANL
Stefano Gandolfi, LANL
Steven Gardiner, Fermilab
Luca Girlanda, University of Salento, Italy
Alejandro Kievsky, INFN-Pisa, Italy
Alessandro Lovato, ANL
Laura E. Marcucci, University of Pisa, Italy
Emanuele Mereghetti, LANL
Rocco Schiavilla, ODU/JLab
Michele Viviani, INFN-Pisa, Italy
Robert Wiringa, ANL