NUCLEI

Nuclear Computational Low-Energy Initiative

A SciDAC-5 Project

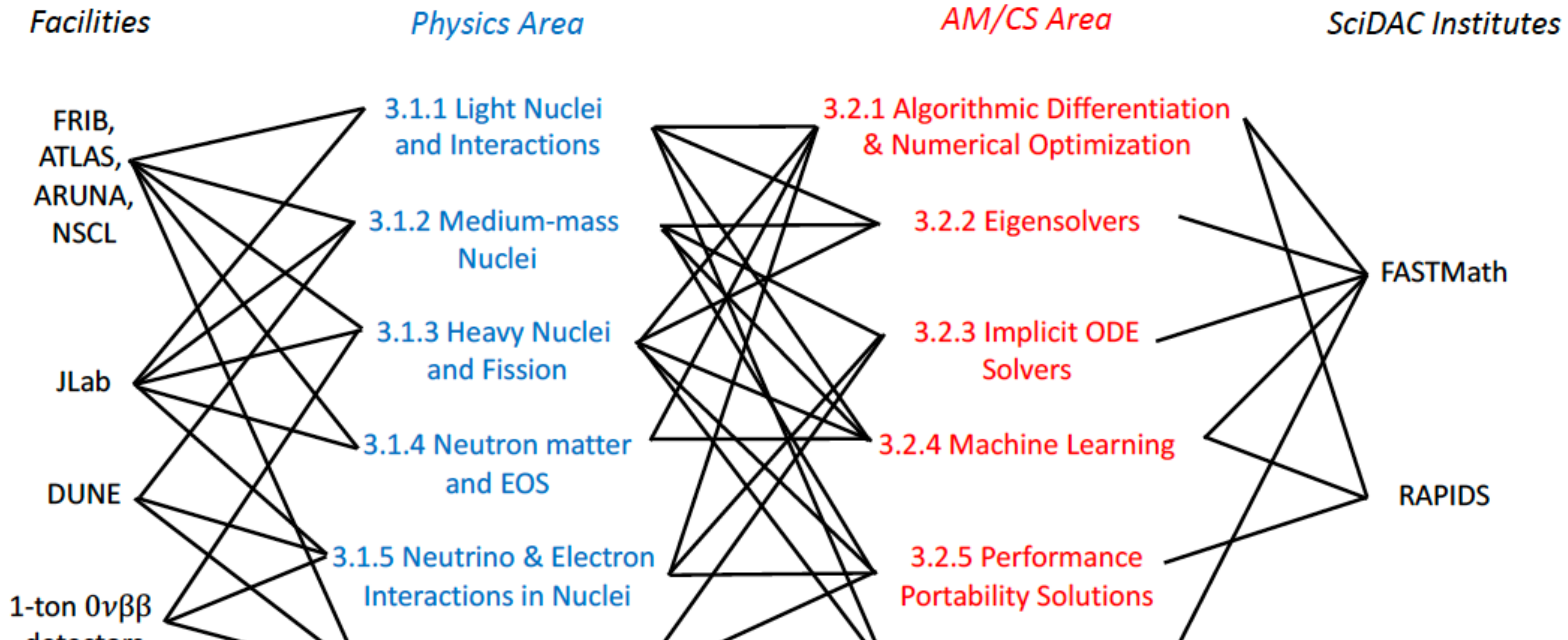
Thomas Papenbrock, with input from many colleagues

Software Infrastructure for Advanced Nuclear Physics Computing (SANPC)

Jefferson Lab, June 20, 2024

i. Properties and interactions of light nuclei and multinucleon systems
ii. Precision calculations of nuclear matrix elements for fundamental symmetries
iii. Neutrino and electron interactions in nuclei and dense matter
iv. Nuclear structure and properties of nuclei
v. Nuclear fission

Connecting DOE facilities and SciDAC Institutes



Facilities

FRIB, ATLAS, ARUNA, NSCL

JLab

DUNE

1-ton $0\nu\beta\beta$ detectors

Physics Area

3.1.1 Light Nuclei and Interactions

3.1.2 Medium-mass Nuclei

3.1.3 Heavy Nuclei and Fission

3.1.4 Neutron matter and EOS

3.1.5 Neutrino & Electron Interactions in Nuclei

3.1.6 Fundamental Symmetries

AM/CS Area

3.2.1 Algorithmic Differentiation & Numerical Optimization

3.2.2 Eigensolvers

3.2.3 Implicit ODE Solvers

3.2.4 Machine Learning

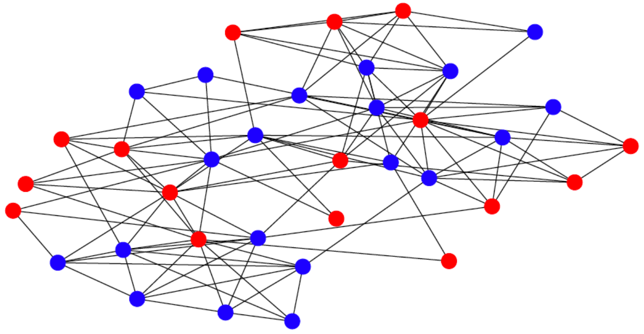
3.2.5 Performance Portability Solutions

3.2.6 Uncertainty Quantification

SciDAC Institutes

FASTMath

RAPIDS



Lots of NP and AM/CS connections

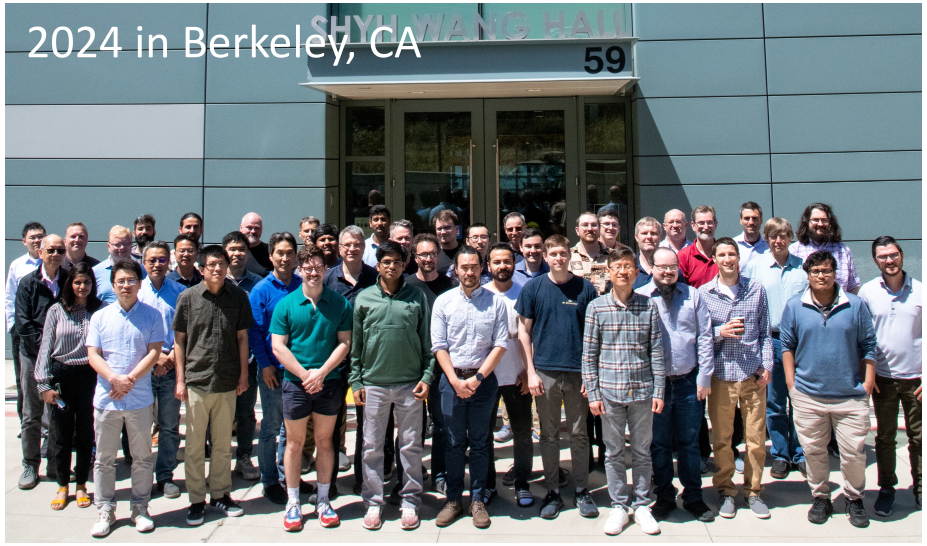
Who is NUCLEI?

Participating Institutions and Investigators (SciDAC-5)

[Color denotes Physics or Computer Science & Applied Mathematics
Postdocs are indicated by (p) and graduate students by (g); all others are faculty or laboratory staff.]

Argonne National Laboratory
J. Fox (p), A. Lovato, A. McCoy, M. Menickelly, S. Narayanan, J. ONeal, K. Raghavan, R. Wiringa
Iowa State University
P. Maris, J. Vary
Lawrence Berkeley National Laboratory
E. Ng, D. Rouson , S. Wild, C. Yang
Lawrence Livermore National Laboratory
C. Balos, K. Kravvaris, N. Schunck, P Siwach (p), M. Verriere, C. Woodward
Los Alamos National Laboratory
J. Carlson, S. Gandolfi, M. Grosskopf, I. Tews, H. Yuchi
Massachusetts Institute of Technology
C. Feng (g), Y. Marzouk
Michigan State University
H.M. Aktulga, T.S. Blade (g), E. Flynn (g), M. Gajdosik (g), K. Godbey, O.M. Gul (g), H. Hergert, Caleb Hicks (g), D. Lee, Y.-Z. Ma (p), W. Nazarewicz, J. Wylie (g)
Oak Ridge National Laboratory
T. Djaervs (p), G. Hagen, B. Hu (p), G. Jansen, S. Lee, T. Papenbrock
Ohio State University
R. Furnstahl, M. Hisham (g), P. Millican (g), P. Sharma (g), S. Sundberg (g)
University of North Carolina at Chapel Hill
M. Dai (g), J. Engel
University of Notre Dame
R. Stroberg
University of Oregon
B. Norris
Washington University in St. Louis
S. Pastore, M. Piarulli


2023 in Knoxville, TN


2024 in Berkeley, CA

Many-Fermion Dynamics for Nuclear Structure

- No-Core Shell Model (No-Core Configuration Interaction)
  - expand A-body wavefunction in orthonormal harmonic oscillator basis, consisting of Slater-Determinants of A single-particle states
  - express Hamiltonian H_{ij} in this basis
  - obtain lowest eigenstates of resulting (sparse, symmetric) matrix
  - complete basis $\longrightarrow$ exact result
    - caveat: complete basis is infinitely large . . .
- MFDn (Fortran legacy code)
  - parallel F90/95 code using MPI + OpenMP (CPUs) / OpenACC (GPUs)
  - construct and stores nonzero MEs in many-body matrix H_{ij}
  - obtain lowest eigenpairs using LOBPCG or Lanczos algorithm
- Input
  - 2-body (and 3-body) nuclear potential in harmonic oscillator basis
- Output
  - energies, radii, and magnetic and quadrupole moments
  - reduced one-body density matrix elements
  - wavefunctions (eigenvectors)
- MFDn postprocessor
  - use MFDn wavefunctions to calculate 1- and 2-body observables, e.g. electroweak transition matrix elements and form factors

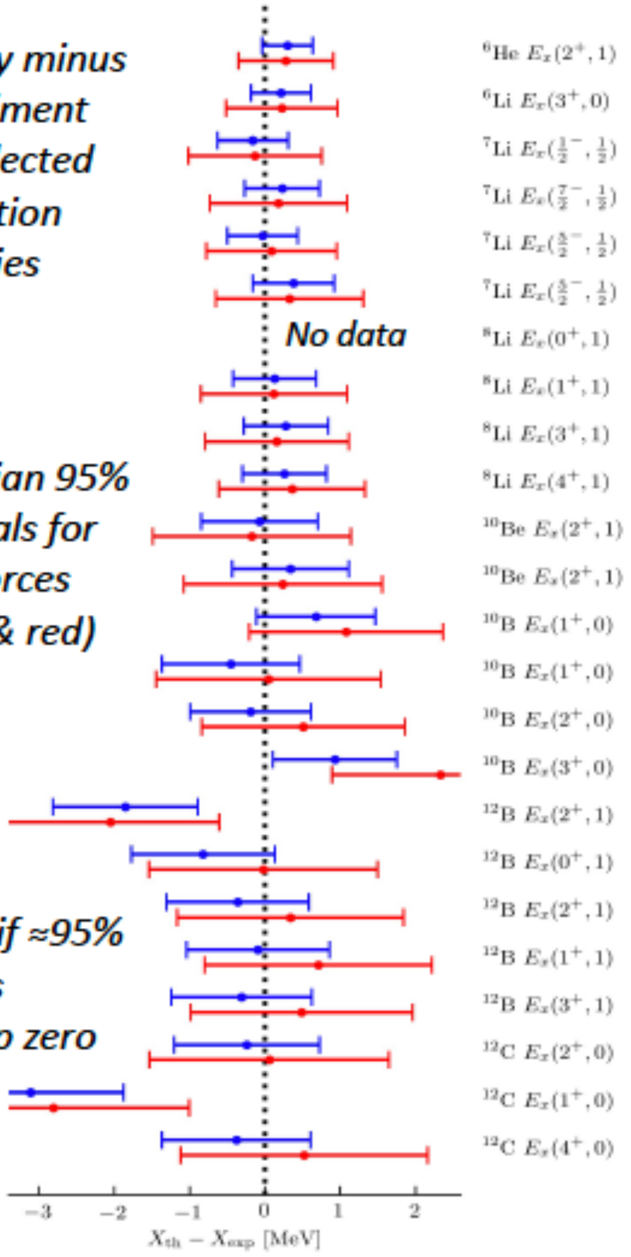
Courtesy of P. Maris

Excitation energies from effective field theory with quantified uncertainties

Theory minus experiment for selected excitation energies

Bayesian 95% intervals for two forces (blue & red)

Check if ≈95% of bars overlap zero



Courtesy of P. Maris

Objectives

- Predict properties of ground and excited states of light nuclei with robust theoretical error estimates.
- Test consistent LENPIC chiral effective field theory (EFT) interactions with 2- and 3-nucleon forces.
- Extend and test a Bayesian statistical model that learns from the order-by-order EFT convergence pattern to account for correlated excitations.

Impact

- First test of novel chiral nucleon-nucleon potentials with consistent three-nucleon forces.
- Demonstrates understanding of theoretical uncertainties due to chiral EFT expansion.
- Accounting for correlations produces agreement with experimental excitation energies (see figure).
- Exceptions in ^{12}C and ^{12}B indicate different theoretical correlations in the nuclear structure.

Accomplishments

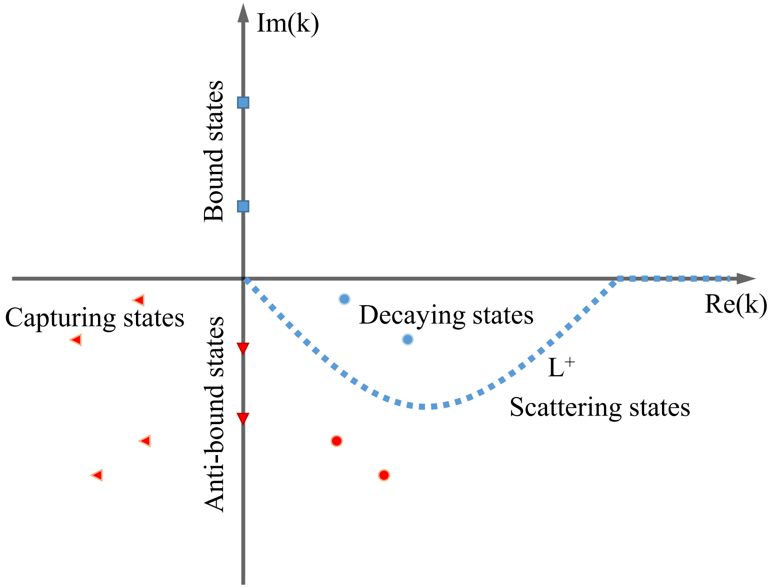
P. Maris et al, Phys. Rev. C **103**, 054001 (2021); Editors' Suggestion; arXiv: 2012.12396 [nucl-th]

Gamow Shell Model (GSM) Code for Many-Body Calculations of Nuclear Open Quantum Systems

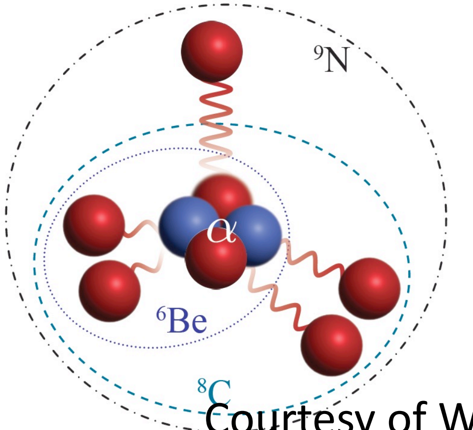
- Gamow Shell Model (GSM) has been developed to study the many-body states occurring at the limits of the nuclear chart, i.e. drip-line nuclei
- GSM is a configuration interaction model based on Berggren basis, which contains bound, resonant and scattering states
- GSM requires the diagonalization of complex symmetric matrices, which present difficulties for numerical methods

GSM Code by N. Michel et al.[1,2] is a scalable parallel implementation of GSM

- Resonant states targeted with GSM are situated in the middle of scattering states, hence require finding the interior eigenpairs
- Jacobi-Davidson (JD) method, which can directly target the interior eigenvalues and eigenvectors, is used in the GSM code
- Preconditioning and angular momentum projection techniques are implemented to ensure rapid convergence; hybrid MPI/OpenMP parallelization and 2D decomposition are adopted for scalability
- Demonstrated scaling to hundreds of cores; currently limited to CPU architectures only



Numerous nuclear physics applications under NUCLEI, including the recent study of the nested nucleus ^{9}N: Phys. Rev. Lett. 131, 172501 (2023)



Courtesy of W. Nazarewicz

1. N Michel, W Nazarewicz, M Ploszajczak, T Vertse, J. Phys. G: Nucl. Part. Phys. 36 (2009) 013101.
2. N Michel, HM Aktulga, Y Jaganathen, Comp. Phys. Comm. 247 (2020), 106978

Quantum Monte Carlo calculations

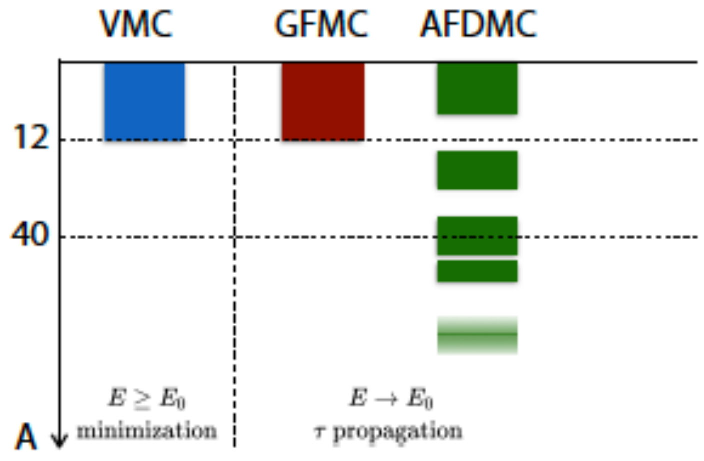
Variational Monte Carlo (VMC)

Green’s Function Monte Carlo (GFMC)

Auxiliary Field Diffusion Monte Carlo (AFDMC)

All codes use **MPI** and **OpenMP**, GFMC uses **ADLB** for load balancing.

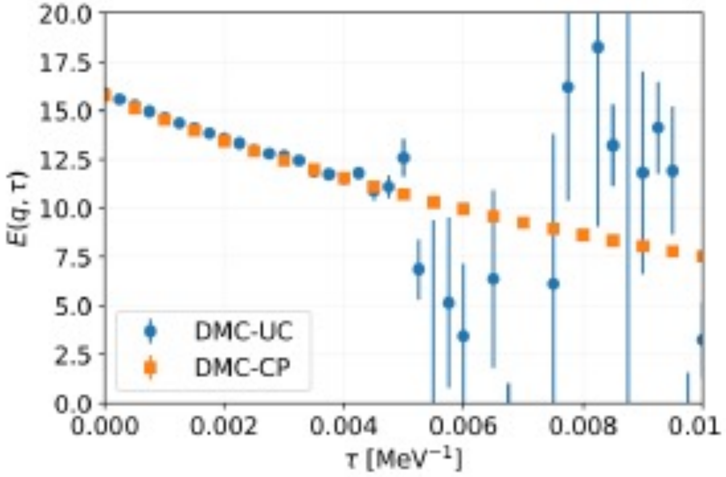
Porting to **GPU** in progress



VMC GFMC AFDMC	light systems	A ≤ 12
AFDMC	light to medium-heavy nuclei, infinite matter	A ~ 50

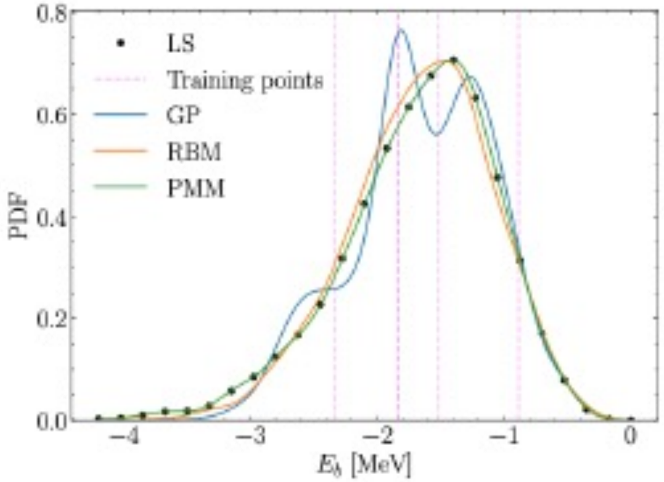
Courtesy of D. Lonardoni

Courtesy of Lorenzo Andreoli



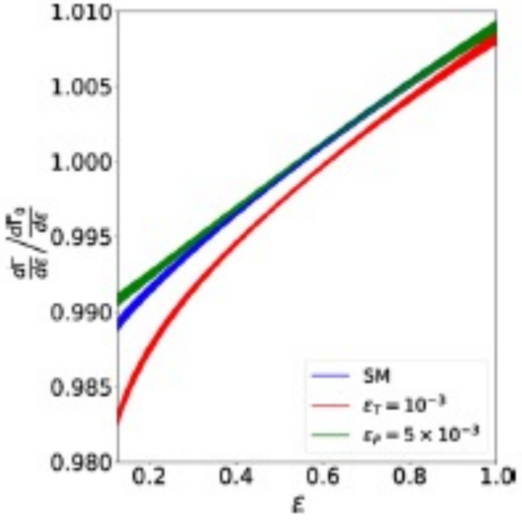
Static and dynamic properties of atomic nuclei with high-resolution potentials

Alex Gnech,[1,2] Alessandro Lovato,[3,4] and Noemi Rocco[5]



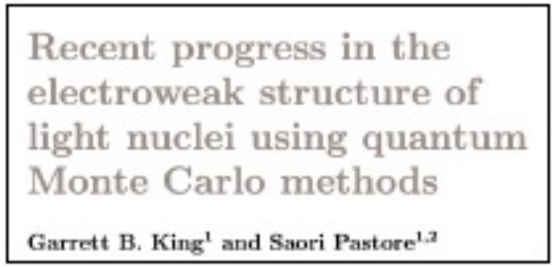
Emulators for scarce and noisy data:
application to auxiliary field diffusion Monte Carlo for the deuteron

Rahul Somasundaram,[1,2,*] Cassandra L. Armstrong,[3]
Pablo Giuliani,[4,5] Kyle Godbey,[4] Stefano Gandolfi,[1] and Ingo Tews[1]



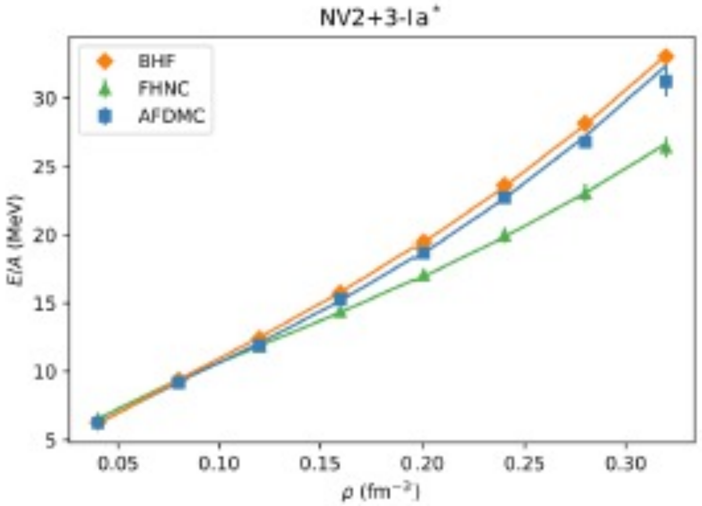
Ab initio calculation of the β-decay spectrum of ^{6}He

G. B. King, A. Baroni, V. Cirigliano, S. Gandolfi, L. Hayen, E. Mereghetti, S. Pastore, and M. Piarulli



Recent progress in the electroweak structure of light nuclei using quantum Monte Carlo methods

Garrett B. King[1] and Saori Pastore[1,2]



Benchmark calculations of infinite neutron matter with realistic two- and three-nucleon potentials

A. Lovato, I. Bombaci, D. Logoteta, M. Piarulli, and R. B. Wiringa

Courtesy of Lorenzo Andreoli

Neural-network quantum states

Neural networks can provide a compact and efficient representation of the nuclear many-body wave function, capturing correlations more efficiently than traditional QMC methods.

- Training leverages the variational principle

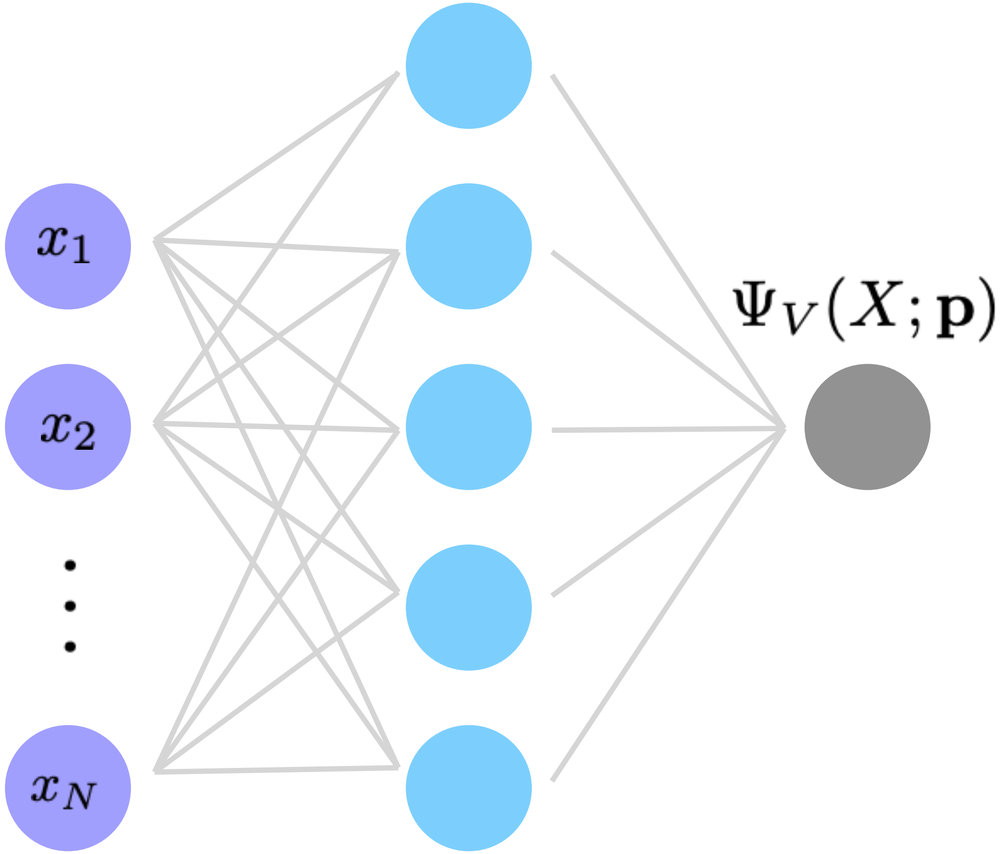
$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

- Hilbert space sampled with VMC methods

$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

- Code entirely developed over the last three years in Python - JAX

- Efficiently scales up to ~1,000 GPUs

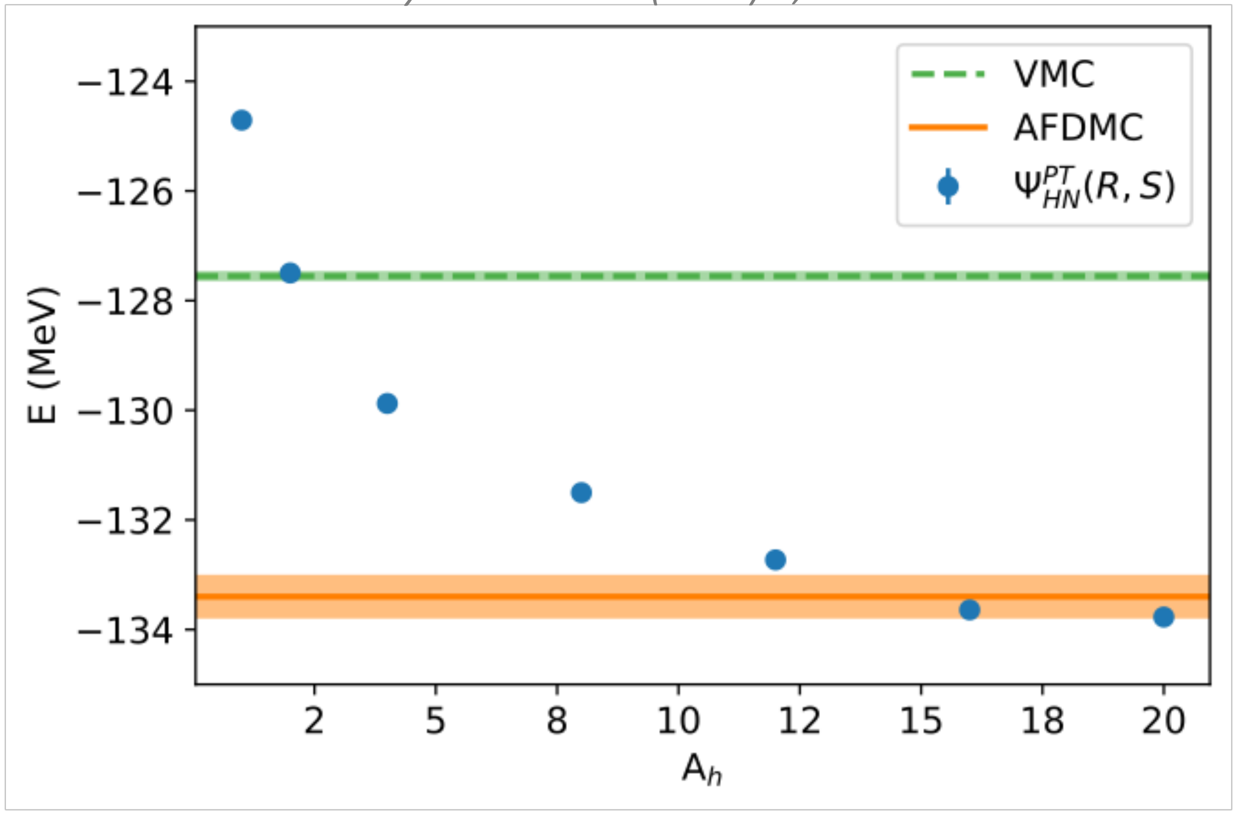


Courtesy of A. Lovato

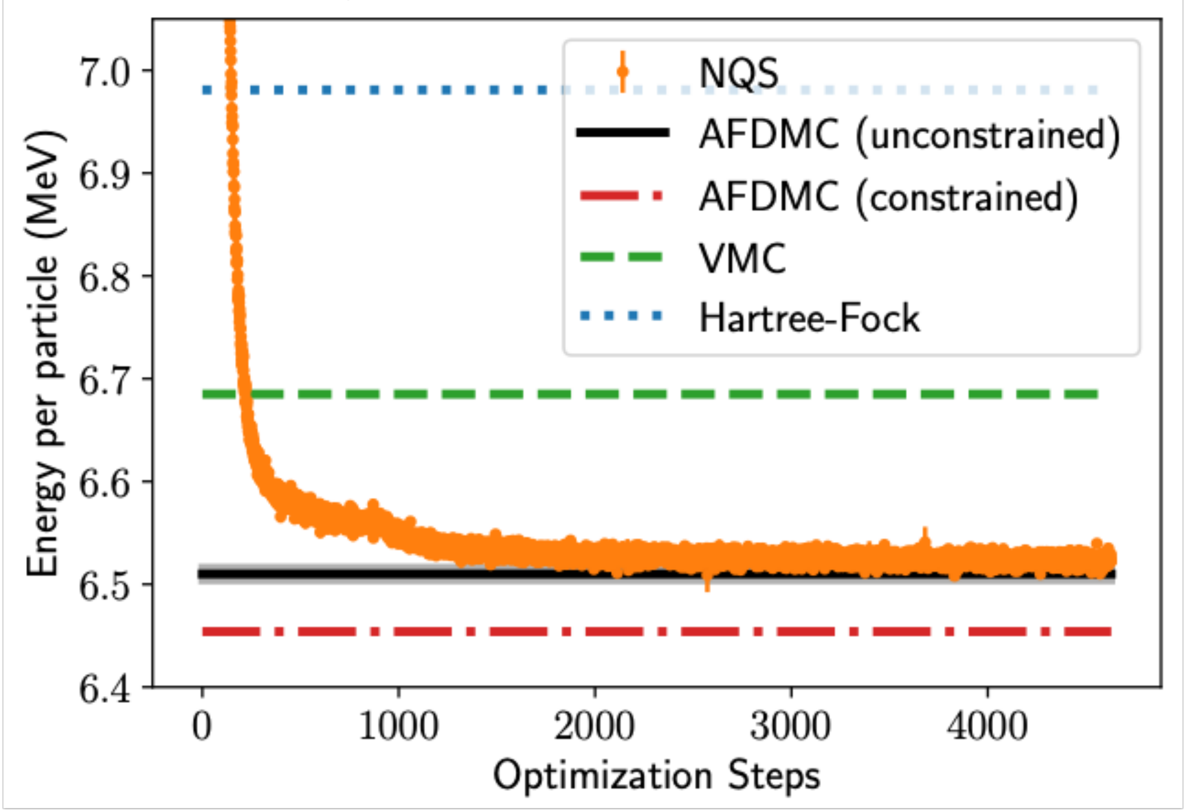
Neural-network quantum states

Successfully applied to both finite nuclei and infinite systems

Phys. Rev. Res. 4 (2022) 4, 043178



Phys. Rev. Res. 5 (2023) 3, 033062



Goal: reach medium-mass nuclei and neutron-star matter with high-resolution interactions

Courtesy of A. Lovato

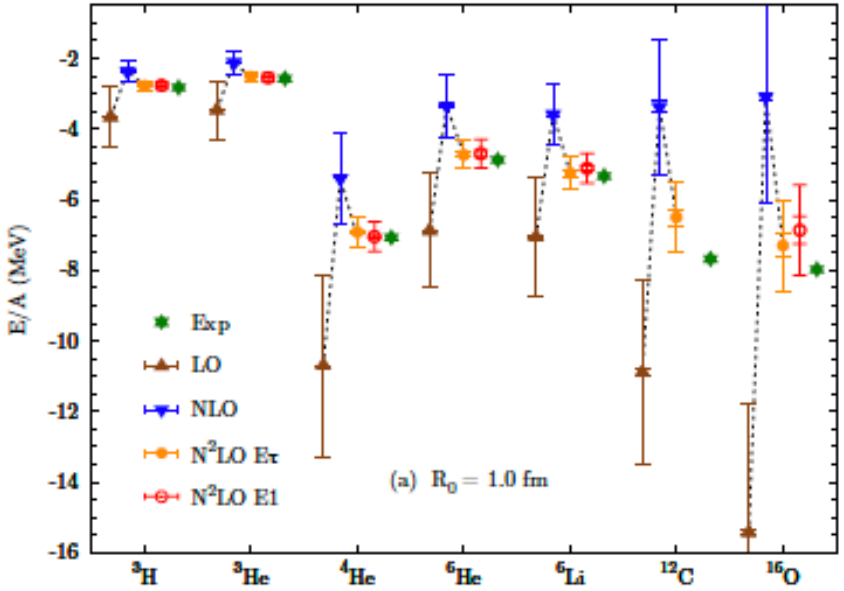
Auxiliary Field Diffusion Monte Carlo:

- Solve for the many-body Schroedinger equation through an evolution in imaginary time. Multidimensional integrals solved with Monte Carlo sampling.
- Code written in Fortran 2003, MPI, uses all cores available per node.
- Configuration distributed across cores. Load balancing needed to dynamically move configurations, not embarrassing parallel.
- Scales well up to over 100k cores with 100k MPI threads.
- Typical production runs take about 10 to 100 nodes up to 16 hours. Checkpoint, so time and resources can be decided based on availability.
- Moderate memory need, OMP not efficient. Use of GPUs under exploration, but will need to use not all available cores.
- AFDMC very powerful to calculate properties and transitions of nuclei up to A=20 and infinite matter.

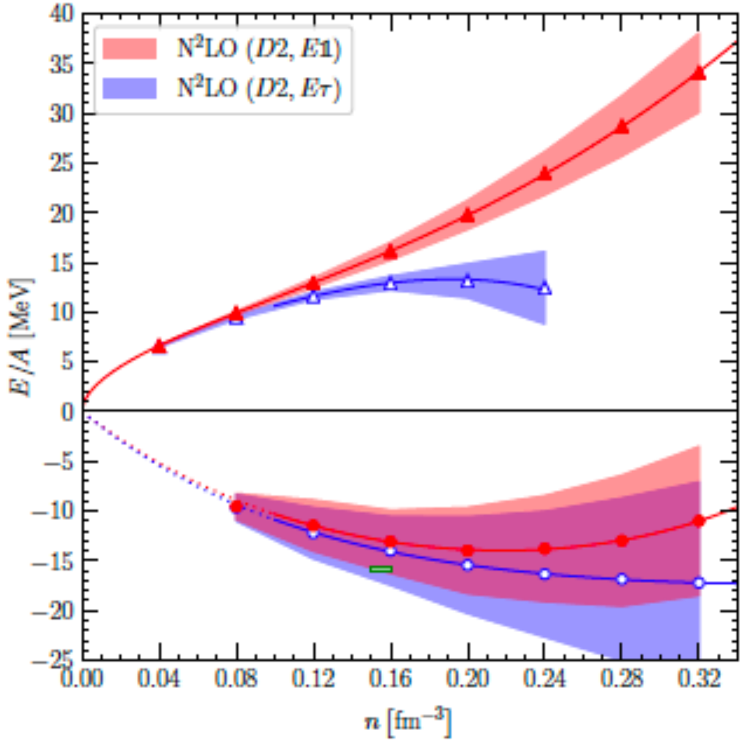
Courtesy of S. Gandolfi

Examples:

Nuclear ground state energy and nuclear and neutron matter EOS with uncertainty quantification:



Lonardoni, et al., PRL (2018), PRC (2018).



Lonardoni, et al., Phys. Rev. Research 2, 022033(R) (2020).

Also nuclear radii, magnetic moments, electro-weak transitions, distributions, and others.

Courtesy of S. Gandolfi

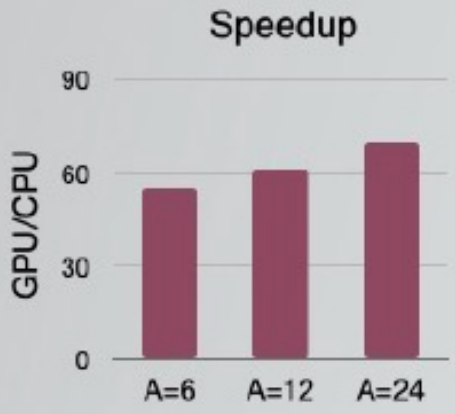
Nuclear Lattice Effective Field Theory

1. Profiling & hotpoint analysis
2. Kernel-by-kernel optimization
3. Parallel tasks
4. Reducing redundant MPI communication

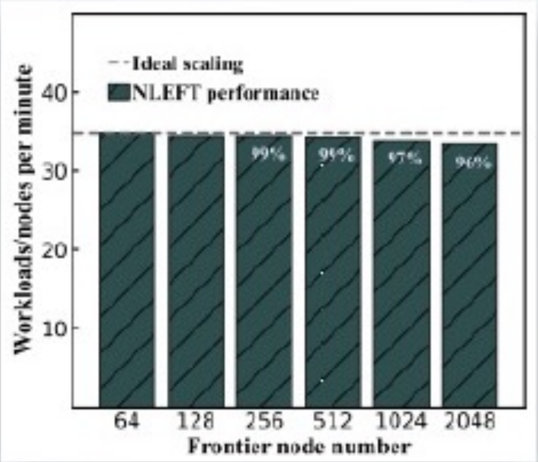
Hybrid: MPI(C++) & GPU(CUDA/HIP)

Summit

Number of CUDA kernels ~ 70
GPU usage ~ 80%



Frontier

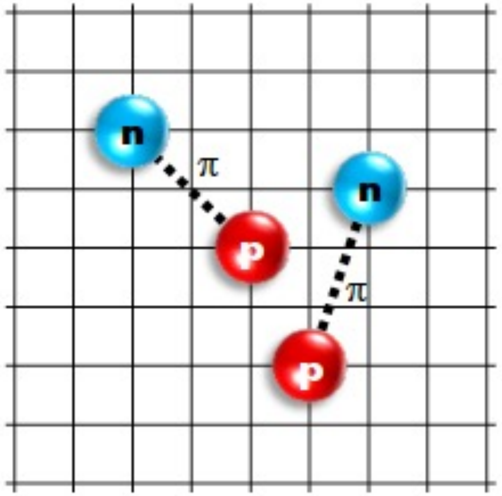


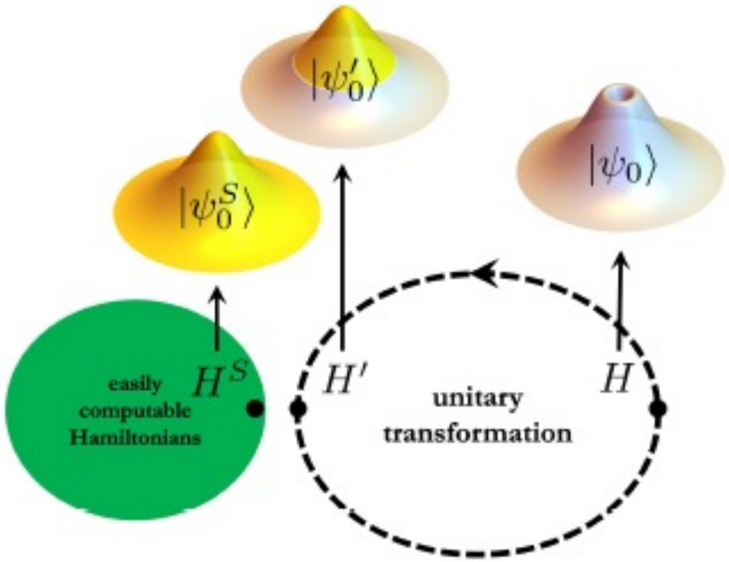
scaling performance with NMVe

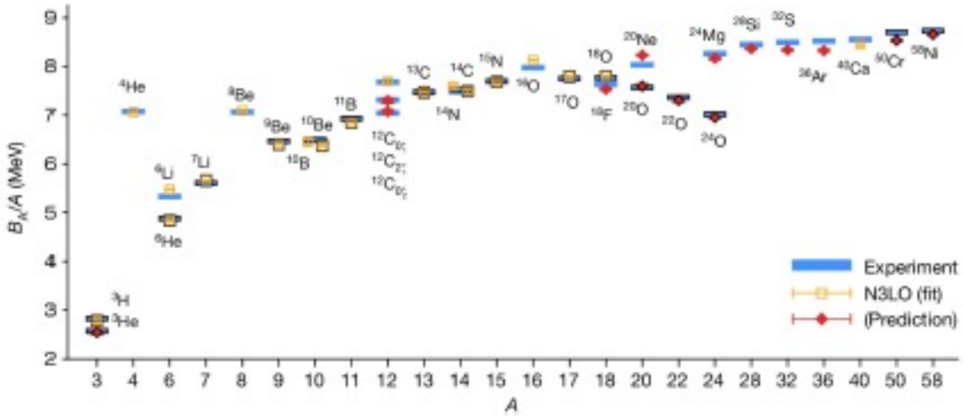
OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

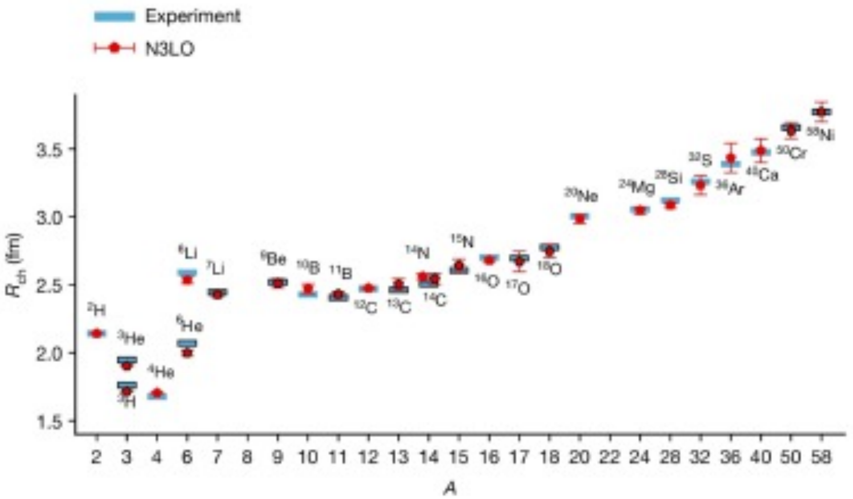
Courtesy of Dean Lee

Nuclear Lattice Effective Field Theory









Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, Lee, Li, Lu, M. Kim,
Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Courtesy of Dean Lee

In-Medium Similarity Renormalization Group

- **In-Medium Similarity Renormalization Group Codes**
  - IMSRG & Multireference IMSRG (*Hergert*)
  - Valence-Space IMSRG (*Stroberg*)
  - In-Medium Generator Coordinate Method (*Hergert & Yao (external)*)
- **Languages:** C/C++, Fortran, some Python
- **Libraries:**
  - SUNDIALS (ODE Solvers) – FastMATH SciDAC Institute
  - Linear Algebra: Armadillo, (vendor) BLAS, (vendor) LAPACK
  - GNU Scientific Library, GNU Multiprecision Library, HDF5
- **Current Target Platforms:**
  - Intel/AMD – typical university clusters & NERSC
- **Future Plans:**
  - Platforms: leadership class CPU/GPU systems (with next-gen IMSRG(3) and more complex GCM calculations)
  - Automatically scalable code (e.g., through Kokkos?)

Courtesy of H. Hergert

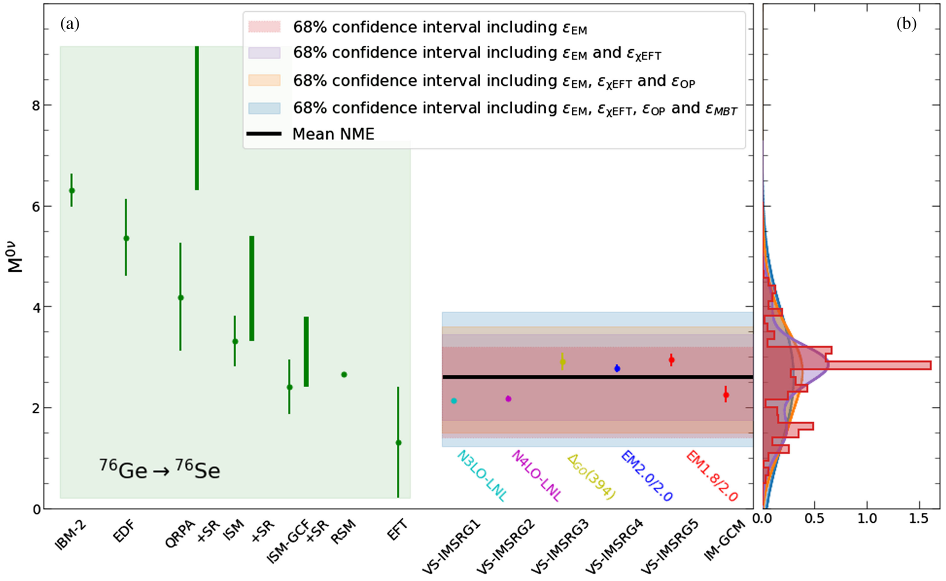
Ab Initio Uncertainty Quantification of Neutrinoless Double-Beta Decay in ^{76}Ge

Objectives

- The observation of neutrinoless double beta decay (NLDBD) would yield profound insights into the nature of neutrinos, their mass, and it might help explain the dominance of matter over antimatter in our universe.
- We perform *ab initio* calculations of the nuclear (decay) matrix elements (NMEs) in ^{76}Ge, which are necessary to reliably extract the neutrino mass scale from experimental data, and identify the primary drivers of theoretical uncertainties in current systematic state-of-the-art approaches.

Impact (as of now)

- We combine strong and electroweak interactions from (chiral) Effective Field Theory, complementary many-body methods – Valence-Space In-Medium Similarity Renormalization Group (VS-IMSRG) and In-Medium Generator Coordinate Method (IM-GCM) – and novel emulators to achieve the first comprehensive *ab initio* uncertainty quantification of the ^{76}Ge NME.
- Multioutput Multifidelity Deep Gaussian Processes are introduced as an emulator for general data and applied to *ab initio* results from different model space sizes.
- The application of IM-GCM to nuclei with triaxiality and shape coexistence also yields the first *ab initio* results for the structure of collective states in ^{76}Ge and ^{76}Se.



Comparison of NLDBD NMEs in ^{76}Ge from nuclear models and *ab initio* calculations. (a) NMEs from phenomenological models and results from VS-IMSRG and IM-GCM using different chiral interactions. Error bars of phenomenological NMEs reflect the discrepancy between calculations from different groups. (b) Posterior distribution function of the NME using a novel VS-IMSRG emulator with 8188 non-implausible chiral interactions from which confidence intervals are extracted.

Accomplishments (as of now)

- Published in PRL 132, 182502 (2024)

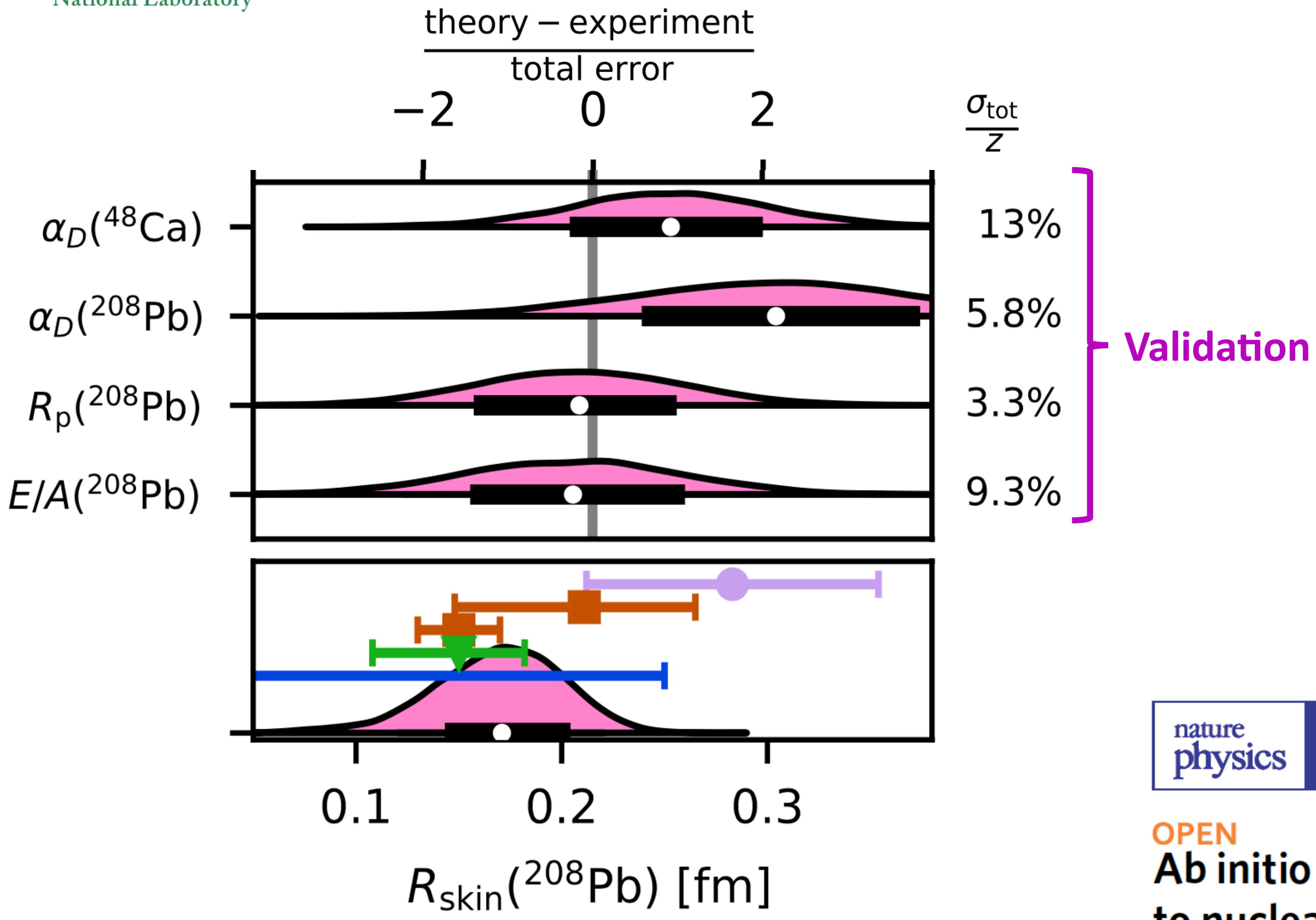
Courtesy of H. Hergert

Nuclear Coupled Cluster Oak Ridge (NUCCOR)

- Modern Fortran, MPI, OpenMP
- BLAS and Nuclear Tensor Contraction Library (CUDA, HIP)
- Runs at scale on Frontier
- Libraries: HDF5, SUNDIALS (for time evolution & symmetry projection)

Oak Ridge
National Laboratory

Neutron skin of ^{208}Pb

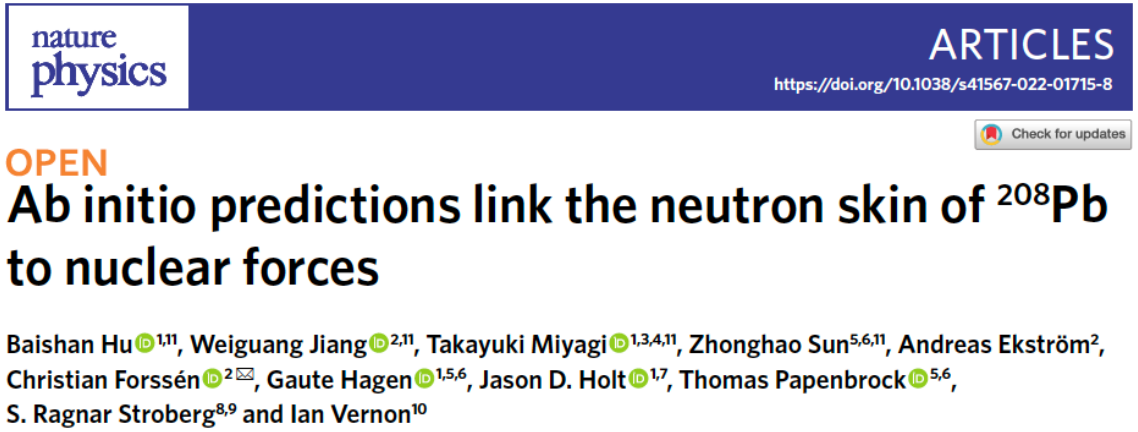


Posterior predictive distribution for the neutron skin in ^{208}Pb (experiments: electroweak (purple), hadronic (red), electromagnetic (green), and gravitational waves (blue) probes)

The size of the neutron skin of ^{208}Pb constrains the size of neutron stars.

Parity-violating e⁻ scattering (via Z boson) couples dominantly to neutrons.

Ab initio prediction more precise (and smaller) than experiment. Theory used history matching and Bayesian inference.


nature physics
ARTICLES
https://doi.org/10.1038/s41567-022-01715-8

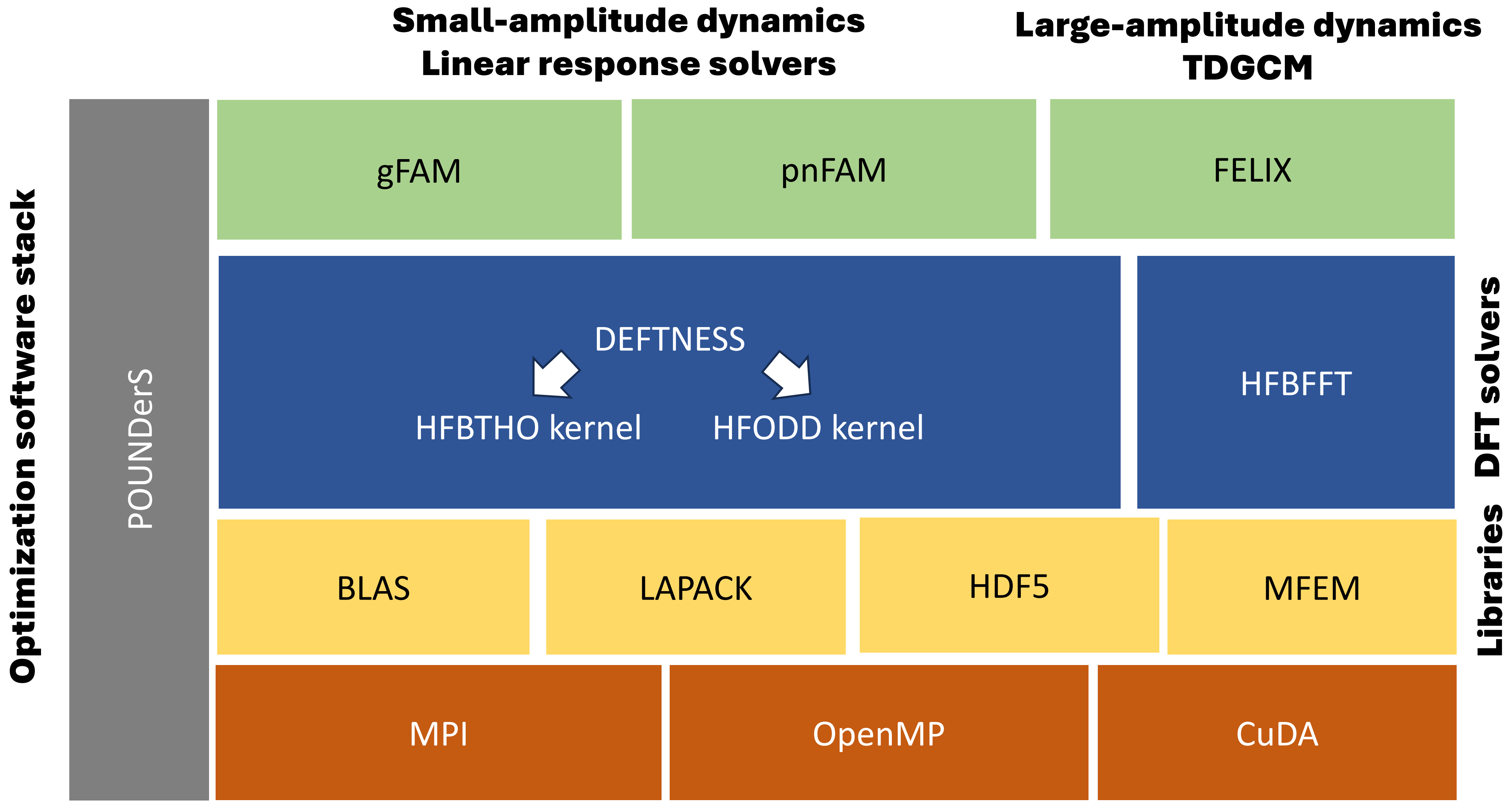
Check for updates

OPEN

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

Density Functional Theory: Infrastructure



Small-amplitude dynamics
Linear response solvers

Large-amplitude dynamics
TDGCM

Optimization software stack

POUNDerS

gFAM

pnFAM

FELIX

DEFTNESS

HFBTHO kernel

HFODD kernel

HFBFFT

DFT solvers

BLAS

LAPACK

HDF5

MFEM

Libraries

MPI

OpenMP

CuDA

Courtesy of N. Schunck

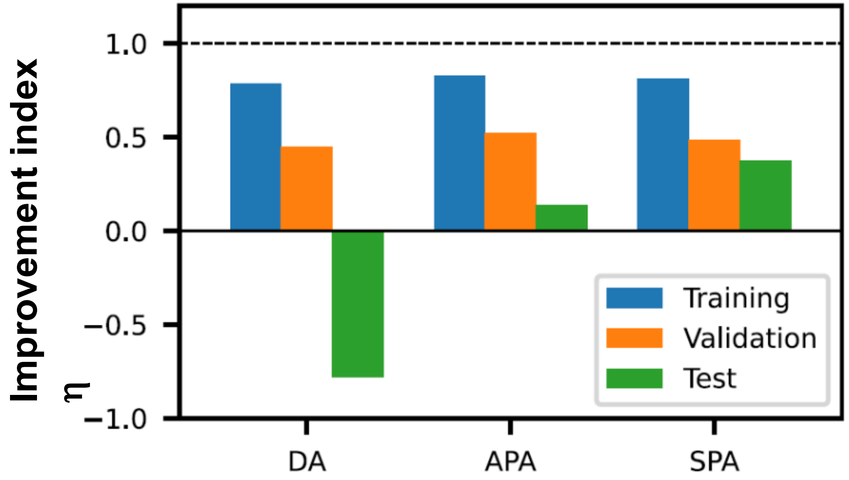
Thou Shalt Not Extrapolate: Quantifying the Unknown

Objectives

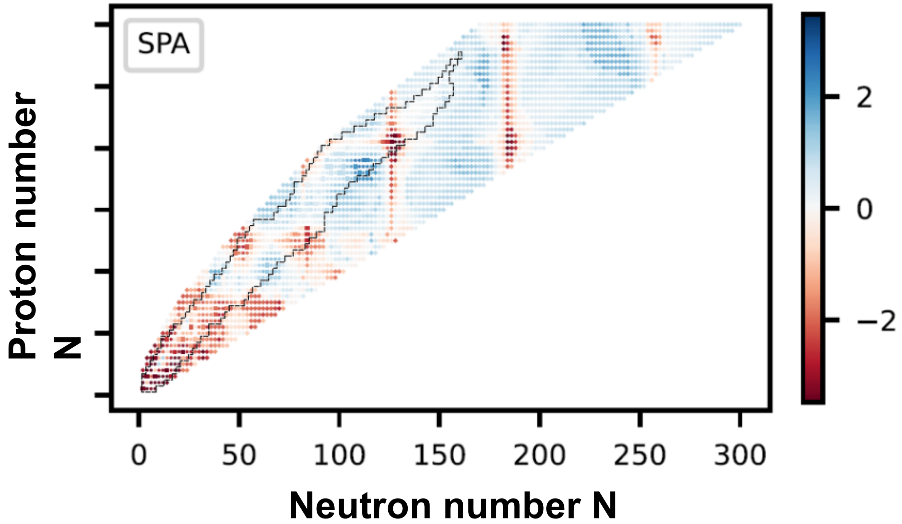
- Predictions of nuclear properties far from stability are based on theoretical models that must be corrected for systematic bias
- We developed a feature-learning novel method to compute reliable estimates of the model bias even in nuclei where experimental information is not available

Impact

- We proved that simple estimates of the model bias based only on proton and neutron numbers are unstable and lead to uncontrolled extrapolation errors
- Our feature learning approach gives robust estimates of model bias and is potentially generalizable to other observables and models



Positive (negative) values of the improvement index indicate the model bias correction has improved (degraded) predictions. Without feature selection (DA), fitting the model bias can degrade predictions while with selected-feature learning (SPA), predictions are systematically better



With feature learning, the model bias has learned the characteristic patterns of closed shells even outside the fitting range.

Accomplishments

- R. Navarro Perez and N. Schunck, "*Controlling extrapolations of nuclear properties with feature selection*", Phys. Lett. B **833**, 137336 (2022)

Courtesy of N. Schunck

Summary

- Several different codes / solvers
  - coupled cluster method, exact diagonalization (NCSM), similarity renormalization group (IMSRG) nuclear lattice EFT, quantum Monte Carlo
- Maintained by few individuals / groups
  - Some openly shared, some shared upon request
- Many benchmarks
- Interesting and impactful physics results
- Most codes/solvers run at scale on leadership computing facilities