Ab initio No-Core Shell Model calculations of light nuclei on current HPC Systems

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7th LENPIC workshop, March 11-13, 2024
HISKP, Bonn, Germany

Outline

- Current HPC systems
- Ab Initio Nuclear Structure
- NCSM Calculations of Light Nuclei
- Summary and Outlook

HPC Collaborators (incomplete . . .)

Metin Aktulga (MSU), Abdullah Alperen (MSU),
Brandon Cook (NERSC), Nan Ding (LBNL), Patrick Fasano (ANL),
Dossay Oryspayev (BNL), Meiyue Shao (Fudan U.),
Chao Yang (LBNL), . . .

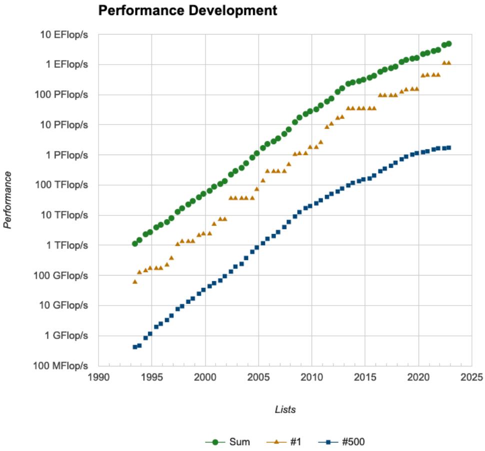
Made possible by

- DOE/SciDAC-5 project NUCLEI
- NERSC Exascale Science Applications Program for Perlmutter
- HPC allocations at ALCF (INCITE) and at NERSC

Computational resources: Moore’s Law

Computational Nuclear Structure needs High-Performance Computing

- Highly nontrivial to achieve good performance
- Multi-level parallelism
    - Distributed memory MPI between nodes
    - Shared memory OpenMP multi-threading
    - Accelerators (GPUs)
- Increasing performance gap between processing and memory performance



Need to collaborate with applied mathematicians and computer scientists

Top 12 HPC systems (Nov 2023)

1. Frontier (Oak Ridge, US), AMD CPU & AMD GPU, 1,194 PFlop/s
2. Aurora (Argonne, US), Intel CPU & Intel GPU, 585 PFlop/s
3. Eagle (Microsoft, US), Intel CPU & NVIDIA GPU, 561 PFlop/s
4. Fugaku (RIKEN, Japan), Fujitsu CPU, 442 PFlop/s
5. LUMI (Finland), AMD CPU & AMD GPU, 380 PFlop/s
6. Leonardo (Italy), Intel CPU & NVIDIA GPU, 239 PFlop/s
7. Summit (Oak Ridge, US), IBM CPU & NVIDIA GPU, 149 PFlop/s
8. MareNostrum (Spain), Intel CPU & NVIDIA GPU, 138 PFlop/s
9. Eos SuperPOD (NVIDIA, US), Intel CPU & NVIDIA GPU, 121 PFlop/s
10. Sierra (Livermore, US), IBM CPU & NVIDIA GPU, 95 PFlop/s
11. Sunway TaihuLight (China), Sunway CPU, 93 PFlop/s
12. Perlmutter (NERSC, US), AMD CPU & NVIDIA GPU, 79 PFlops/s

…

18. JUWELS (Jülich, Germany), AMD CPU & NVIDIA GPU, 44 PFlops/s

…

27. Polaris (Argonne, US), AMD CPU & NVIDIA GPU, 26 PFlops/s

DOE – High Performance Computing hardware

- Oak Ridge Leadership Computing Facility
  - Summit (2018 – current)
    4,608 nodes, 2 IBM CPUs & 6 NVIDIA V100 GPUs/node
  - Frontier (2022 – current)
    9,402 nodes, 1 AMD CPU & 4 AMD MI250X GPUs/node
- Argonne Leadership Computing Facility
  - Theta (2017 – 2023), retired Dec. 31, 2023
    4,392 nodes, 64-core Intel Xeon Phi (KNL)
  - Polaris (2023 – current)
    560 nodes, 1 AMD CPU & 4 NVIDIA A100 GPUs/node (testbed)
  - Aurora (2023, pre-production)
    10,624 nodes, 2 Intel CPUs & 6 Intel PVC GPUs/node
- National Energy Research Scientific Computing Center
  - Perlmutter-GPU (2022 – current)
    1,536 nodes, 1 AMD CPU & 4 NVIDIA A100 GPUs/node
  - Perlmutter-CPU (2023 – current)
    3,072 nodes, 2 64-core AMD CPUs/node

Performance Portability and Productivity (P3)

Current HPC systems have diverse hardware

- Multi-core (many-core) CPUs
  - with hyper-threading ('oversubscribing cores') ✓
  - with SIMD instruction set (vectorization) ✓
- Reconfigurable memory
  - e.g. HBW memory on Intel Xeon Phi (Knights Landing, KNL) ✓
- Accelerators (GPUs)
  - NVIDIA, AMD, Intel, . . .
  - require GPU-enabled source code
    - typically vendor specific (CUDA, Intel OneAPI, . . .) ✓
    - some with support for more than one vendor (OpenACC, . . .) ✓
    - rarely support for all vendors (OpenMP target offload, Kokkos, . . .) ←
- Developing and maintaining efficient codes
  - hardware specific code
- Challenge: one source that
  - runs on range of hardware (Portability)
  - performs well on range of hardware (Performance Portability)
  - so that domain scientists can do their domain science (Productivity)

Allocations on DOE Leaderschip Computing Facilities

ALCC: ASCR Leadership Computing Challenge

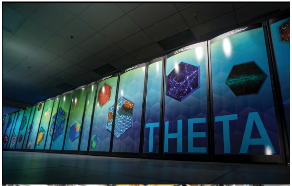
INCITE: Innovative and Novel Computational Impact on Theory and Experiment

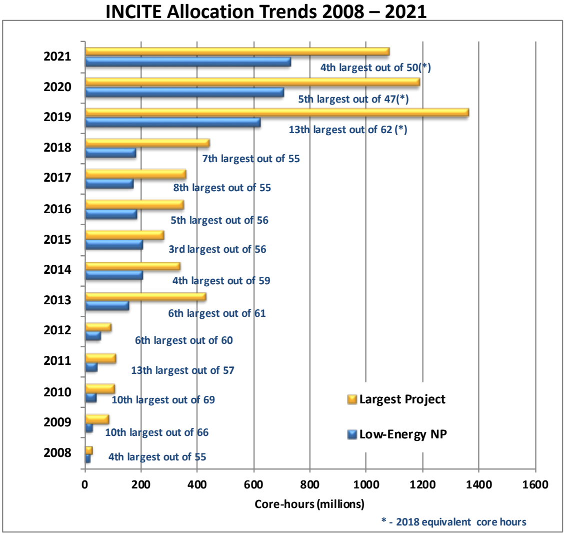
In 2023: 56 INCITE projects awarded

- INCITE proposals reviewed by domain scientists as well as by HPC experts on code-readiness, but decided by ASCR
- INCITE awards require quarterly progress reports
- OLCF – 29 active projects in fall 2022, across all sciences
    - 15 INCITE and 14 ALCC projects
    - 2 INCITE Nuclear Structure and Reactions projects
    - all INCITE and ALCC projects on OLCF have demonstrated good performance on GPUs (including NucPhys codes)
- ALCF – 32 projects in 2021, across all sciences
    - 16 INCITE and 16 ALCC projects in 2021
    - 1 INCITE and 1 ALCC Nuclear Structure and Reactions project
    - starting from 2024, all INCITE and ALCC projects on ALCF have to demonstrate good performance on GPUs
    - not all NucPhys codes targeting ALCF have been ported to GPUs
        - MFDn with NN potentials has been ported to NVIDIA GPUs

INCITE allocations over time by NUCLEI/UNEDF

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING



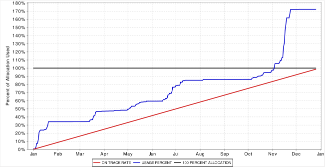


INCITE usage by MFDn and QMC on Theta @ ALCF

2021: Excellent

NucStructReact_6 Machine: THETA

Allocation Node Hours: 500,000 Data Dates: 2021-01-01 through 2021-12-26
Usage Node Hours: 861,539 (172.3%) Allocation Dates: 2021-01-01 through 2022-01-02



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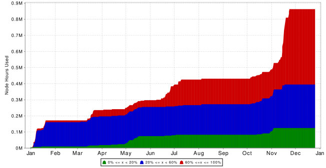
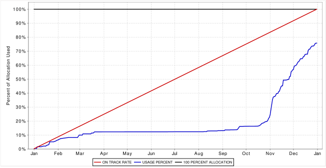


- 125% use allowed through Nov
- available resources checked at submission, not at runtime

2023: Poor

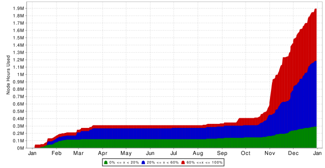
NucStructReact_6 Machine: THETA

Allocation Node Hours: <null> Data Dates: 2023-01-01 through 2024-01-02
Usage Node Hours: <null> (<null>) Allocation Dates: <null> through <null>



NucStructReact_6 Machine: THETA

Allocation Node Hours: 0 Data Dates: 2023-01-01 through 2024-01-02
Usage Node Hours: 0 (0) Allocation Dates: <null> through <null>



- missed N3LO 3NF milestone
- may negatively impact future allocations …

National Energy Research Scientific Computing center

Powering **Scientific Discovery** for 50 Years

- About 10,000 users
  (compared to about 1,500 on ALCF & OLCF each)
- Many more projects than on ALCF & OLCF
- Requests for NERSC resources have low threshold
  - virtually any scientists with a DOE grant
    can obtain a modest NERSC allocation
  - allocations decided by DOE domain science program managers
- Number of Nuclear Physics projects in 2022: 74
- Amount of resources for Nuclear Physics:
  10 % of NERSC total resources
- Node hours awarded to us in 2022: 60,000 on Cori @ NERSC
  compared to 750,000 on Theta @ ALCF

Ab Initio Nuclear Structure allocations 2024 – 2025

SciDAC5/NUCLEI approaches targeting current DOE HPC platforms

- Quantum Monte Carlo methods Aurora @ ALCF
  - Variational Monte Carlo (VMC)
  - Green's Function Monte Carlo (GFMC)
  - Auxiliary-Field Diffusion Monte Carlo (AFDMC)
  - . . .
- Configuration Interaction:
  Expansion of many-body wavefunction
  in Slater determinants of single-particle wavefunctions
  - Traditional Shell Model codes
  - No-Core Shell Model Perlmutter @ NERSC, Aurora @ ALCF
  - Coupled Cluster Summit, Frontier @ OLCF
  - . . .
- Lattice Simulations
  - Nuclear Lattice Effective Field Theory Summit, Frontier @ OLCF
- . . .

Computational Challenges

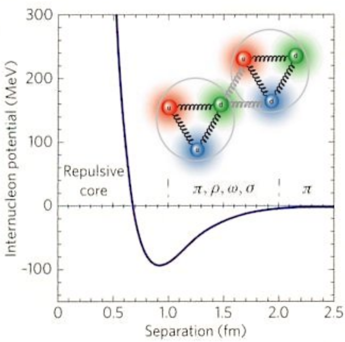
- Strong interactions, with both short-range and long-range pieces
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Self-bound quantum many-body problem,
  with $3A$ degrees of freedom in coordinate (or momentum) space, as well as spin degrees of freedom
- Uncertainty quantification for calculations needed
  - for comparisons with experiments
  - for comparisons between different methods
- Sources of numerical uncertainties
  - statistical and round-off errors
  - systematical errors inherent to the computational method
    - Monte Carlo methods: sensitivity to the trial wave function
    - Configuration Interaction methods: finite basis space
    - Lattice Simulations: finite volume and lattice spacing
  - uncertainties in the nuclear interactions

Nuclear Interactions

$$\hat{\mathbf{H}}_{\text{rel}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

Nuclear interaction not well-determined

- In principle calculable from QCD
- Constrained by (fitted to) experimental (scattering) data



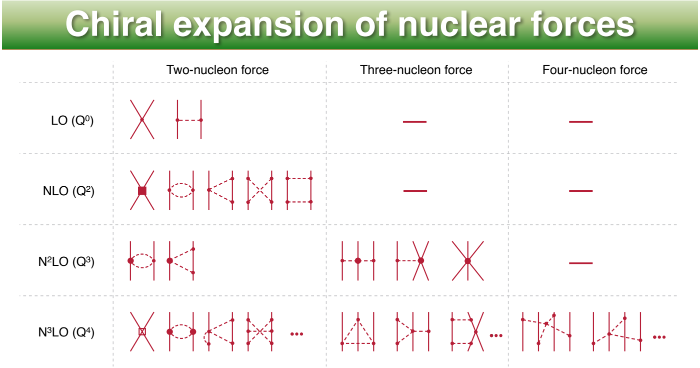
Alphabet of realistic NN potentials

- Argonne potentials (AV18 + . . .)
- Bonn potentials
- Chiral EFT interactions
  - Δ-less
  - Δ-full
  - pion-less
- Daejeon16 (based on Idaho-N^{3}LO)
- . . .

Most NN potentials need 3N forces for agreement with data for nuclei

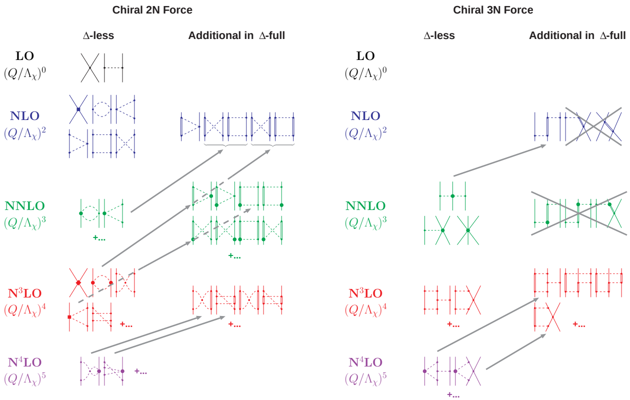
Nuclear Interactions from chiral EFT

- Controlled power series expansion in $Q = \max(p, M_\pi)/\Lambda_B \sim 0.3$
- Hierarchy for many-body forces $V_{NN} \gg V_{NNN} \gg V_{NNNN}$
  - 3NFs appear at N^{2}LO, 4NFs appear at N^{3}LO



- Allows for quantification of uncertainties due to the interaction

Δ-full Chiral EFT Interactions



$m_\pi \sim$ 140 MeV
$m_\rho \sim$ 770 MeV
$m_N \sim$ 940 MeV
$m_N \sim$ 1210 MeV
$m_\Delta - m_N \sim$ 270 MeV

several diagrams get 'promoted' to lower orders

3NFs start at NLO

in particular

Fujita–Miyazawa term

If pions are relevant for chiral EFT,
then what about the role of the nucleon-Δ mass difference?

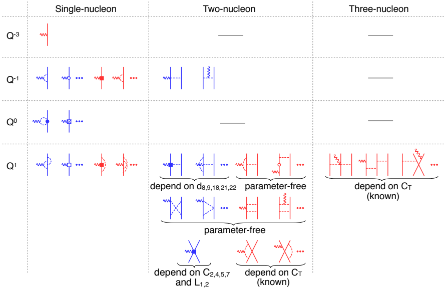
Machleidt and Entem, Phys. Rept. 503 (2011);
see also Piarulli and Tews, Front. Phys. doi: 10.3389/fphy.2019.00245

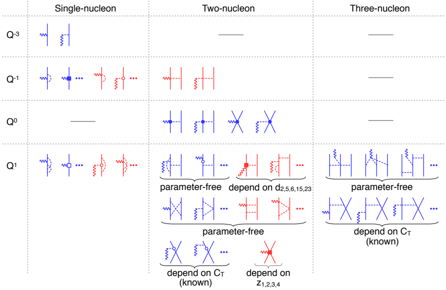
NN Potential and Scattering Data

- NN potentials fitted to phase-shifts
  - propagation of experimental uncertainties?
  - fitted up to what energy?
- Experiments for *pp* and *pn* scattering, but not for *nn* scattering
  - analysis in terms of isoscalar $T = 0$ and isovector $T = 1$ channels
- NN scattering data constrain only the on-shell NN potential, but not the off-shell behavior
  - many NN potentials describe NN scattering data, but differ for $A > 2$
  - wave functions not unique (unitary transformations)
  - for $A > 2$ nuclei we may also need 3N interactions
- Additional physics input
  - chiral effective field theory
  - fit select observables from light nuclei (which?)
- Additional consideration
  - suitability for computational framework (e.g. local vs. nonlocal)
- Implicit assumption
  - NN potential in vacuum and in nuclei (nuclear matter) is the same

Electroweak Operators from Chiral EFT

figures from Epelbaum, arXiv:1908.09349





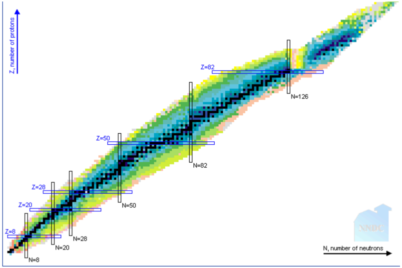
em charge and current operators; **axial** charge and current operators

- Chiral EFT two-body corrections to M1 operator at NLO and N^{3}LO
- Two- and three-body corrections to charge operator at N^{3}LO
- Two-body corrections to axial charge at NLO and N^{3}LO
- Leading two-body corrections to axial current at N^{2}LO and N^{3}LO
- Three-body corrections to axial current at N^{3}LO

Configuration Interaction Methods

- Shell Model

  Maria Goeppert Mayer,
  Nuclear Configurations in the Spin-Orbit Coupling Model. I. Empirical Evidence,
  Phys. Rev. 78, 16 (1950) and
  II. Theoretical Considerations,
  Phys. Rev. 78, 22 (1950)



  Eugene Wigner, Maria Goeppert Mayer, J. Hans D. Jensen, 1963 Nobel Prize

- Coupled Cluster methods (CC)
  - in particular suitable for closed-shell nuclei
  - in past decade significant improvements for select open-shell nuclei

  Hagen, Papenbrock, Hjorth-Jensen, Dean, Rept. Prog. Phys. 77, 096302 (2014)

- In-Medium Similarity Renormalization Group (IM-SRG)

  Hergert, Bogner, Morris, Schwenk, Tsukiyama, Phys. Rep. 621, 165 (2016)

- No-Core Shell Model / No-Core Configuration Interaction

  Barrett, Navrátil, Vary, Prog. Part. Nucl. Phys. 69, 131 (2013)

No-Core Shell Model

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i|\Phi_i\rangle$
- Express Hamiltonian in basis $\langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core: All A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result (at least for states below threshold)
  - caveat: complete basis is infinite dimensional
- In practice
  - truncate basis
  - study behavior of observables as function of truncation
- Computational challenge
  - construct large ($10^{10} \times 10^{10}$) sparse symmetric matrix H_{ij}
  - obtain lowest eigenvalues & -vectors corresponding to low-lying spectrum and eigenstates

Note: Computational method, not a model

No-Core Configuration Interaction method

Basis Expansion

- Expand A-body wave function in basis functions

$$\Psi(r_1,\ldots,r_A) = \sum a_i \Phi_i(r_1,\ldots,r_A)$$

- Use basis of single Slater Determinants of Single-Particle states

$$\Phi_i(r_1,\ldots,r_A) = \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

- Single-Particle basis states $\phi_{ik}(r_k)$
  - eigenstates of SU(2) operators $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$, and $\hat{\mathbf{J}}_\mathbf{z}$ with quantum numbers n, l, s, j, m
  - radial wavefunctions
    - Harmonic Oscillator (HO) — allows for exact factorization of Center-of-Mass
    - Coulomb–Sturmian — Caprio, Maris, Vary, PRC86, 034312 (2012); PRC90, 034305 (2014)
    - Natural orbitals — Fasano, Constantinou, Caprio, Maris, Vary, PRC105, 054301 (2022)
    - …

Truncation Schemes

- *M*-scheme: Many-Body basis states $|\Phi_i\rangle$ eigenstates of $\hat{\mathbf{J}}_{\mathbf{z}}$

$$\hat{\mathbf{J}}_{\mathbf{z}}|\Phi_i\rangle = M|\Phi_i\rangle = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

  - two runs (positive and negative parity) gives entire spectrum
- $N_{\rm max}$ truncation: Many-Body basis states $|\Phi_i\rangle$ satisfy

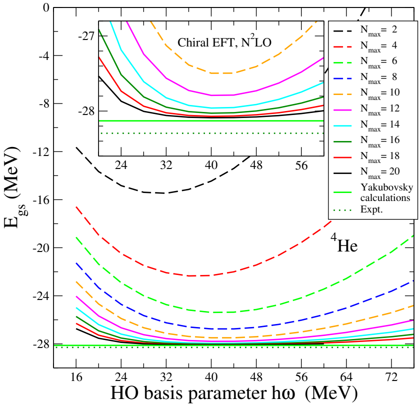
$$\sum_{k=1}^{A} \left(2\, n_{ik} + l_{ik}\right) \leq N_0 + N_{\rm max}$$

  - exact factorization of Center-of-Mass motion in HO basis
- Alternatives:
  - Full Configuration Interaction (FCI), truncation on Single-Particle basis only commonly used in valence shell model, quantum chemistry, . . .
  - Importance Truncation Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model Abe *et al*, PRC86, 054301 (2012)
  - Truncation based on dominant SU(3) or $\mathrm{Sp}(3,\mathbb{R})$ symmetries

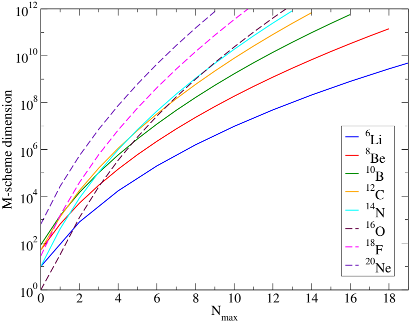
    Dytrych *et al*, PRL111, 252501 (2013); McCoy, Caprio, Dytrych, Fasano, PRL 125, 102505 (2020)
  - . . .

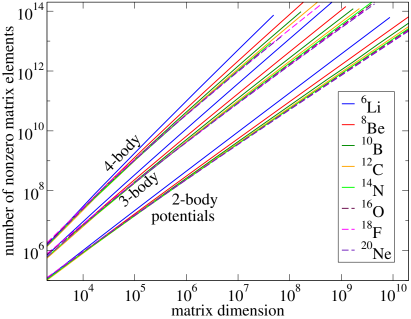
Convergence of basis expansion

- Variational: for any finite truncation of the infinitely-large basis, eigenvalue is an upper bound for the ground state energy
- Smooth approach to asymptotic value with increasing basis space
- Convergence: independence of both truncation paramere $N_{\max}$ and HO basis parameter $\hbar\omega$
    - different methods using the same interaction give same results within numerical uncertainties



Computational Challenge





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$, preferably $N_{\text{max}} = 10$ or 12 for meaningful extrapolation and numerical error estimates
- Largest calculation with NN-only potentials: ^{12}Be at $N_{\text{max}} = 12$
  - dimension of 35 billion, with 60 trillion nonzero matrix elements
  - needed all of Theta at ALCF (or all of Cori-KNL at NERSC)

McCoy, Caprio, Maris, Fasano, arXiv:2402.12606

Extrapolation to the Complete Basis

Challenge: achieve numerical convergence for No-Core CI calculations using a finite amount of CPU time on current HPC systems

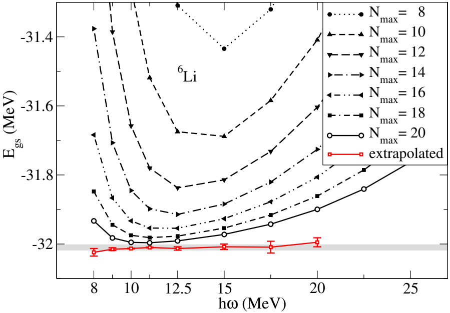
- Perform a series of calculations with increasing N_{max} truncation
- Extrapolate to infinite model space ⟶ exact results
  - Empirical: binding energy exponential in N_{max}

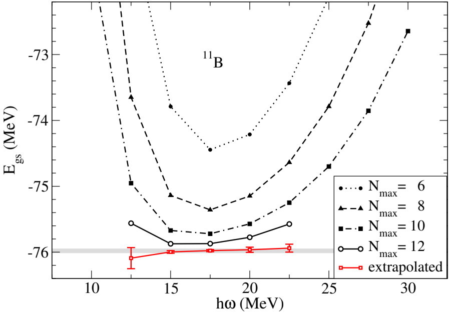
    $$E^{\hbar\omega}(N) = E^{\hbar\omega}_{\infty} + a_1 \exp(-a_2 N)$$

    to determine $E^{\hbar\omega}_{\infty}$
  - use $\hbar\omega$ and N_{max} dependence to estimate numerical error bars

    Maris, Shirokov, Vary, PRC79, 014308 (2009)
- Extrapolate using exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$ motivated by IR and UV behavior of wavefunction, based on s.p. asymptotics
  Coon *et al*, PRC86, 054002 (2012); Furnstahl *et al*, PRC86, 031301(R) (2012); More *et al*, PRC87, 044326 (2013); Wendt *et al*, PRC91, 061301 (2015); Gazda *et al*, PRC106, 054001 (2022);. . .
- Use Machine Learning/Artificial Neural Networks
  Negoita *et al*, PRC99, 054308 (2019); Jiang it at al, PRC100, 054326 (2019); Knöll *et al*, PLB839, 137781 (2023); . . .
- Bayesian inference?

Empirical exponential extrapolation of binding energies

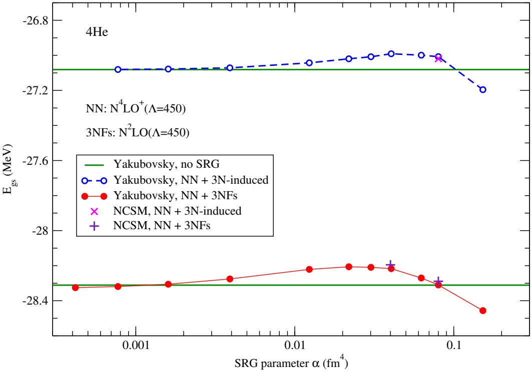




- Use 3 consecutive N_{max} values to determine $E_\infty^{\hbar\omega}$
- Optimal $\hbar\omega$ where $|E_\infty^{\hbar\omega} - E^{\hbar\omega}(N_{\text{max}})|$ is minimal (above var. min.)
- Numerical uncertainty estimate: Maximum of
  - difference in $E_\infty^{\hbar\omega}$ for two successive extrapolations
  - half the variation in $E_\infty^{\hbar\omega}$ over 8 MeV interval around optimal $\hbar\omega$
  - 20% of $|E_\infty^{\hbar\omega} - E^{\hbar\omega}(N_{\text{max}})|$ at optimal $\hbar\omega$

Similarity Renormalization Group (SRG) evolution

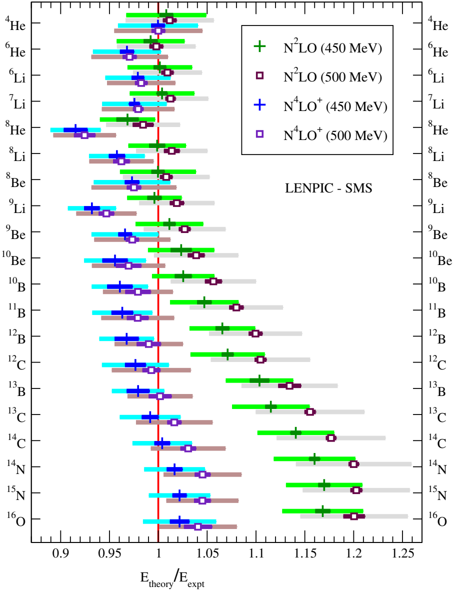
- Apply unitary transformation on Hamiltonian
  to improve numerical convergence in finite HO model spaces



- No change in observables provided that
  - any induced many-body interactions are included
  - same SRG evolution is applied to operators for observables
- Effect of induced 4-body interactions
  - small down to $\alpha < 0.1$ fm^4
  - grow rapidly for $\alpha > 0.2$ fm^4

PM, Le, Nogga, Roth, Vary, Front. Phys. 11 1098262 (2023)

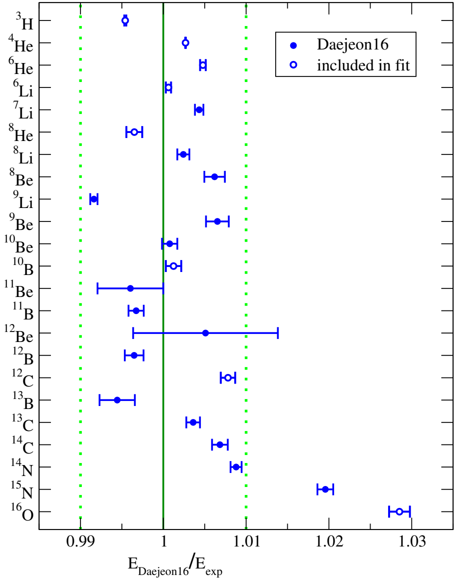
Binding Energies with LENPIC-SMS chiral EFT



PM, Le, Nogga, Roth, Vary,
Front. Phys. 11 1098262 (2023)

- NN potential up to N^{4}LO$^+$
- 3NFs at N^{2}LO
- SRG evolved to $\alpha = 0.08$ fm^4
- LECs fitted to
  - NN scattering data
  - ^{3}H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

Binding energies with Daejeon16

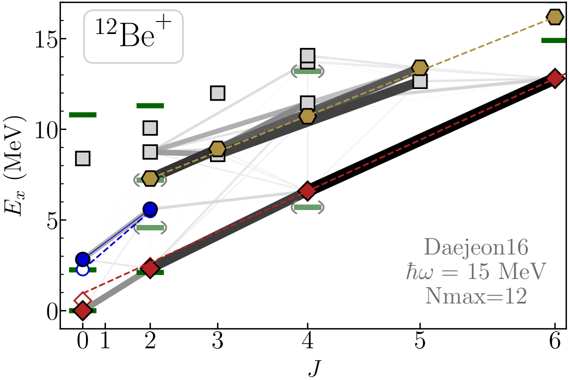


(PM, Shin, Caprio, Vary, in preparation)

- NN interaction, based on SRG evolved chiral EFT, using phase-equivalent transformations to fit select *p*-shell nuclei
- Ground state energies agree with experiment to within 1% for all *p*-shell nuclei up to A=14
- Correct J^π for ^{10}B (fitted)
- Parity inversion ^{11}Be
- Correct J^π for ^{12}B
- Energies of narrow excited states also agree with data

Special Case: Low-lying levels of ^{12}Be

McCoy, Caprio, PM, Fasano
arXiv:2402.12606



- Short $K = 0$ rotational band
  - ground state band at low $N_{\max}$
  - dominated by $N_{\max} = 0$ configs
  - closed-shell neutrons
- Long $K = 0$ rotational band
  - ground state band at high $N_{\max}$
  - dominated by $N_{\max} = 2$ configs
- $K = 2$ rotational band

MFDn moving towards Exascale

Exascale computing enables calculations for

- larger model spaces for *p*-shell nuclei
- unnatural parity states?
- ’cross-shell’ nuclei (e.g. neutron-rich B, C, N isotopes)?
- *sd*-shell nuclei?

Towards Exascale

- Incite 2024 Allocation on Aurora @ ALCF
    - expected (?) fourth quarter 2024 – first quarter 2025
    - have to demonstrate performance ’by this summer’

Porting MFDn to run efficiently on Aurora requires significant effort

- eigensolver
- matrix construction with NN potentials
- including 3N interactions on GPUs

Timeline

- April - June 2024 for initial port of MFDn to OpenMP target offload

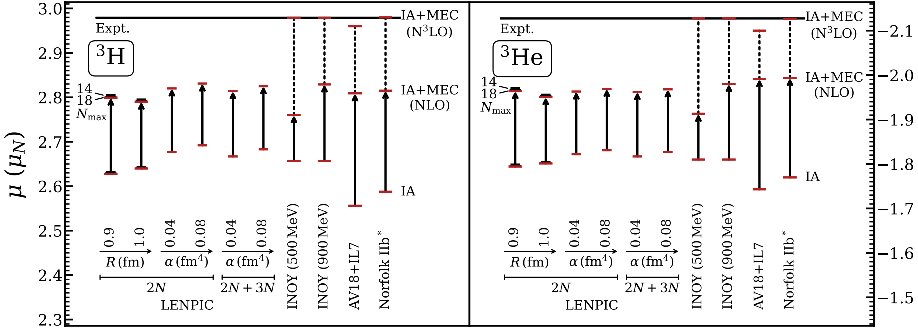
LENPIC moving forward?

Moving forward with LENPIC SMS interactions
and consistent electroweak operators towards Exascale computing

- Spectra with consistent N^3LO 3NFs,
  in combination with NN potentials at N^3LO, N^4LO, and N^4LO^+
- Radii, magnetic moments, and quadrupole moments
  - SRG evolution at 2-body level
  - consistent 2-body operators up to N^3LO
  - importance of 3-body operator?
  - convergence of expectation values of 'long-range' operators?
- E0, M1, and E2 transitions
  - with consistent 2-body operators at N^3LO
- β decay
  - with consistent 2-body operators at N^3LO
- Benchmark vs Faddeev–Yakubovsky calculations

Magnetic moment at N^{2}LO (LENPIC SCS)

Pal, Sarker, Fasano, PM, Vary, Caprio, Basili, PRC108, 024001 (2023)



- Consistent M1 operator with LENPIC-SCS interactions up to N^{2}LO
- Magnetic observables of *p*-shell nuclei (Fasano, PhD thesis (2023))
- Need consistent M1 operators at N^{3}LO

LENPIC moving forward!

- Consistent N^{3}LO 3N interaction, SRG evolved
  - Bochum, Jülich, Darmstadt
- Consistent electroweak 2-body operators up to N^{3}LO
  - Bochum
- Express e.w. (non-scalar) operators in HO basis and evaluate TBMEs for electroweak operators
  - Jülich, Darmstadt
- SRG evolution of e.w. operators (w/o induced 3-body operators)
  - Jülich, Darmstadt
- Talmi-Moshinski transformation of e.w. operators
  - Darmstadt
- Evaluate expectation values of e.w. operators using wave-functions obtained with MFDn
  - Ames, IA
- Benchmark against Faddeev–Yakubovsky calculations
  - Jülich, Cracow
- Chiral uncertainties
  - Columbus, OH

Concluding remarks and Summary

- Moving towards Exascale computing
  - challenging and exciting
- Should open up new opportinities
  - reduced numerical incertainties
  - extend calculations to larger nuclei?
  - explore unnatural parity spectrum?
  - explore intruder states?
- Consistent interactions and e.w. operators up to N^{3}LO
  - reduced chiral uncertainties