HPC for Ab Initio Nuclear Structure and Reactions

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NSAC Longe Range Plan Town Hall Meeting
Nuclear Structure, Reactions, and Astrophysics
Nov 14 – 16, 2022
Argonne National Laboratory

Objectives

Obtain predictive description of nuclei and their internal structure in terms of protons and neutrons with quantified uncertainties

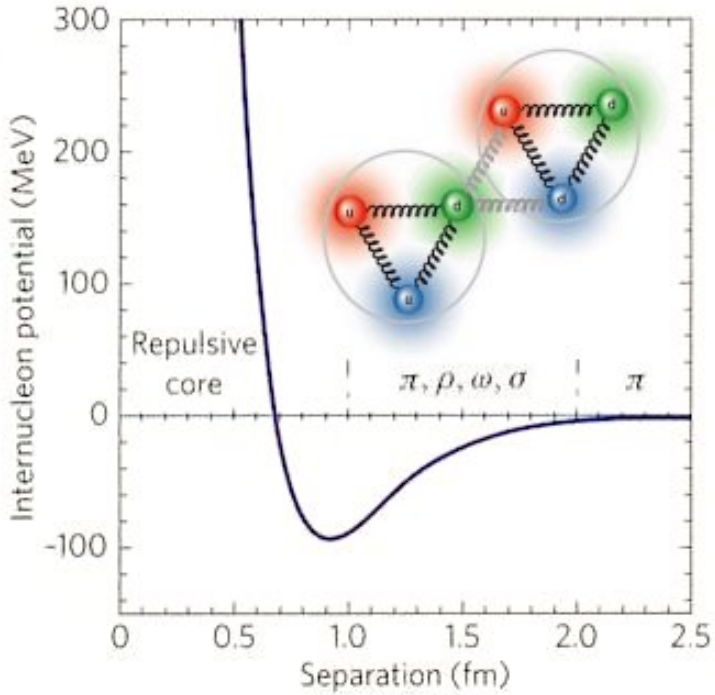
- Bound states of protons and nucleons
  - binding energies, spectra (including resonances)
  - wavefunctions
  - densities
- Wavefunction and densities
  input for calculation of electroweak observables
  - M1 and E2 moments and transitions
  - beta decay
  - nuclear reactions
- Cross-cutting:
  Wavefunction and densities also needed as input for e.g.
  - QCD physics (EIC)
  - fundamental symmetries (double-beta decay)

Computational Challenges

- Self-bound quantum many-body problem, with $3A$ degrees of freedom in coordinate (or momentum) space, as well as spin degrees of freedom
- Strong interactions, with both short-range and long-range pieces
  - Purely phenomenological potentials
  - Phenomenological interaction based on meson-exchange models
  - Interactions based on chiral Effective Field Theory (EFT)
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Interaction parameters fitted to data
  - Choice of which data to fit
  - Choice of being Predictive or Descriptive
- Uncertainty quantification
  - Sources of numerical uncertainty
    - statistical and round-off errors
    - systematical errors inherent to the computational method
    - uncertainties in the nuclear interactions

Nuclear Interactions

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

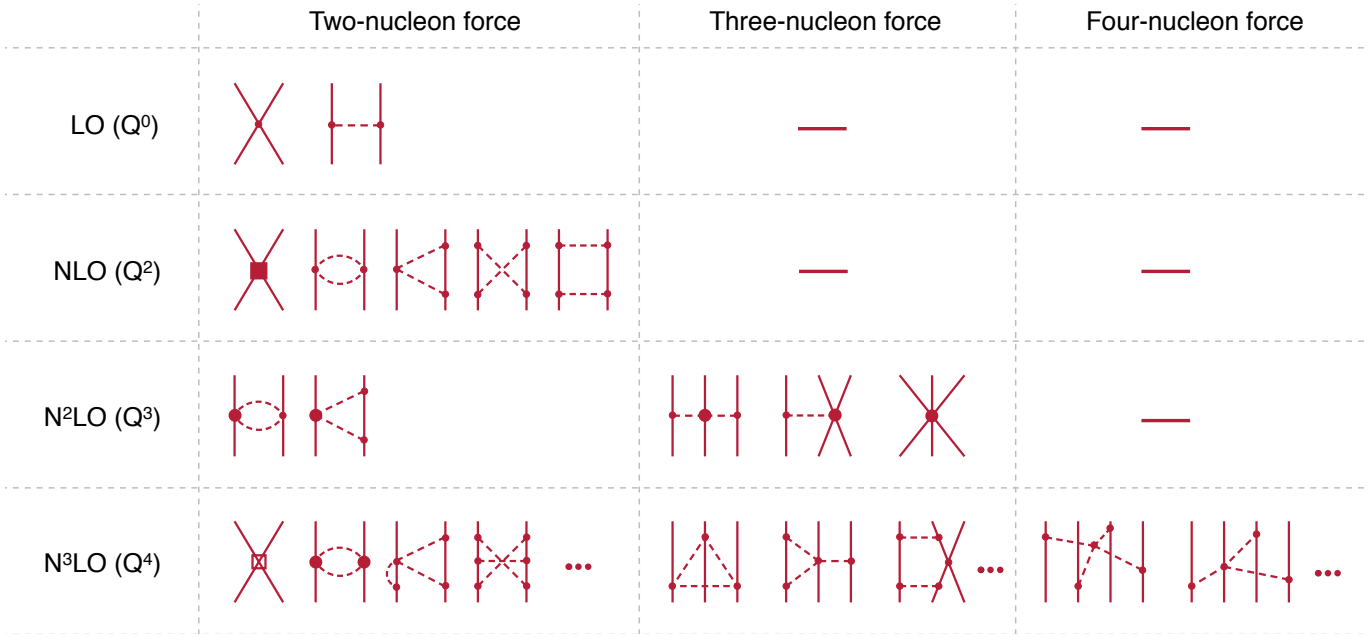


- In principle: calculable from QCD
- In practice: fitted to experiment
- NN potential fitted to phase-shifts
  - fitted up to what energy?
  - propagation of uncertainties?
  - data for *pp* and *pn* scattering, but not for *nn* scattering
- NN scattering data constrain only the on-shell NN potential, but not the off-shell behavior
  - different NN potentials describe same NN scattering data
  - wavefunctions not unique
    $\rightarrow$ potential issue when using ab initio wavefunctions as input for e.g. reaction calculations
- Most NN potentials need 3NFs 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
  - Alternative formulation with Δ DoF: 3NFs appear at NLO

Chiral expansion of nuclear forces



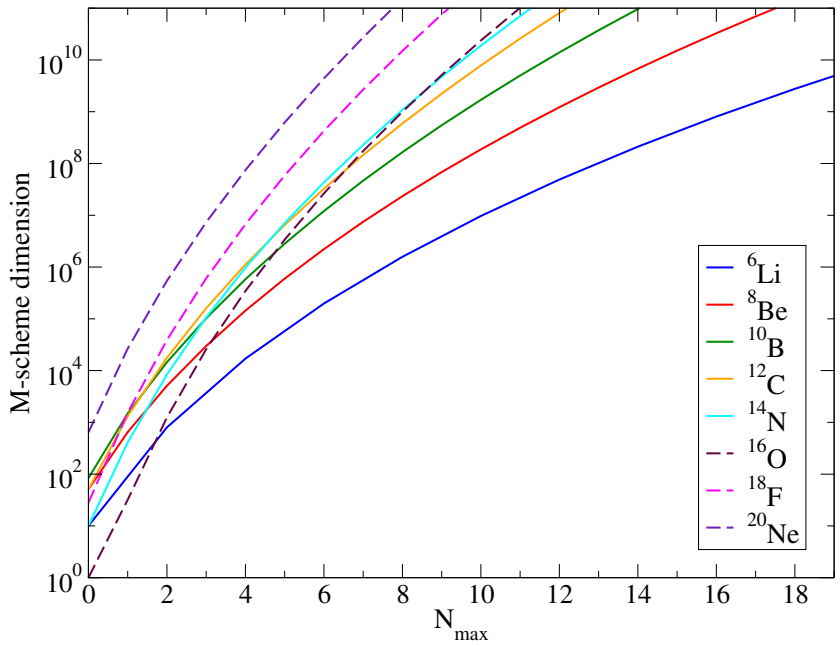
- Allows for quantification of uncertainties due to the interaction

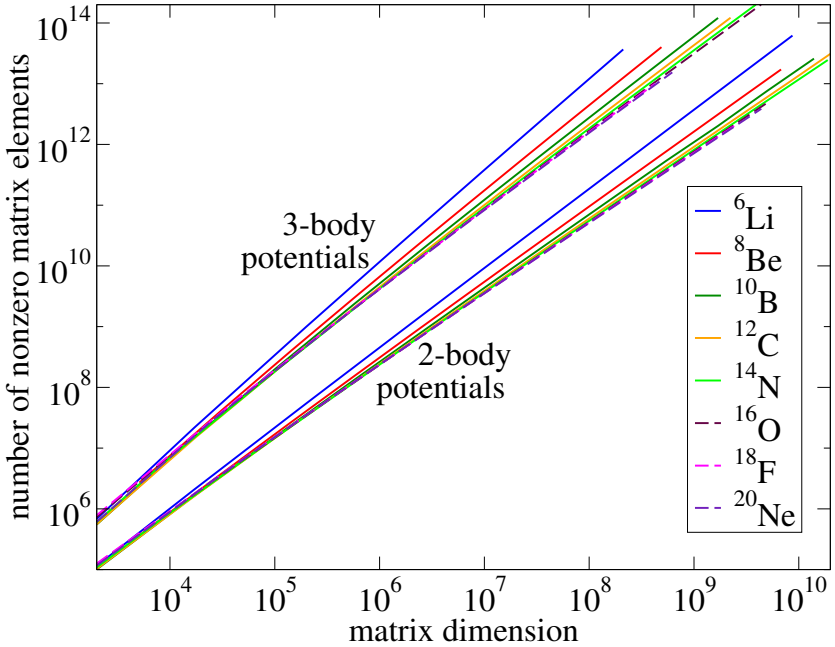
HPC Computational Methods

Currently running on DOE HPC centers

- Quantum Monte Carlo (QMC) (Theta @ ALCF, Perlmutter @ NERSC)
  - Variational Monte Carlo (VMC)
  - Green's Function Monte Carlo (GFMC)
  - Auxiliary-Field Diffusion Monte Carlo (AFDMC)
- Lattice Simulations (Frontier @ ALCF)
  - Nuclear Lattice Effective Field Theory (NLEFT)
- Configuration Interaction: Expansion of many-body wavefunction in Slater determinants of single-particle wavefunctions
  - No-Core Shell Model (NCSM) (Theta @ ALCF, Perlmutter @ NERSC)
  - Coupled Cluster (CC) (Frontier @ OLCF)
  - In-Medium Similarity Renormalization Group (IM-SRG)
  - Valence-Space Shell Model (Perlmutter @ NERSC)
    - valence interactions based on ab initio calculations near closed-shell
- Density Functional Theory not discussed in this presentation
- ...

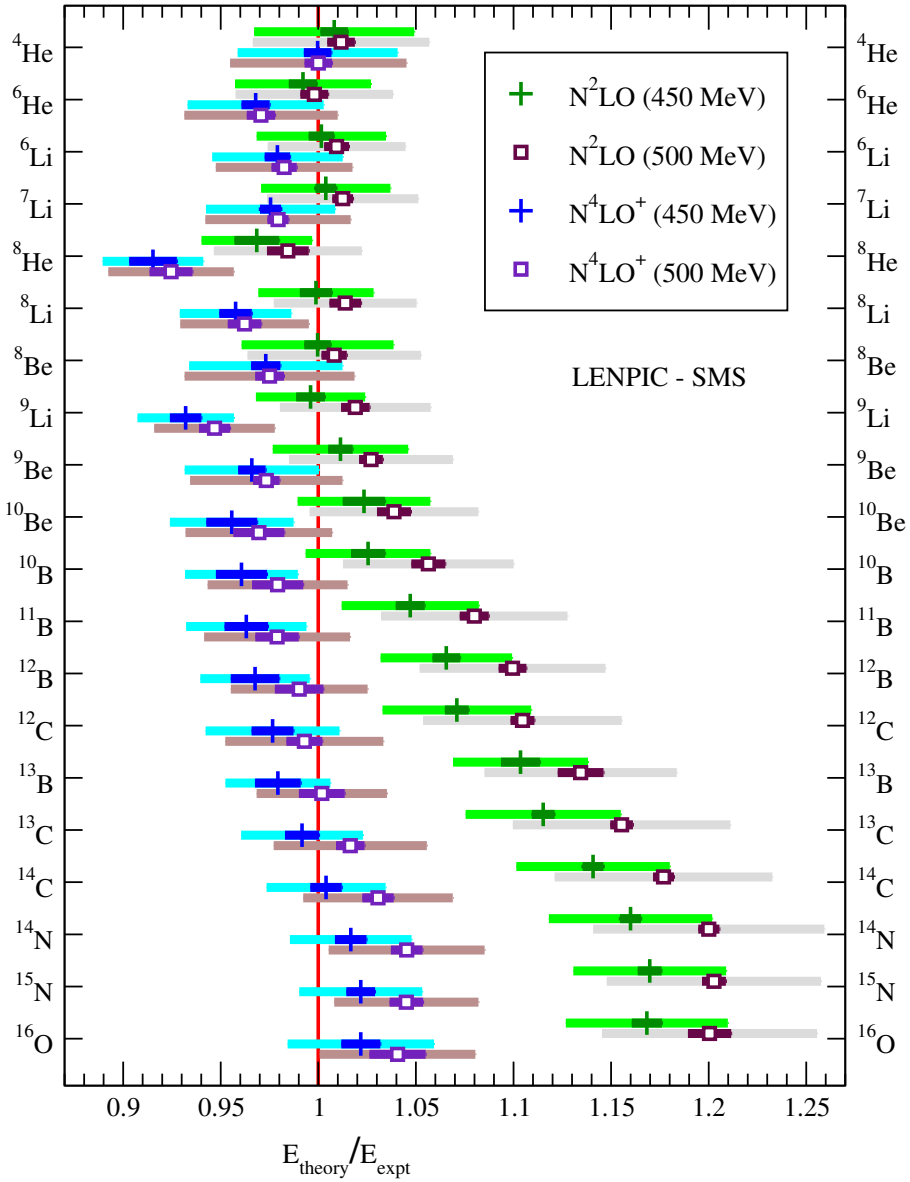
No-Core Shell Model – Main Challenge





- Increase of basis with increasing A and $N_{\max}$
  - use symmetry considerations to control basis size
  - medium-heavy nuclei: CC, IM-SRG, ab initio Valence-Space, . . .
- More relevant measure for computational needs
  - number of nonzero matrix elements
- Higher N-body interactions
  - significant increase in computational cost
  - potential solution: normal-ordering ?

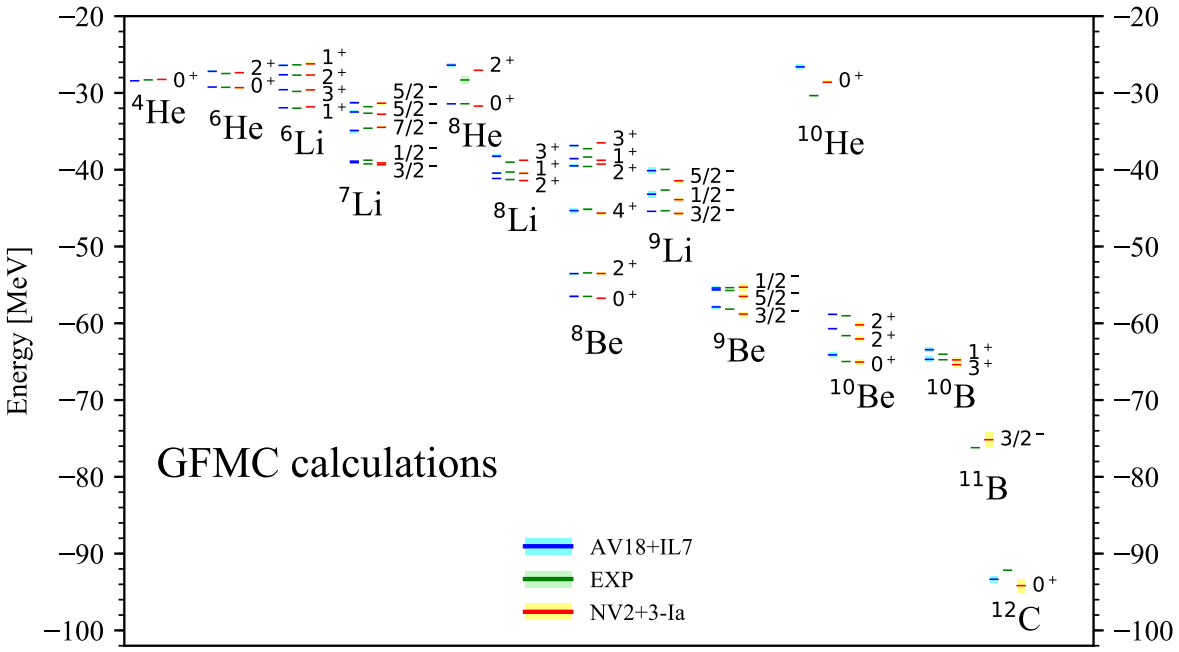
NCSM: Binding Energies from chiral EFT



PRC103, 054001 (2021); PRC, in press; Front.Phys, submitted

- NN potential up to N^4LO^+
- 3NFs at N^2LO
- SRG evolved to improve numerical convergence
- LECs fitted to
  - NN scattering data
  - ^3H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

QMC: Binding Energies and Spectra

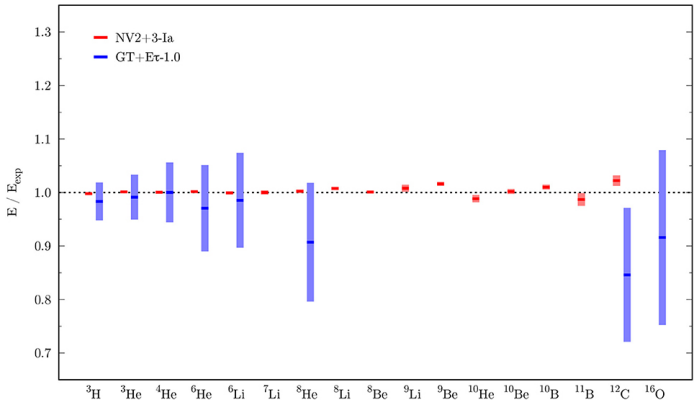


PRL 120, 052503 (2018)

Ground state and excited state energies

- AV18 + IL7 (blue)
- Norfolk Δ-full χEFT (red)
- Monte Carlo uncertainties only

Front.Phys. 8, 117 (2020)

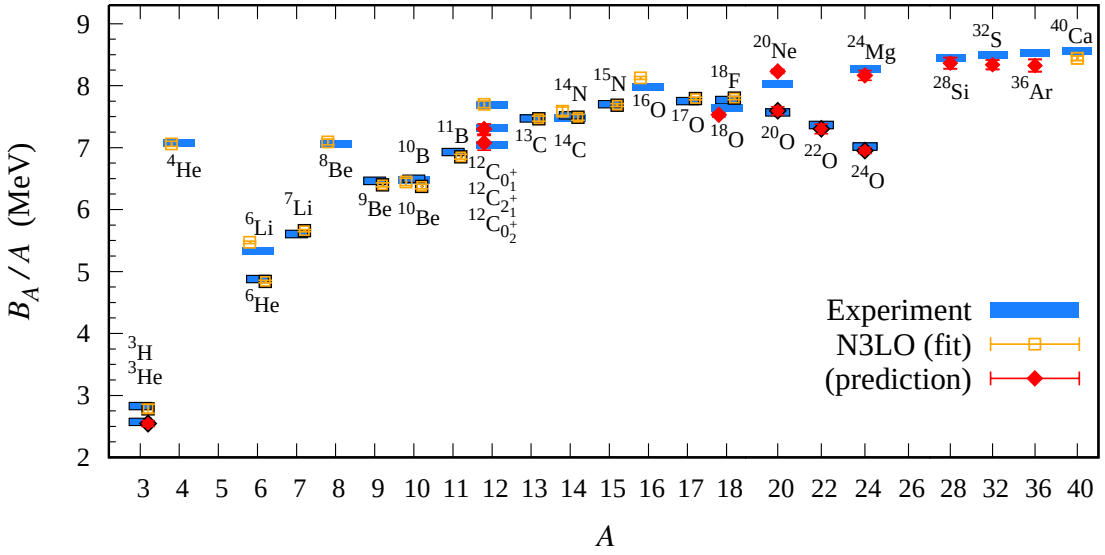


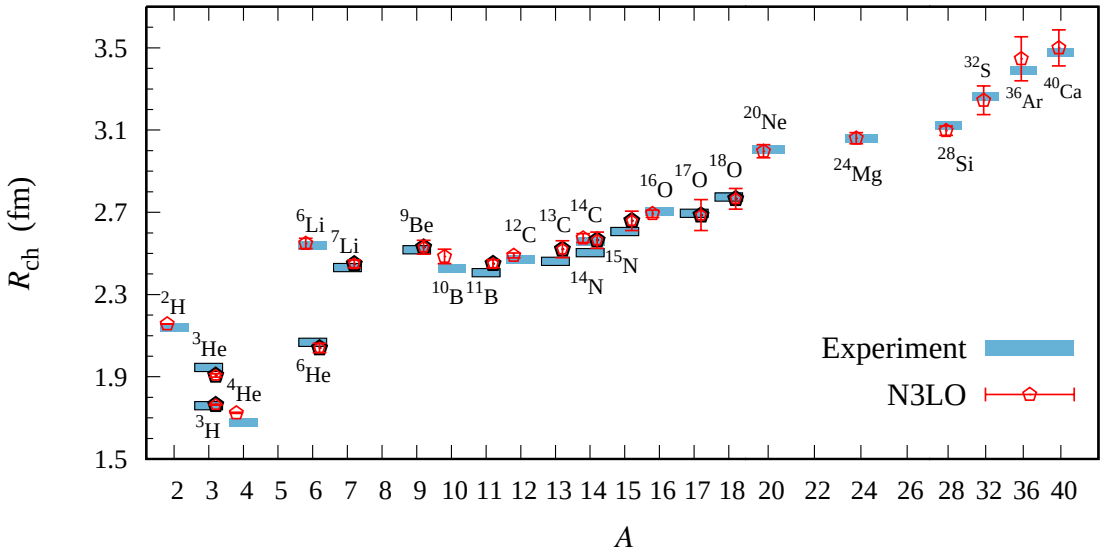
Ratio of binding energies

- GFMC results for Δ-full χEFT (red)
- AFDMC for local N^{2}LO χEFT (blue) w. chiral uncertainty estimates

NLEFT: Energies and Radii from chiral EFT

arXiv:2210.17488





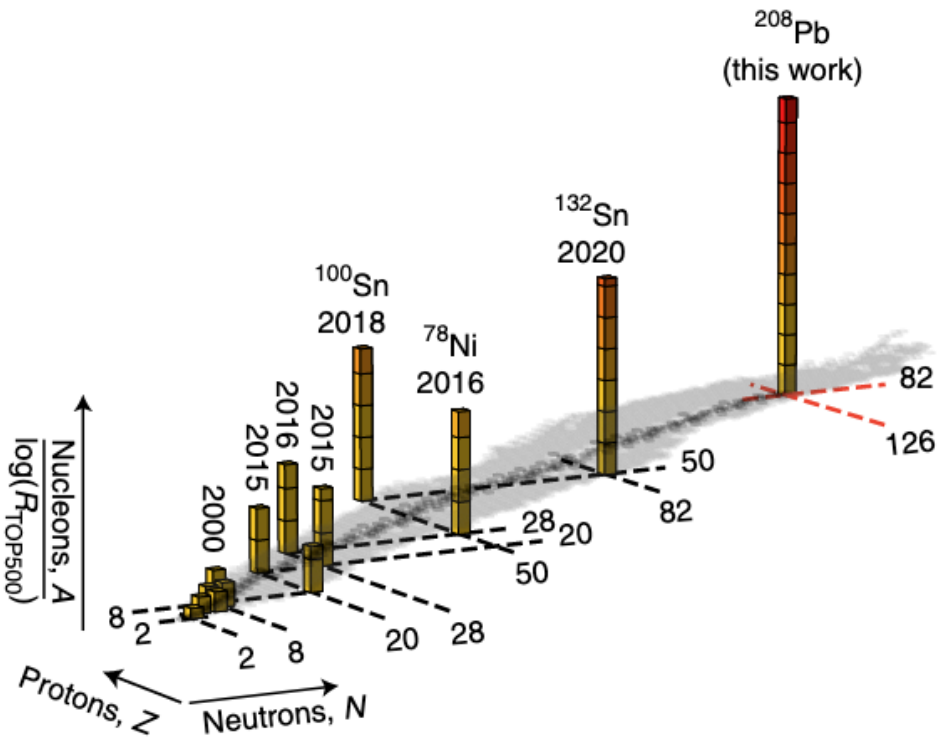
Nuclear lattice simulations

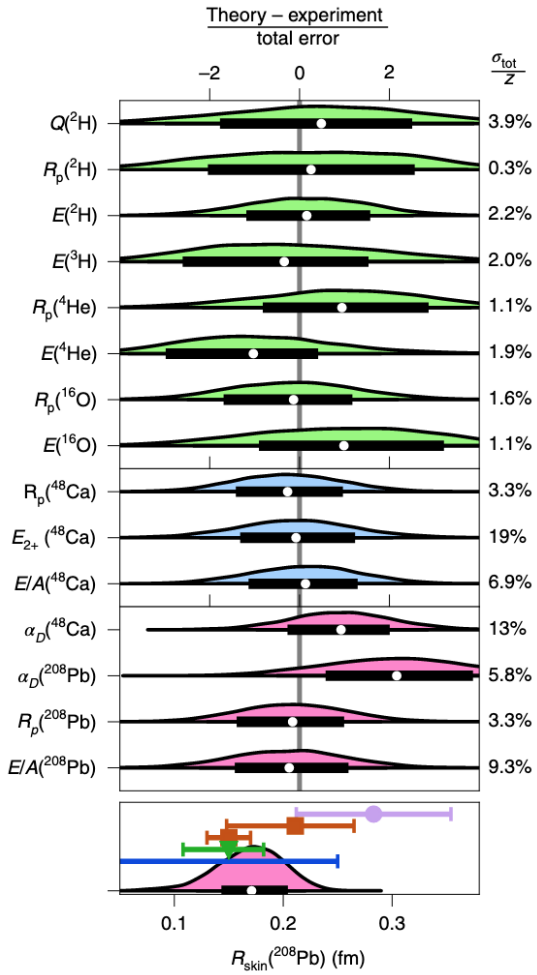
- chiral EFT interaction up to N^3LO (N^3LO 4NFs omitted)
- uncertainties include Monte Carlo uncertainties and finite volume uncertainties
- estimated systematic uncertainties $\approx$ 0.1 MeV/A
- estimated interaction uncertainties $<$ 0.1 MeV/A
- systematic and interaction uncertainties for radii TBD

Extending the Landscape to ^{208}Pb

- CC, IM-SRG, MBPT calculations to estimate method uncertainty
- Use emulator to sample 17-dimensional parameter space of LECs

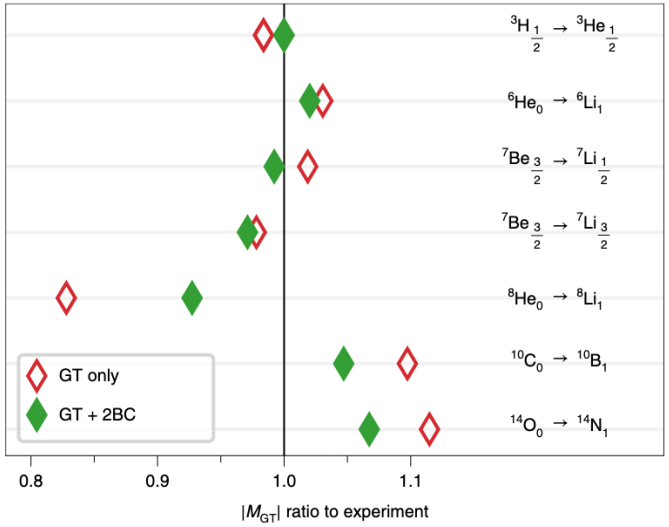
NATURE PHYSICS 18, 1196 (2022)



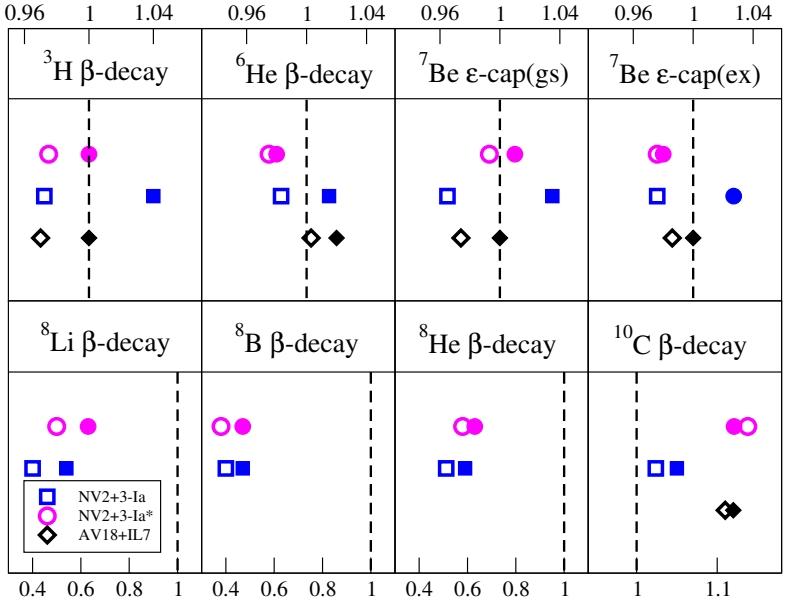


Ab Initio Reactions: Beta-decay light nuclei

Nature Physics 15, 428 (2019)



PRC 102, 025501 (2020)



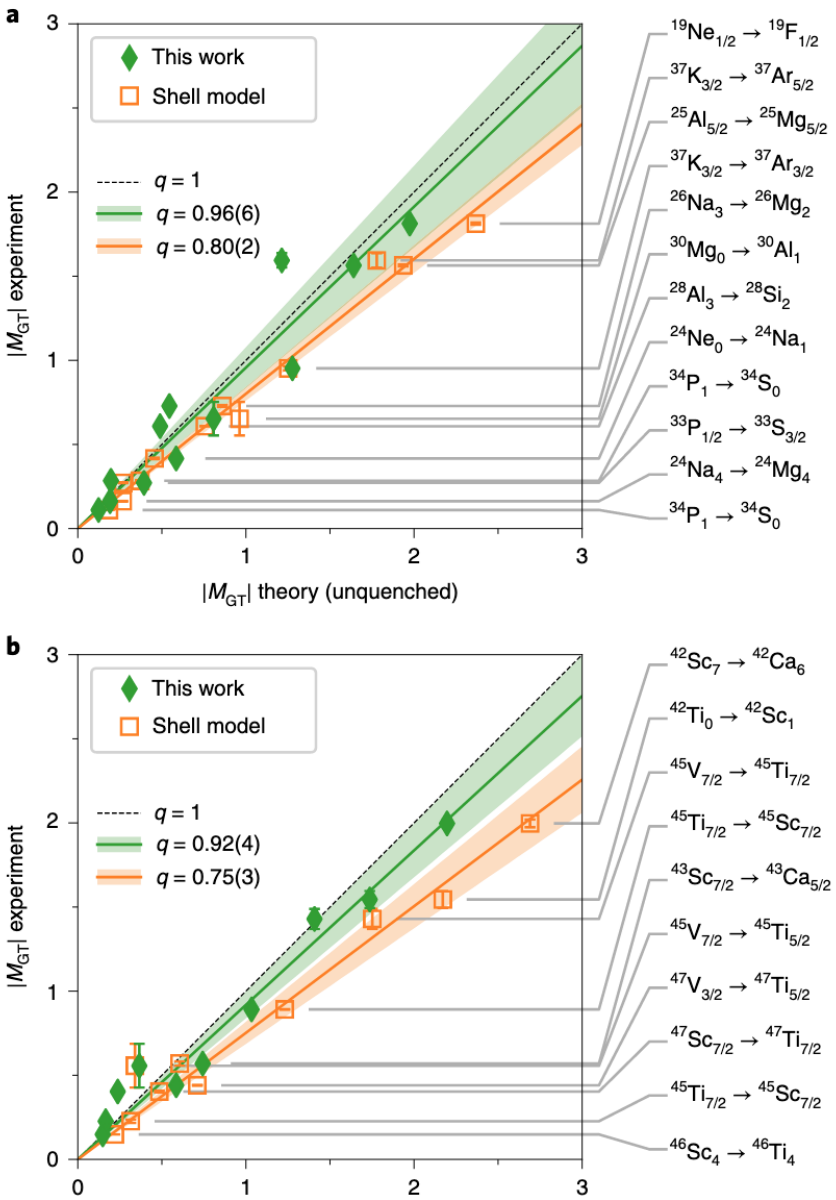
NCSM calculations

- N^{4}LO NN potential
- N^{2}LO 3NFs w. local and nonlocal regulators fitted to triton β-decay
- Chiral EFT 2-body current

GFMC calculations

- AV18 + IL7
- Norfolk Δ-full χEFT
- LO axial current (open)
- N^{3}LO axial current (solid)

Ab Initio Reactions: Beta-decay



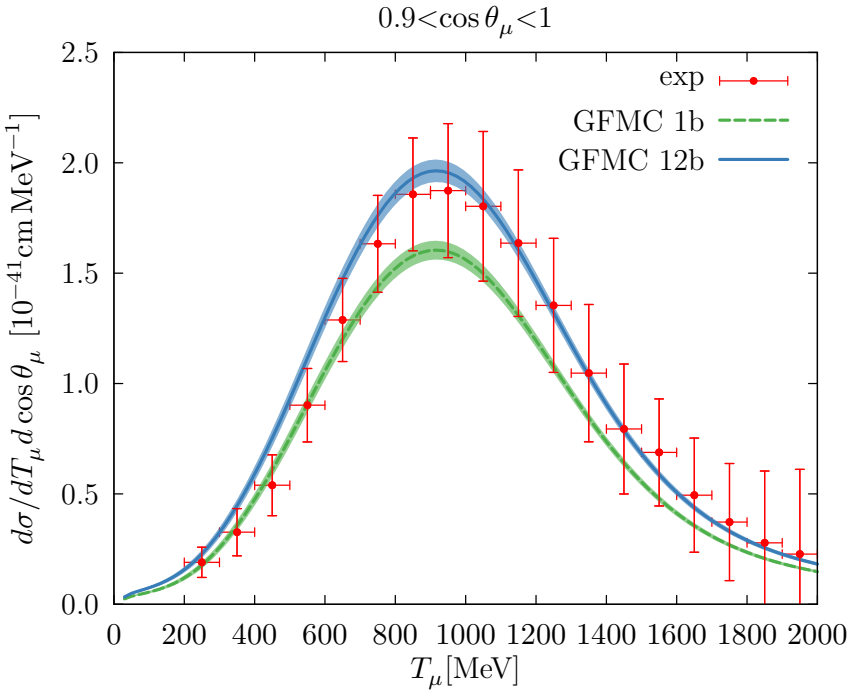
Nature Physics 15, 428 (2019)

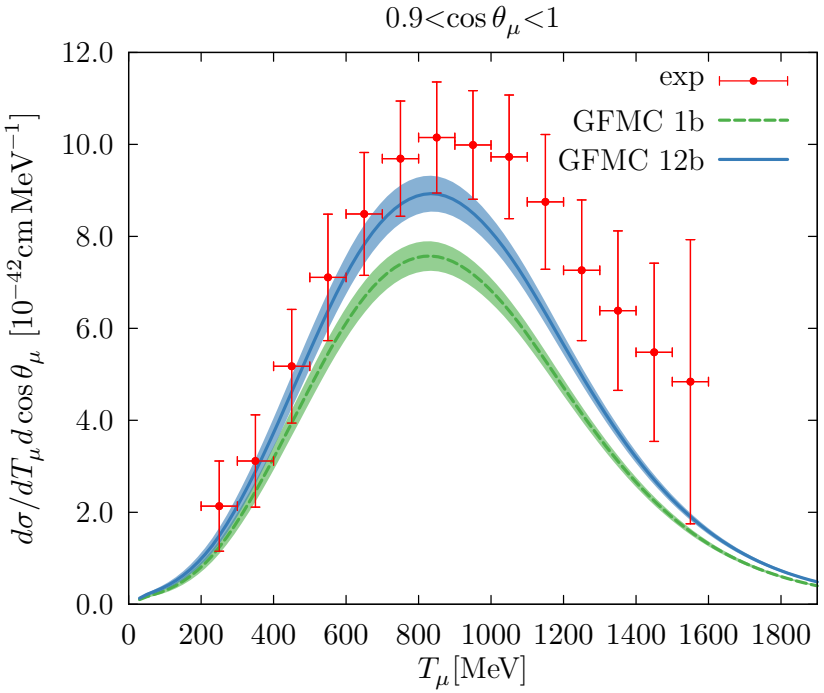
Valence Shell Model

- Phenomenological shell model does not reproduce β-decay data
- IM-SRG Valence-Space model close to β-decay data
  - N^{4}LO NN potential
  - N^{2}LO 3NFs w. local and nonlocal regulators fitted to triton β-decay
  - 2-body chiral EFT current
- No need for 'quenching'

Ab Initio Lepton-Nucleus Scattering

PRX 10, 031068 (2020)

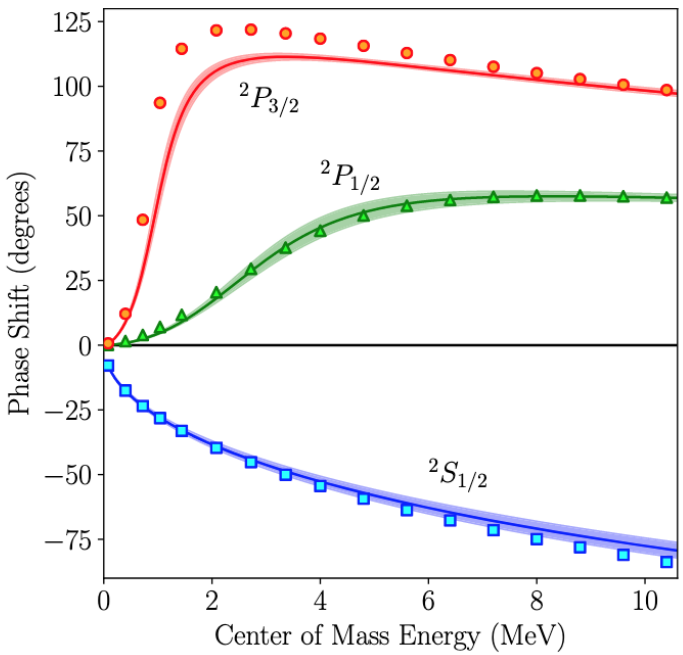


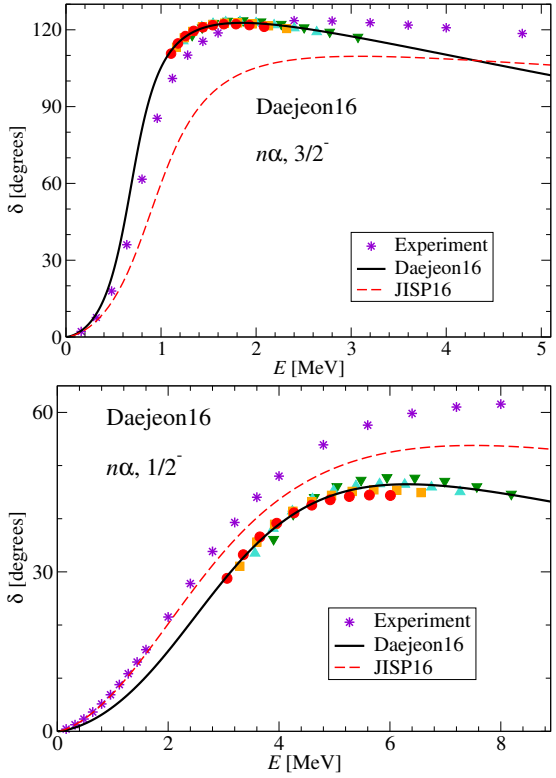


- MiniBooNE Charge Current QuasiElastic neutrino scattering data
  overall 10.7% (left) and 17.4% (right) normalization uncertainty not included
- GFMC calculations of ^{12}C wavefunction using AV18 + IL7
- One-body axial current (green)
- Plus 2-body meson-exchange current (blue)

Ab Initio neutron-α Scattering in resonance region

PHYSICAL REVIEW C **102**, 024616 (2020)





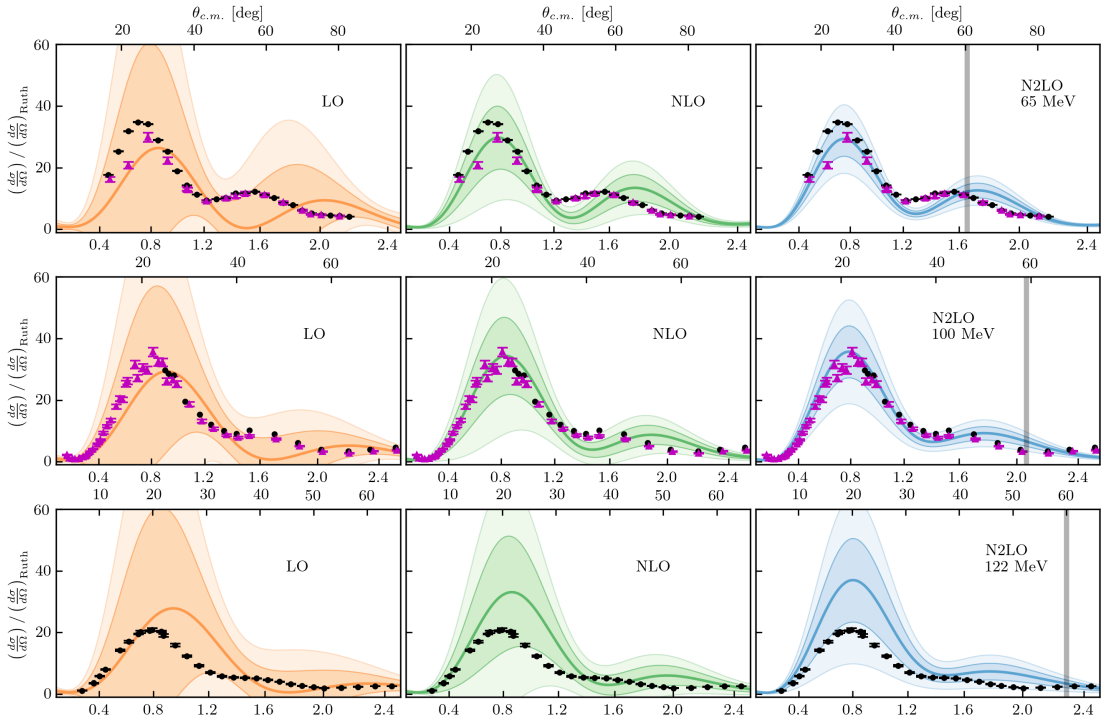
PRCC98 044624 (2018)

- NCSM with Continuum
- N^{4}LO NN potential
- N^{2}LO 3NFs local-nonlocal
- Uncertainties based on LEC parameter sampling using emulators

- Single-State Harmonic Oscillator Representation of Scattering Eqns
- Phenomenological NN potential based on N^{3}LO NN potential
- No uncertainty estimates (yet)

Ab Initio NA Scattering beyond resonance region

- Projectile energies in 50 $\sim$ 200 MeV
  - Leading-order spectator expansion of multiple scattering theory
    - consistent LO optical potential using density from NCSM
    - chiral EFT up to N^{2}LO (NN-only)
    - differential cross section ^{12}C$(p,p)^{12}$C



- Chiral uncertainties increase with projectile energy
- Uncertainties of spectator expansion?

arXiv:2112.02442 (PRC, in press); Front.Phys, submitted

Moving forward: Physics Goals

- Uncertainty quantification on all computational results
  - including uncertainties from the method, interactions, operators, ...
- Consistent chiral EFT for interactions and electroweak operators
  - need reliable UQ
  - reconcile different formulations of chiral EFT
  - need to be able to incorporate 4NFs (at least approximately)
- Extend the NCSM well into the *sd*-shell
  - use of symmetry-inspired truncations
- Extend medium (and heavy) mass nuclei towards the drip-line
  - ab initio Valence-Space SM interactions with uncertainties?
- Resonances (open quantum systems) with UQ
  - NCSM-Continuum, Gamov Shell Model, ...
  - novel developments ?
- Nuclear reactions with UQ
  - NCSMC, Resonating Group Method, ...
  - Beyond LO in spectator expansion ?
  - novel developments ?

From an HPC perspective

- Successes of ab initio nuclear structure calculations enabled
  - by acces to DOE's HPC platforms
  - by collaborations with applied mathematicians and computer scientists for code development and performance optimization
  - by applying for, and being awarded, early science projects at DOE HPC centers

Moving forward, it is critical that we have ongoing interdisciplinary collaborations between nuclear physicists, applied mathematicians, and computer scientists in order to fully exploit the opportunities offered by future hardware and software HPC developments

- Keep up with HPC hardware developments
  - performance-portable codes
  - HPC quantum computers? (next session)
- Extensive use of emulators
- Extensive use of AI/ML (next session)

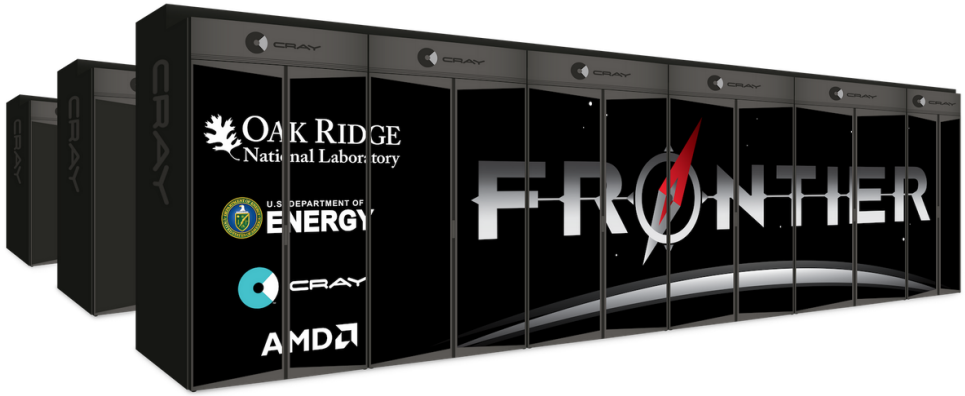
Also need ongoing collaborations with statisticians

DOE HPC centers: Hardware developments

Also need access to HPC hardware

- Oak Ridge Leadership Class Facility
  - Summit (OLCF-4, 2018 – . . .), IBM CPU w. NVIDIA GPU
  - Frontier (OLCF-5, 2022 – . . .), AMD CPU w. AMD GPU
- Argonne Leadership Class Facility
  - Theta (ALCF-3, 2017 – 2023), Intel CPU KNL (many-core)
  - Aurora (ALCF-4, 2023 – . . .), Intel CPU w. Intel Accelerator
- National Energy Research Scientific Computing center
  - Cori (NERSC-8, 2016 – 2022), Intel CPU, mostly KNL (many-core)
  - Perlmutter (NERSC-9, 2022 – . . .),
    AMD CPU only partition and AMD CPU w. NVIDIA GPU partition
  - NERSC-10, passed CD-0, designed for 2026 deployment

Perlmutter's Phase I cabinets without the doors attached reveal the blue and red lines of its direct liquid cooling system.



Oak Ridge and Argonne Leadership Class Facilities

Allocations on DOE's Leadership Class HPC centers through

ALCC: ASCR Leadership Computing Challenge

INCITE: Innovative and Novel Computational Impact on Theory and Experiment

Breaking News: 56 INCITE projects awarded for 2023
to accelerate science and engineering research

- OLCF – currently 29 active projects, across all sciences
  - currently active: 15 INCITE and 14 ALCC projects
  - 2 INCITE Nuclear Structure and Reactions projects
  - all current projects on OLCF have demonstrated good performance on GPUs (including NP codes)
- ALCF – 32 projects in 2021, across all sciences
  - 2021: 16 INCITE and 16 ALCC projects
  - 1 INCITE and 1 ALCC Nuclear Structure and Reactions project
  - moving forward, projects on ALCF will have to demonstrate good performance on GPUs, once Theta retires (end of 2023)
  - not al codes from the Nuclear Structure and Reaction project currently running at ALCF have been ported to GPUs (yet)
    - at least one has been ported to NVIDIA GPUs

NERSC allocations for Nuclear Physics

- Amount of resources for Nuclear Physics: 10 % of total resources
- Number of Nuclear Physics projects in 2022: 74
- Amount of resources requested for 2022:
  - 15 % – QCD (hot and cold) (i.e. 1.5 times NP resources)
  - 3.4 % – Astrophysics
  - 2.4 % – Nuclear Structure and Reactions
  - 2.3 % – Experiment (mostly data analysis and simulations)
- Resources requested for 2023 on CPUs (out of 1,964 k available)
  - 5,270 k – QCD (hot and cold) (i.e. 2.6 times NP resources)
  - 1,589 k – Astrophysics
  - 772 k – Nuclear Structure and Reactions
- Resources requested for 2023 on GPUs (out of 927 k available)
  - 2,794 k – QCD (hot and cold) (i.e. 3 times NP resources)
  - 1,238 k – Astrophysics
  - 96 k – Nuclear Structure and Reactions

  not many 'Nuclear Structure and Reactions' codes are GPU-ready?

Concluding remarks

- Successes of ab initio nuclear structure calculations enabled by interdisciplinary collaborations with applied mathematicians, computer scientists, and statisticiancs
- Need ongoing support for collaborations with statisticians for UQ
  - currently through SciDAC
- Need ongoing support for collaboration with applied mathematicians and computer scientists for code development
  - currently through SciDAC and early-science programs
- Need dedicated HPC-oriented domain scientists
  - workforce development of future computational nuclear physicists
- GPUs pose a challenge for performance portability
  - large-scale HPC users benefitted from early-science programs at HPC centers to port and optimize codes for the latest hardware
  - challenge for broader computational Nuclear Structure and Reactions community to keep up with hardware development