High-Performance Computing for Nuclear Physics

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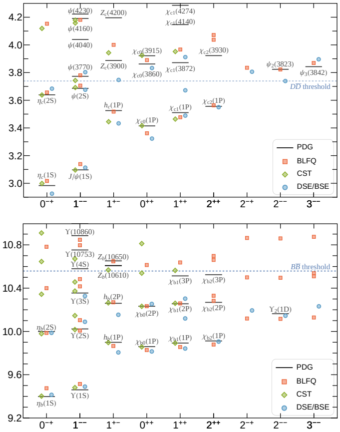
James P. Vary 80th Jubilee
Planet Earth, June 05, 2023

Hadrons: Relativistic Quantum Field Theory

- Lattice QCD
  - highly efficient computational methods and implementations thanks to decades of code development and optimization by dedicated computational scientists
- Dyson–Schwinger Equations
  - Dynamical Chiral Symmetry Breaking pions emerge as Goldstone bosons
  - Bethe–Salpeter Eqn for mesons
  - Relativistic Faddeev Eqn for baryons
  - Spectra, decay constants, form factors
- Light-front methods
  - Direct access to light-front observables
  - Discrete Light-Cone Quantization
  - Basis Light-Front Quantization



Gross *et al*, 50 Years QCD, 2212.11107 [hep-th]

Nuclei: Nonrelativistic Quantum Mechanics

- Few-Body methods
  - Faddeev Equation for $A = 3$ system
    - typically in momentum space
  - Faddeev–Yakubosky Equations for $A = 4$ systems
    - can nowadays be pushed to $A = 5$ and 6
  - Hyperspherical Harmonics
    - up to $A = 6$
- Many-Body methods
  - Monte-Carlo methods
  - Nuclear Lattice Simulations
  - Configuration Interaction (CI) methods
    - Valence-Space Shell Model
    - No-Core Shell Model (NCSM)
    - In-Medium Similarity Renormalization Group (IM-SRG)
    - Coupled Cluster (CC)
  - Self-Consistent Green's Function (SCGF) methods
  - Many-Body Perturbation Theory (MBPT)
  - Density Functional Theory (DFT)
  - ...

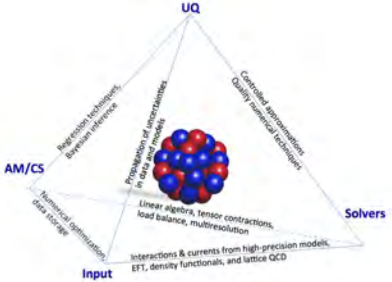
Computational resources: Moore's Law

All computational methods benefit from 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

SciDAC

- Partnerships between DOE Office of Advanced Scientific Computing Research and DOE Domain Science programs
- Five-year collaborative grants, created in/around 2000
- Currently in 5th cycle
- Three SciDAC-5 programs in Nuclear Physics
  - Femtoscale Imaging of Nuclei using Exascale Platforms (Cloët)
  - Fundamental nuclear physics at the exascale and beyond (Edwards)
  - Nuclear Computational Low Energy Initiative (NUCLEI) (Papenbrock)
- James Vary and Esmond Ng (AM/CS, LBNL) played essential role in creating successful SciDAC-2 UNEDF proposal in 2006
- UNEDF evolved to NUCLEI



UNEDF (2007–2012), NUCLEI (2012–2017; 2017-2022; 2022–2027)

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

Participating Institutions and Investigators

Ames National Laboratory
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University of Washington
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Color denotes:

- Physics
- Computer Science & Applied Mathematics

NUCLEI

Nuclear Computational Low-Energy Initiative
A SciDAC-5 Project

About ▾ People ▾ Science ▾ Deliverables ▾ Tools ▾ Internal ▾ Links

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
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P. Maris, J. Vary
Lawrence Berkeley National Laboratory
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Lawrence Livermore National Laboratory
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Los Alamos National Laboratory
J. Carlson, S. Gandolfi, M. Grosskopf, E. Lawrence, I. Tews
Massachusetts Institute of Technology
C. Feng (g), Y. Marzouk
Michigan State University
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Oak Ridge National Laboratory
T. Djaervs (p), G. Hagen, B. Hu (p), G. Jansen, S. Lee, T. Papenbrock
Ohio State University
R. Furnstahl, A. Garcia (g), P. Millican (g)
University of North Carolina at Chapel Hill
J. Engel
University of Notre Dame
R. Stroberg
University of Oregon
B. Norris
Washington University in St. Louis
S. Pastore, M. Piarulli

For more information on NUCLEI, please contact tpapenbr@utk.edu

Early-Science Projects

- Collaboration with Computer Scientists to port and optimize select codes to next-generation HPC hardware
  - Support from HPC centers and hardware vendors
  - Early access to proto-type and/or actual production hardware
  - New hardware & software not necessarily stable: finding and reporting bugs is 'part of the job'
- Early-Science Projects for Many-Fermion-Dynamics-nuclear
  - Pre-2007: Distributed parallel only, using MPI
  - Early Science Project for Jaguar @ ORNL, 2008 – 2010
    - Implementing hybrid MPI/OpenMP in MFDn
      PM, Vary, Navratil, Ormand, Nam, and Dean,
      Origin of the anomalous long lifetime of ^{14}C, PRL106, 202502 (2011)
  - NESAP for Cori-KNL @ NERSC, 2014 – 2017
    - Expose at least two levels of paralellism in inner-loops, such that most inner-loop can be vectorized on KNL
  - NESAP for Perlmutter-GPU @ NERSC, 2019 – 2022
    - Port to GPUs using OpenACC target offload

Collaborating with AM/CS

- Both SciDAC and Early Science Projects resulted in significant performance improvements
- SciDAC also resulted in algorithmic improvements
- Early Science Projects: focus on hard-ware specific performance
  - often also leads to performance improvements on other hardware
- Building long-term personal connections with applied mathematicians and computer scientists
  - collaborating with Esmond Ng and Chao Yang for nearly 20 years
  - ongoing collaboration with former postdocs
- Taken seriously in design criteria for future HPC platforms
  Evaluating the Potential of Disaggregated Memory Systems for HPC applications, Nan Ding, PM, Hai Ah Nam, *et al.*, submitted for publication
  - performance consequences of having modest memory on each compute node, with seperate memory banks for codes that need it
  - Hai Ah Nam, now project director for NERSC-10 https://www.nersc.gov/systems/nersc-10/

Computational Challenges

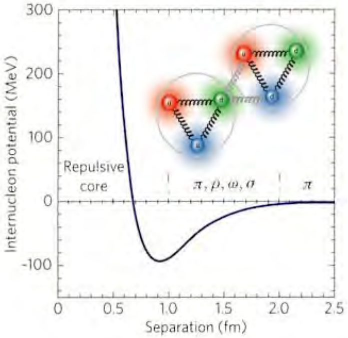
- Self-bound quantum many-body problem, with $3A$ degrees of freedom in coordinate (or momentum) space, as well as spin degrees of freedom
- Strong interactions, with both short-range and long-range pieces
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher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

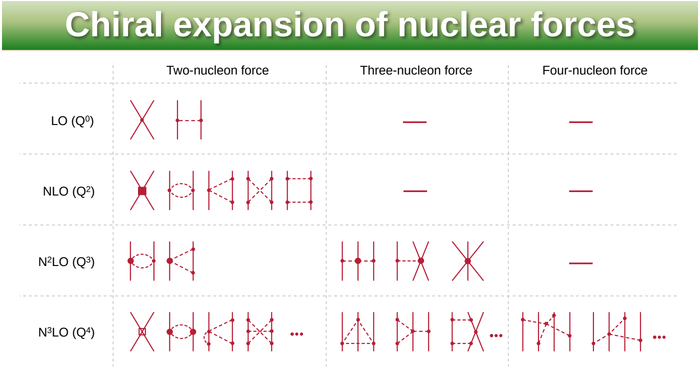
Most NN potentials need 3N forces for agreement with data for nuclei

NN Potential and Scattering Data

- Typically, cross-section data converted to phase-shifts
- NN potentials fitted to phase-shifts
  - propagation of experimental uncertainties?
  - fitted up to what energy?
- Experimental cross-section data 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 $A > 2$
  - some give good description of
    - binding energies & spectra (may need 3NFs)
    - select electroweak observables (may need corrections beyond IA)
  - wave functions not unique (unitary transformations)
- Additional (physics) input
  - chiral effective field theory
  - select observables from light nuclei (which?)
  - more or less suitable for intended computational framework

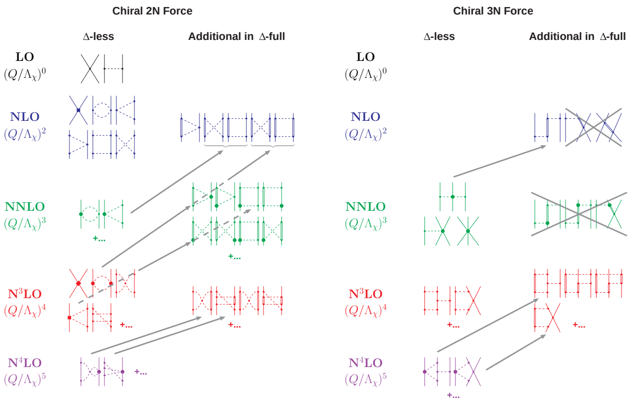
Nuclear Interactions from chiral EFT

- 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

Daejeon16 Potential

Shirokov, Shin, Kim, Sosonkina, Maris, Vary, PLB761, 87 (2016)

Nonlocal NN potential in finite Harmonic Oscillator (HO) basis, based on χEFT interactions

- Start with Idaho N^{3}LO NN potential ($\Lambda = 500$ MeV)
- Similarity Renormalization Group (SRG) evolution at 2-body level to $\lambda = 1.5$ fm^{-1} to improve convergence in HO basis
- Tuned to select light nuclei including excited states using Phase-Equivalent Transformations (PETs)
  - Seven PET angles: ${}^1s_0$, ${}^3sd_1$, ${}^1p_1$, ${}^3p_0$, ${}^3p_1$, ${}^3pf_2$, ${}^3d_2$
  - Energy of eleven states:
    - ground states of ^{3}H, ^{4}He, ^{6}Li, ^{8}He, ^{10}B, ^{12}C, ^{16}O
    - several excited states
      $(3^+, 0)$ in ^{6}Li
      $(0^+, 1)$ in ^{6}Li (equivalent to gs ^{6}He),
      $(1^+, 0)$ in ^{10}B
      $(2^+, 0)$ in ^{12}C
- Same description of NN scattering data as Idaho N^{3}LO NN potential, but better description of *p*-shell nuclei

No-Core Shell Model

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

Given a Hamiltonian operator

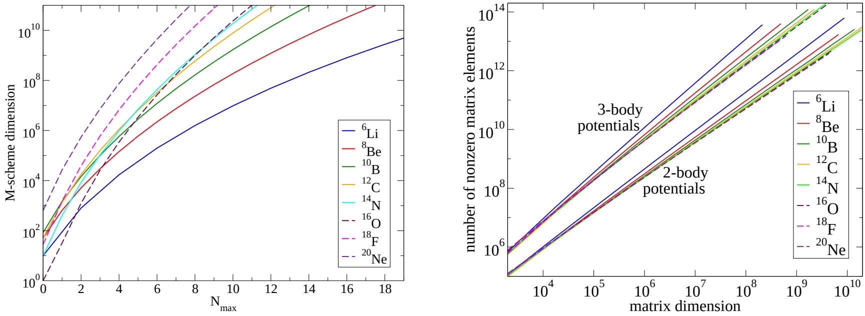
$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\, m\, A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wave function of *A* nucleons

$$\hat{\mathbf{H}}\, \Psi(r_1, \ldots, r_A) = \lambda\, \Psi(r_1, \ldots, r_A)$$

- 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}
- Use wavefunction for evaluating observables
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinitely large
- In practice: truncate basis, extrapolation to complete basis
  - truncation error, extrapolation uncertainties
- Computational challenge
  - construct large ($10^{10} \times 10^{10}$) sparse symmetric matrix H_{ij}
  - obtain lowest eigenvalues & -vectors

Main Challenge



- Relevant measures for computational needs
  - basis size and number of nonzero matrix elements
- 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, . . .
- Higher N-body interactions
  - significant increase in computational cost

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 $\longrightarrow$ exact results
  - Empirical: binding energy exponential in N_{max}

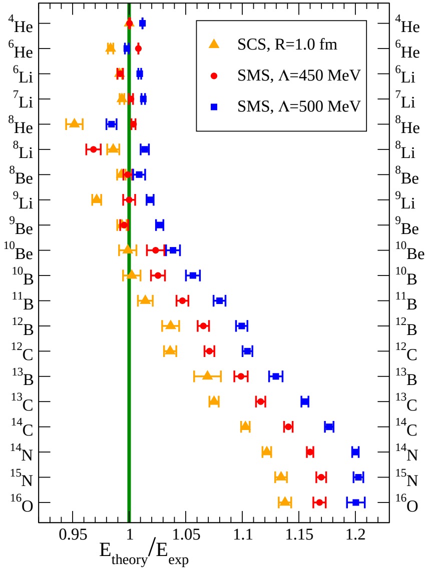
$$E^{\hbar\omega}(N) = E^{\hbar\omega}_{\infty} + a_1 \exp(-a_2 N)$$

    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 analysis emerged from collaborations with statisticians

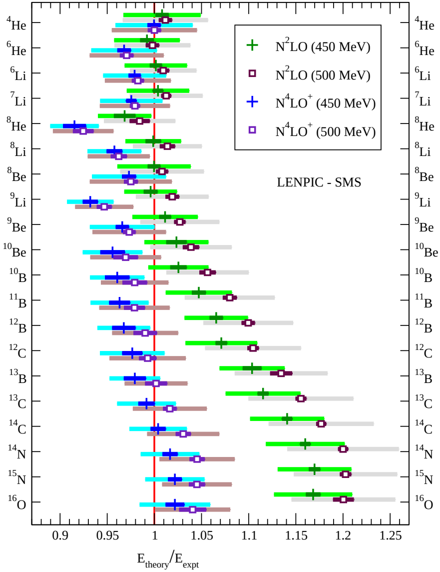
Ground State Energies with LENPIC up to N^{2}LO



PRC103, 054001 (2021)

- Two- and three-body forces up to N^{2}LO
- SRG evolved to improve numerical convergence
- No parameter adjustments
- Large-scale runs with MFDn at ALCF and NERSC
- Error bars:
  Numerical uncertainty from extrapolation to complete basis
- Systematic overbinding for $A > 10$

Binding Energies with LENPIC-SMS chiral EFT



Front.Phys. 11 1098262 (2023)

- 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

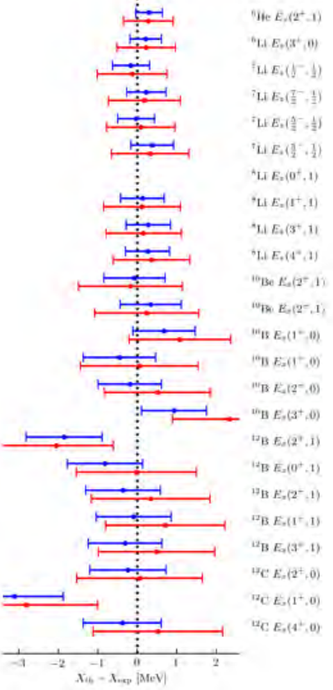
Excitation Energies with UQ

Incorporating correlations
PRC103, 054001 (2021);
following Melendez *et al* PRC100, 044001 (2019)

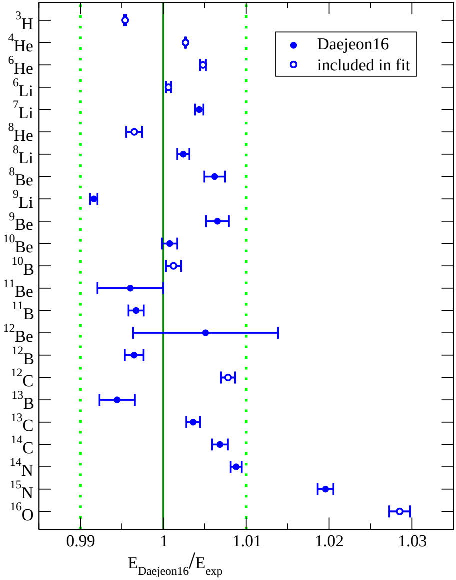
- Need to learn variance $\bar{c}$ and Q but only limited orders up to N^{2}LO
- Use just c_3 to find posterior for Q gives $Q \approx 0.3$
- Use c_2 and c_3 to fit empirical covariance matrix

Excitation energies with 95% DoB

- Uncertainties noticably smaller than uncertainties on gs energies
- Two outliers: 2^+ in ^{12}B and 1^+ in ^{12}C
- Outliers less correlated with gs, suggesting different structure



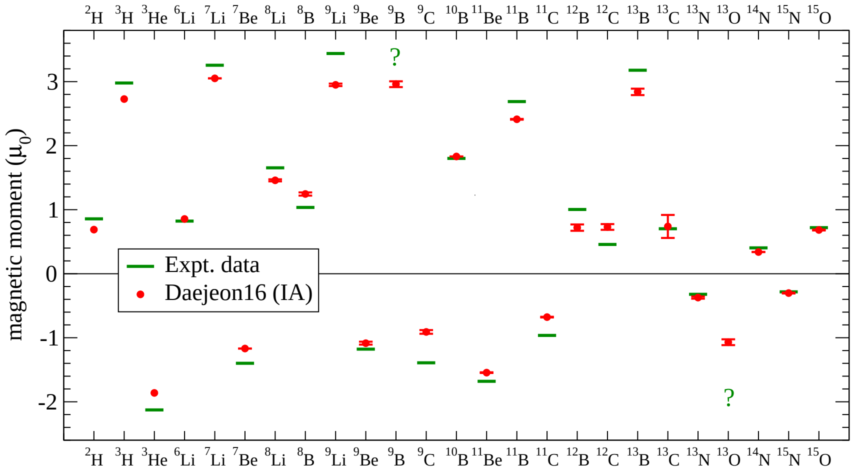
Binding energies with Daejeon16



(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

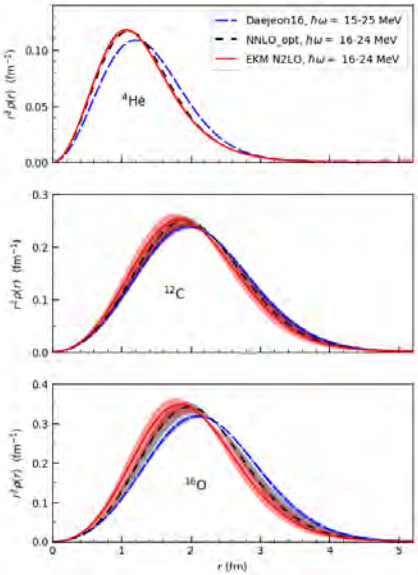
Magnetic Moments thoughout *p*-shell with Daejeon16



- Deviation from data agree with expected MEC corrections
- Nontrivial to construct consistent M1 corrections due to PETs

Charge distribution

- Charge distribution
  - dominated by local proton one-body density
    - center-of-mass motion factorizes in NCSM with $N_{\max}$ truncation
    - depends on interaction
    - slow convergence of asymptotic behavior
  - corrections due to internal structure of nucleons
  - electromagnetic current corrections
  - relativistic corrections
- Elastic form factors
  - Fourier transform of charge distribution



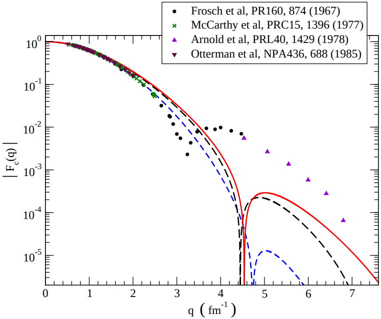
Elastic form factor

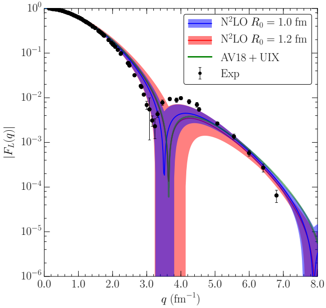
work in progress

$$F_c(q) = \frac{G_p(Q)F_p(q) + (N/Z)G_n(Q)F_n(q)}{\sqrt{1 + Q^2/4m_N^2}}$$

with $G_{p,n}$ proton and neutron form factors

and $Q^2 = q^2 - \left(\sqrt{q^2 + m_A^2} - m_A\right)^2 \approx q^2$ for $q^2 << m_A^2$



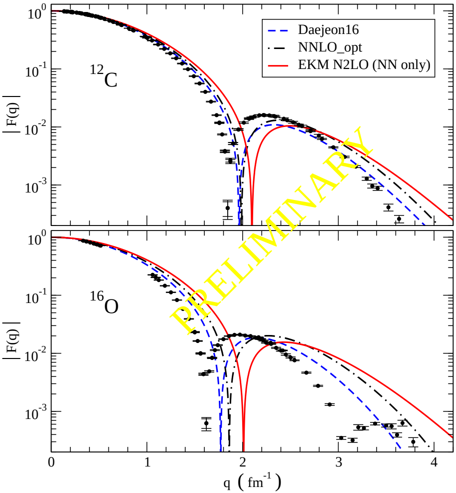


work in progress

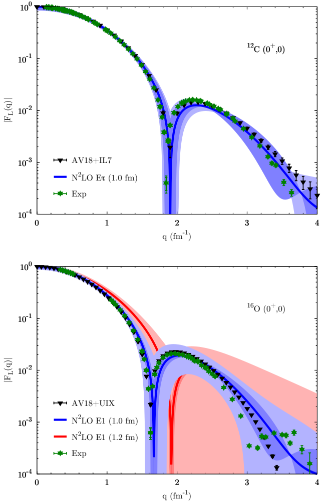
Lynn *et al*, PRC96, 054007 (2017)

Elastic form factors: 12C and 16O

work in progress



Lonardoni *et al*, PRC97, 044318 (2018)



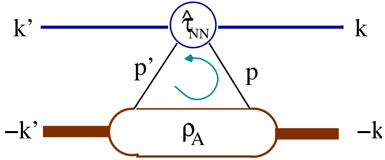
Leading-order spectator expansion for NA scattering

Effective (optical) potential

$$\widehat{U}(q, \mathcal{K}_{NA}, \epsilon) = \sum_{\alpha=n,p} \sum_{K_s} \int d^3\mathcal{K}\, \eta(q, \mathcal{K}, \mathcal{K}_{NA}) \;\; \hat{\tau}_{\alpha}^{K_s}\left(q, \frac{1}{2}\left(\frac{A+1}{A}\mathcal{K}_{NA} - \mathcal{K}\right); \varepsilon\right)$$
$$\rho_{\alpha}^{K_s}\left(\mathcal{K} - \frac{A-1}{A}\frac{q}{2}, \mathcal{K} + \frac{A-1}{A}\frac{q}{2}\right)$$

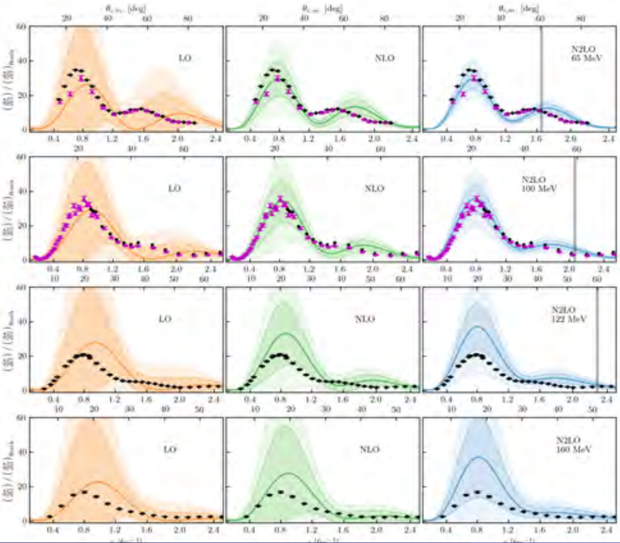
with $\eta(\ldots)$ the Moller factor, relating the NN frame to the NA frame
$\hat{\tau}_{n,p}^{K_s}$ the NN amplitude between projectile and target nucleon ($K_s = 0, 1$)
$\rho_{n,p}^{K_s}$ the (nonlocal) one-body density of the target ($K_s = 0, 1$) and

$$q = p' - p \qquad \mathcal{K} = \frac{1}{2}(p' + p)$$
$$\mathcal{K}_{NA} = \frac{A}{A+1}\left[(k' + k) + \frac{1}{2}(p' + p)\right]$$



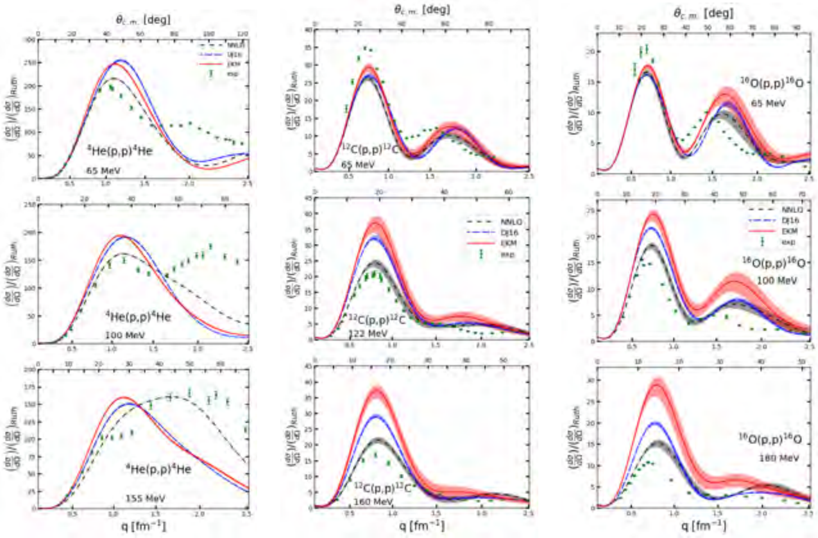
Differential cross section, $^{12}C(p,p)^{12}C$

Baker, Burrows, Elster, Launey, PM, Popa, Weppner, Front.Phys. 10 1071971 (2022)



and with different interactions, for different 0^+ nuclei

in preparation, Burrows, Elster, Popa, Weppner, . . .



Concluding remarks

- Significant progress in last 20–30 years
  in computational low-energy nuclear physics
- Made possible by ongoing collaborations between applied mathematicians, computer scientists, and domain scientists
- Collaboration with applied mathematicians and computer scientists was also crucial for initial BLFQ efforts
  - Vary, Honkanen, Jun Li, PM, Brodsky, Harindranath, Teramond, P. Sternberg, E.G. Ng, C. Yang, *Hamiltonian light-front field theory in a basis function approach*, PRC81, 035205 (2010)
- Long-term collaborations essential for success
- James has been a leading example
  fostering such long-term collaborations
- Looking forward to continue working with James
  and with other collaborators world-wide