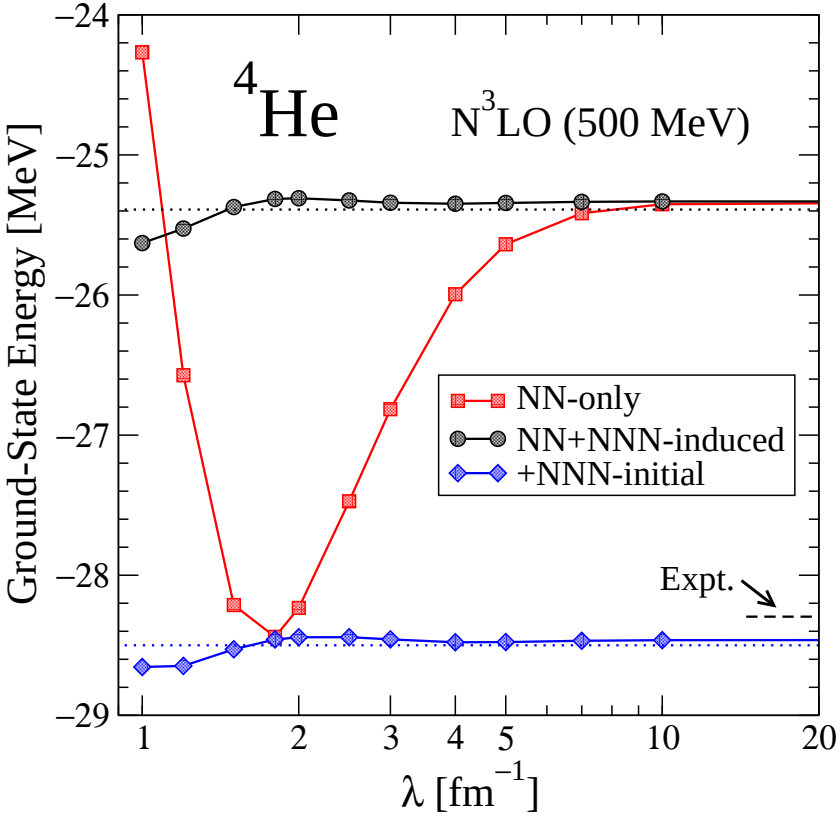
Role and Goals of the Ab Initio Functionals Group

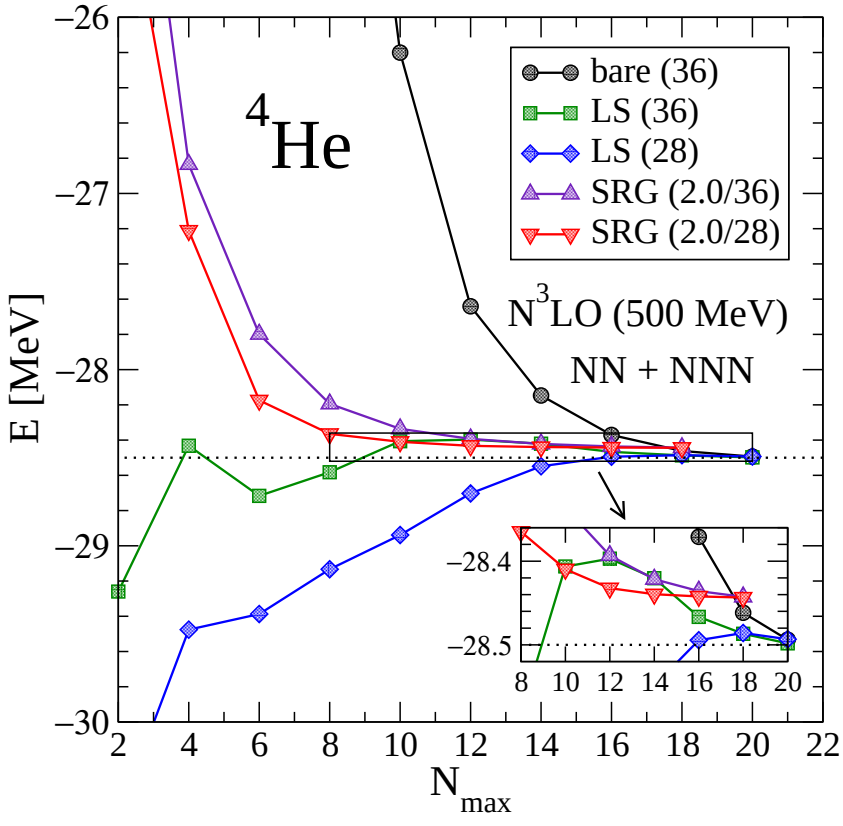
1. Provide interactions for ab initio structure methods
   - low-momentum interactions ($V_{\mathrm{low}\,k}$, SRG)
     - advantageous convergence for some methods
     - driven by requirements of ab initio DFT
     - multiple resolutions: cut-off dependence as a diagnostic
   - 3NF is essential ingredient
     - evolved consistently with NN or fit to chiral EFT basis
     - alternatives: density dependent NN, in-medium SRG
2. Develop novel density dependencies for EDF's based on microscopic interactions
   - universal long-range chiral EFT
   - input to and interaction with DFT applications group
3. Develop complete ab initio (from NN$\cdots$N) DFT
   - test approximations against ab initio (and experiment!)
   - use external fields and Hamiltonian parameters to probe
   - understand conceptual issues (e.g., symmetry breaking)

Interaction (so far) with CS/AM and HPC primarily through Ab Initio Structure and DFT Applications groups.

Year 3 Highlights from Graduate Students

- Eric Jurgenson: Consistent SRG evolution of 3NF

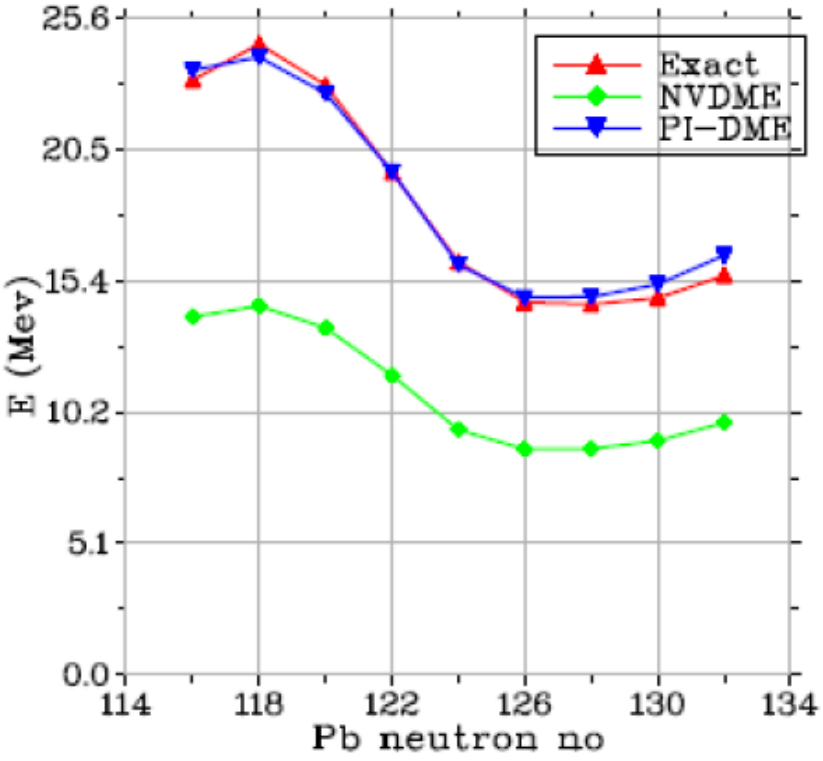


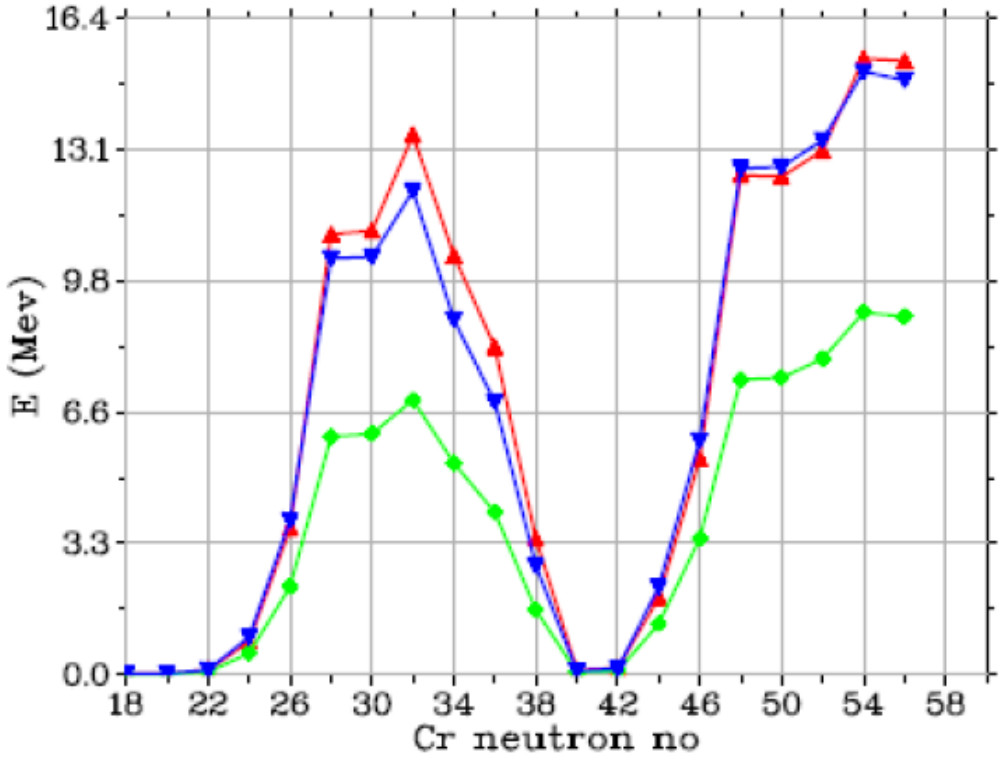


- "Evolution of nuclear many-body forces with the similarity renormalization group," E.D. Jurgenson, P. Navratil and R.J. Furnstahl, arXiv:0905.1873
- HO matrix elements $\Longrightarrow$ ab initio structure

Year 3 Highlights from Graduate Students

- Biruk Gebremariam: Phase-space-averaging extensions of Negele-Vautherin (NV) density matrix expansion (DME)





- Also Biruk: Analytic DME for long-range chiral EFT (3NF!) calculated and delivered to DFT Applications group
- Many papers (with S. Bogner, T. Duguet) in progress!

Year 3 Accomplishments (Deliverables)

- NN$\cdots$N interactions $\Longrightarrow$ 3NF
  - new 3NF: additional $V_{\mathrm{low}\,k}$/SRG fits, SRG-evolved 3NF
  - progress toward density-dependent NN for 3NF (TRIUMF)
  - first in-medium SRG calculations (infinite matter, light nuclei)
- Completed low-k (momentum-space, 3NF) scalar NV-DME
  - "Density matrix expansion for low-momentum interactions," S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. **A39**, 219 (2009)
  - identified limitations of scalar NV-DME based on HFBRAD-implementation and CC comparisons
- Completed DME for long-range chiral EFT NN and 3NF
  - *all* analytic expressions from fully automated tools
  - codes delivered (and freely available)
- Completed improved DME for vector part (PSA Π-DME)
  - parameter free; greatly reduced errors from NV-DME
- Further development of non-empirical pairing using $V_{\mathrm{low}\,k}$
- First steps toward orbital-based DFT (1D models)
  - "Toward ab initio density functional theory for nuclei," J.E. Drut, R.J. Furnstahl, and L. Platter, arXiv:0906.1463 [nucl-th]

Articles and Preprints Citing SCIDAC Support

✓ Published or Posted since Pack Forest 2008

- "Decoupling in the similarity renormalization group for nucleon-nucleon forces," E.D. Jurgenson, S.K. Bogner, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **78**, 014003 (2008)
- "Density matrix expansion for low-momentum interactions," S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. **A39**, 219 (2009)
- "Similarity renormalization group evolution of many-body forces in a one-dimensional model," E.D. Jurgenson and R.J. Furnstahl, Nucl. Phys. A **818**, 152 (2009)
- "Nuclear matter from chiral low-momentum interactions," S.K. Bogner, R.J. Furnstahl, A. Nogga and A. Schwenk, arXiv:0903.3366 [nucl-th], submitted to PRL
- "Evolution of nuclear many-body forces with the similarity renormalization group," E.D. Jurgenson, P. Navratil and R.J. Furnstahl, arXiv:0905.1873, submitted to PRL
- "Toward ab initio density functional theory for nuclei," J.E. Drut, R.J. Furnstahl, and L. Platter, arXiv:0906.1463 [nucl-th], commissioned review for Prog. Part. Nucl. Sci.

Many papers soon from MSU/Saclay collaboration!

Plans for Rest of Year 3 and Year 4 and . . .

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- 3NF fits and tests
  - 3NF project to interface $V_{\mathrm{low}\,k}$ chiral EFT 3NF with NCFC
  - Test new fits with CC and NCFC in larger nuclei (e.g., λ/Λ dependence)
  - Use NCFC in light nuclei for fits of N^{2}LO 3NF coefficients C_D, C_E (and c_i's) for many SRG and smooth $V_{\mathrm{low}\,k}$ cutoffs
- Evolving 3NF with SRG
  - Harmonic oscillator matrix elements for input to NCFCs, CC
  - Understand 3D many-body power counting and use to estimate higher-body interactions; evolve operators
  - Momentum-space evolution of 3NF
  - Validate 3NF chiral basis fits vs. evolved 3NF
- Develop and test in-medium SRG
  - Uniform systems, light closed-shell nuclei
  - Shell model effective interaction
- Upgrade SRG input as it develops (N^{3}LO 3NF, Δ's, . . .)
  - Relies on outside people

Plans for Rest of Year 3 and Year 4 and . . .

- Nuclear matter calculational extensions
  - Full 2nd order calculation with fit 3NF (w/TRIUMF)
  - Asymmetric nuclear matter (just coding to finish)
  - Solve uniform matter with in-medium SRG
  - Explore coupled cluster for nuclear matter (UT/ORNL)
- Nuclear matter studies
  - Complete and publish the G-matrix and BBG study
    $\Longrightarrow$ test power counting with numerical examples
  - Nonperturbativeness in the particle-hole channel
  - Pairing, e.g., in $^3S_1$
  - Nuclear/neutron matter with Jisp-16 (MSU/ISU)
  - 4NF from N^{3}LO chiral EFT at Hartree-Fock
- Validating (or invalidating) NV DME from $V_{\mathrm{low}\,k}$/SRG
  - Compare energies, ρ's to CC, NCFC with same Hamiltonian
    - Vary contact 3NF strength, full 3NF-fitted $V_{\mathrm{low}\,k}$/SRG
  - Compare in external potentials with NCFC, GFMC/AFMC
    - neutron drops

Plans for Rest of Year 3 and Year 4 and . . .

- Further development of Π-DME (MSU,Saclay/Lyon)
  - Finish phase space averaging; alternatives for local k_{F}
  - Write up papers!
  - Validate against exact Hartree-Fock
  - Extend DME to pairing
  - DME beyond HF level — dispersive effects using short-time/factorization methods
- Refit "Skyrme + long-range DME" studies (w/ORNL)
  - Incorporate in HFB DME codes; refit generalized Skyrme
  - Naturalness constraints, higher gradients, look for pion, . . .
  - "Non-empirical" DFT with gradients and volume density dependencies constrained from long-range DME
- Continue 1D (3D) development of orbital-based DFT
  - KLI approximations vs. full OEP
  - Model tests against DME; full comparison
  - Issues: self-interaction, self-pairing, . . .
  - Symmetry breaking, long-range correlations . . .