UNEDF SCIDAC ab-initio progress

Neutron Matter
Light Nuclei
Medium Mass Nuclei

**Universal Nuclear Energy Density Functional**

**Inter-Nucleon NN, NNN Interactions**

**AV18, EFT, V12**

**Theory of Light Nuclei**

**Verification:** NCSM=QMC=CC

**Validation:** nuclei with A=6

**Density Functional Theory**

**Improved functionals**

**remove computationally-imposed constraints**

**global properties of nuclei with A=16**

**Dynamic Extensions of DFT**

**LACM, SCM, TDFFT, ORPA, CI, CC**

**Level densities**

**Low-energy Reactions**

**Heuser-Feshbach**

**Feshbach-Kerman-Koonin Fission**

**mass and energy distributions**

**Validation/Verifications of Codes**

**Constraining Density Functional**

**Strong Ties to Computational Science**

**ANL:**
Pieper, Wiringa

**Iowa State:**
Vary, Maris

**LANL:**
Carlson, Gezerlis, Stetcu, Dupuis

**LLNL:**
Navratil, Ormand

**ORNL/UT:**
Dean, Papenbrock, Hagen

**UW:**
Bulgac
Neutron Matter EOS

Neutron Matter properties less well-known than Nuclear Matter near equilibrium density
Ab Initio calculations can provide guidance to the density functional

Equation of State at Low Densities

Superfluid Density Functional /Ab Initio

Calculate one-, two-body density matrix for matter
Do SLDA & other Density functionals work as well for neutron drops?
Finite range of interaction, weaker pairing,
various trap geometries, ...

Should superfluid densities be included explicitly in density functional?
Neutron Matter Pairing Gap

Pairing Gap at Low Densities

\[ \Delta (\text{MeV}) \]

- \( k_F \text{a} \)

Pairing Gap for Atomic Gas
Experimentally confirmed to \( \sim 10\% \)

Finite Systems:
Neutron Drops

Stringent tests of DFT

EOS
pairing
external fields: quadrupole, spin dependent,...

ADLB Calculations w/ 16,384 processors!
Light Nuclei: Benchmarks and relations to DFT

- Simplified interactions comparison GFMC and NCSM
- Good (0.4 MeV) agreement for energies
- RMS radii need refinement for weakly bound nuclei

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<th>(^6\text{Li})</th>
<th>(^6\text{He})</th>
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SRG/N3LO better than 1% agreement for \(^4\text{He}, ^8\text{He}\) w/ CC, CI (and FY for \(^4\text{He}\))

\(^7\text{Li}\) mSSC

Physics Issues:
- open shell, odd N,Z; weakly bound nuclei
- reliability of evolution from ‘bare’ to lower-momentum interactions
- response to external potentials, one-body density matrix

Important ties to Computational Science: Pieper/Lusk (ADLB), Ng/Vary (MFD),...

\(^{12}\text{C}\) in an external well

12C, N3LO-SRG(\(\lambda =1.5\)), external H.O. field \(\hbar \Omega = 10.0\) MeV, \(N_{\text{max}} = 0, 2, 4, 6\)

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Underway

Started Yr 2

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Ab-initio calculations in medium mass nuclei

Present Status:

CI: \(^{16}\)O and \(^{40}\)Ca with low-momentum potentials in 4p4h
CC: \(^{16}\)O and \(^{40}\)Ca with low-momentum potentials in CCSD(T);
\(^{40,48}\)Ca with bare chiral interactions

Results compatible for \(^{16}\)O but differences for \(^{40}\)Ca, reduced w/ 4p4h
Full CI and CC agree to better than 1% for \(^{8}\)He, \(^{16}\)O, \(^{40}\)Ca Binding w/
SRG evolved N3LO interaction

Coupled Cluster for \(^{40}\)Ca and \(^{48}\)Ca

Configuration Interaction \(^{40}\)Ca
Ab-Initio Relations to DFT

**Comparison of Basic DFT Ingredients:**
- one-body density matrix
  - nearly diagonal (evolution w/ cutoff)
- two-body density matrix

**Comparison of DFT Outputs: Must Agree**
- Energy, one-body densities
- External Fields: monopole, quadrupole
- isospin dependence
- general density perturbations

**Neutron Matter/External Pot.**
- ab initio / DFT

**Light Nuclei:** A up to 12
- nn interactions - ab-initio
- ab-initio / ab-initio

**Medium Nuclei:** A from 16 to 56
- nn interactions - ab initio
- ab initio / DFT