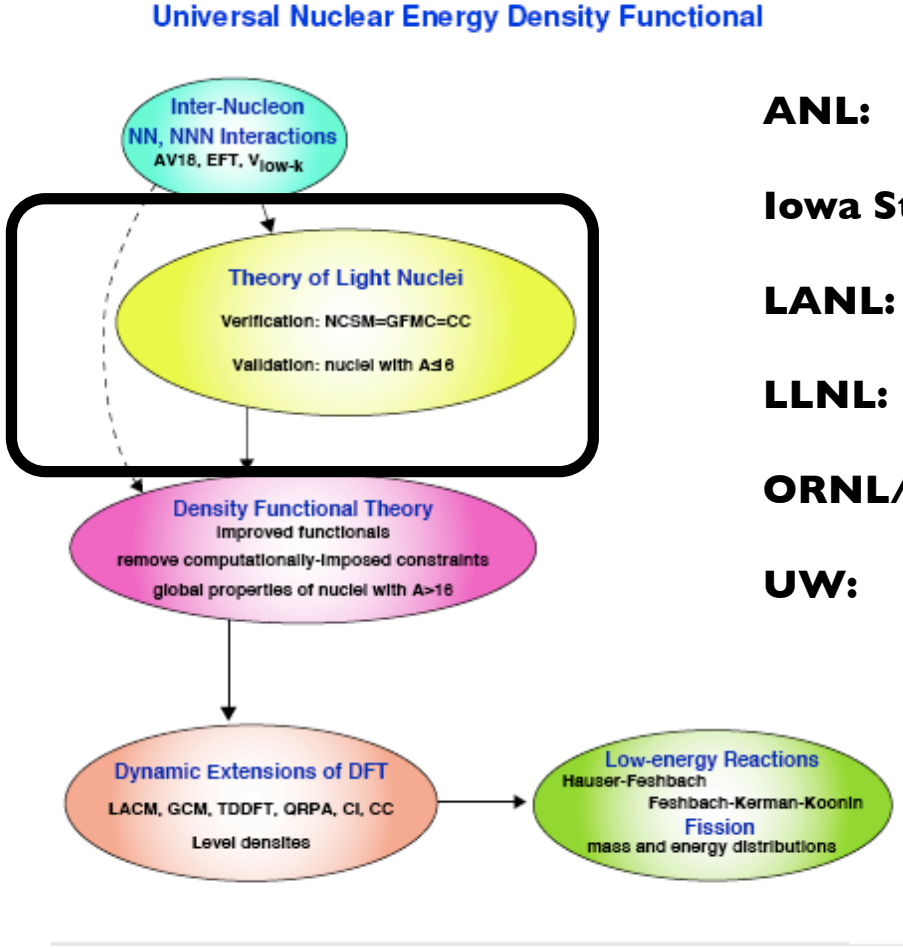
UNEDF SCIDAC ab-initio progress

Neutron Matter
Light Nuclei
Medium Mass Nuclei



ANL:
Pieper, Wiringa

Iowa State:
Vary, Maris

LANL:
Carlson, Gezerlis, Stetcu, Dupuis

LLNL:
Navratil, Ormand

ORNL/UT:
Dean, Papenbrock, Hagen

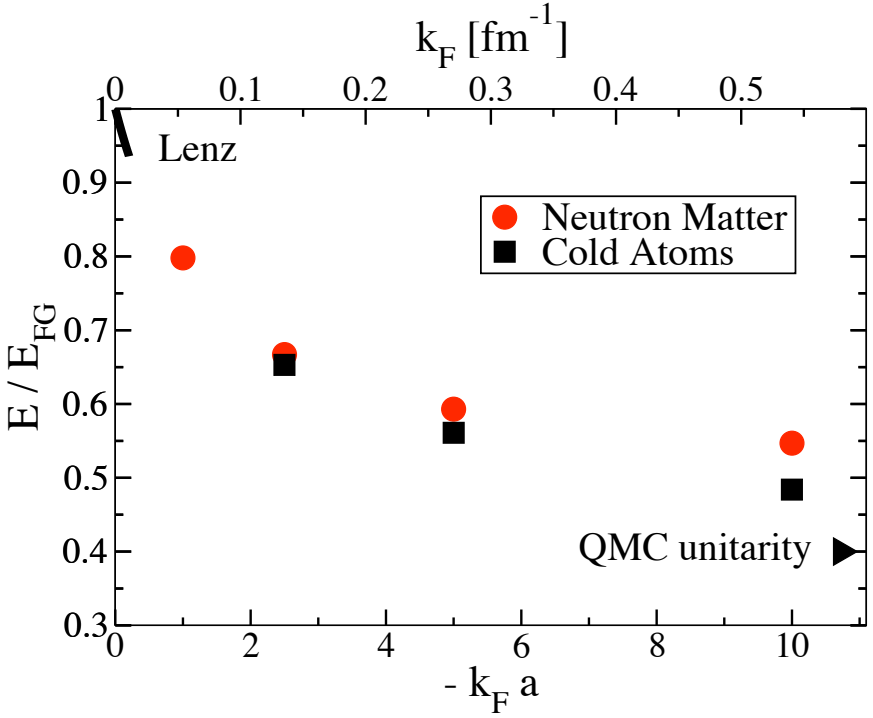
UW:
Bulgac

Validation/Verifications of Codes
Constraining Density Functional
Strong Ties to Computational Science

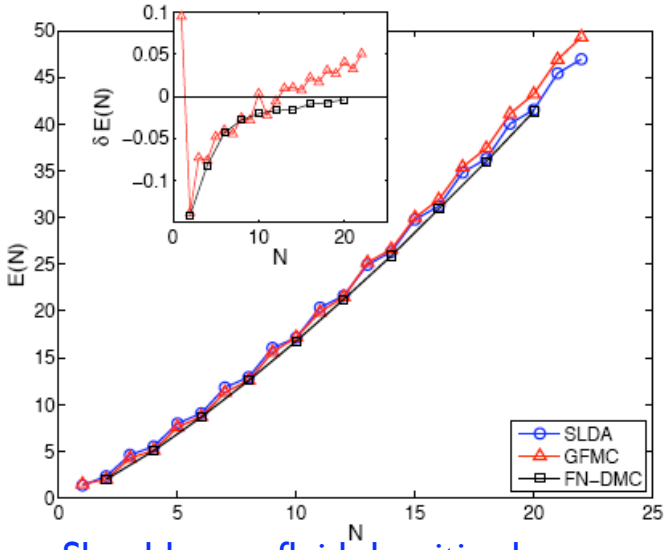
Neutron Matter EOS

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

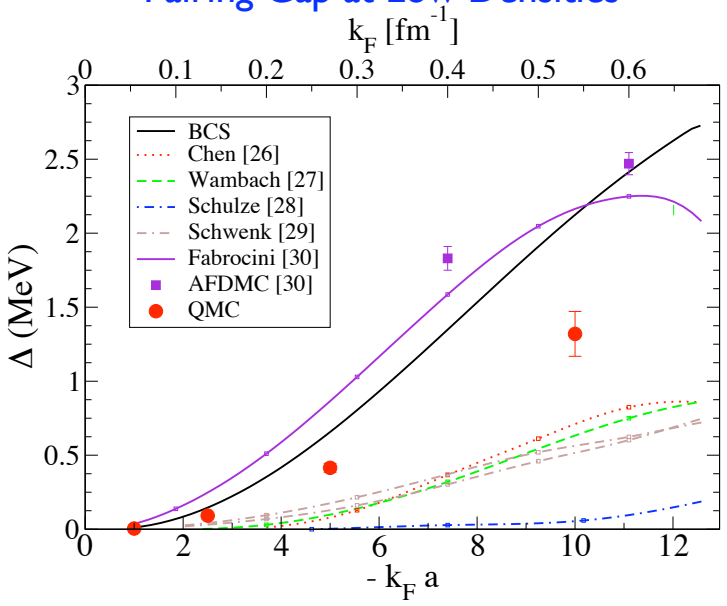


Should superfluid densities be included explicity in density functional?

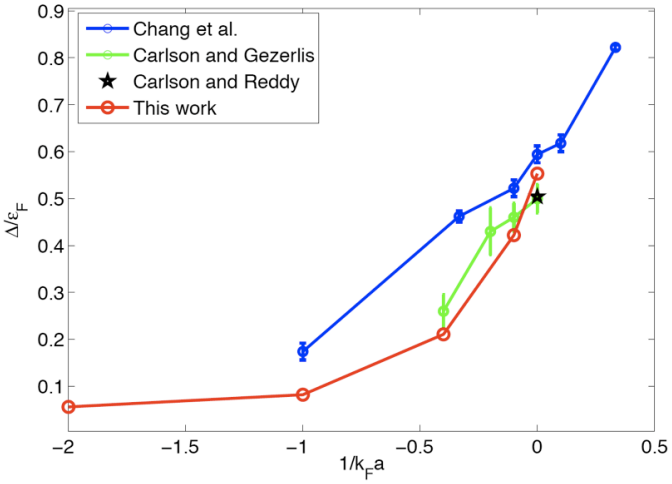
Calculate one-, two-body density matrix for matter
Do SLDA & other Density functionals work as well for
neutron drops?
Finite range of interaction, weaker pairing,
various trap geometries, ...

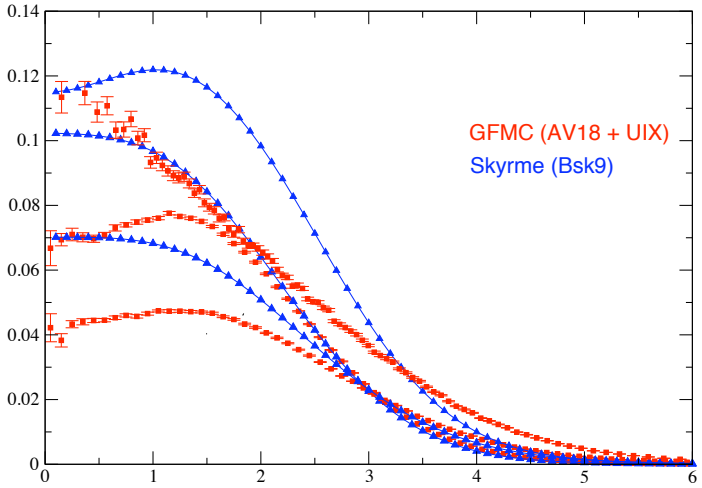
Neutron Matter Pairing Gap

Pairing Gap at Low Densities



Pairing Gap for Atomic Gas
Experimentally confirmed to ~10%





Finite Systems: Neutron Drops

Stringent tests of DFT

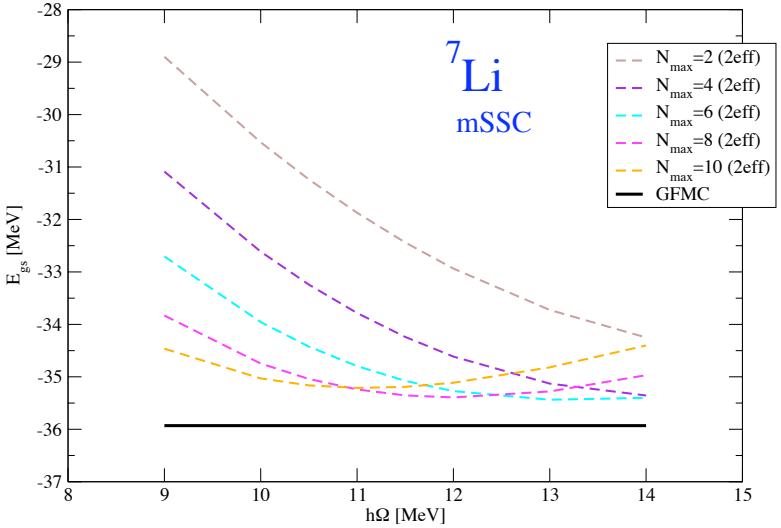
EOS
pairing
external fields: quadrupole, spin dependent,...

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

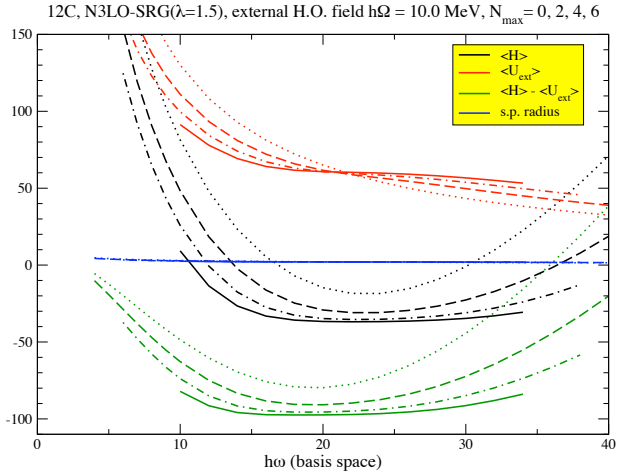
SRG/N3LO better than 1% agreement for ^{4}He, ^{8}He
w/ CC, CI (and FY for ^{4}He)



	^{6}Li	^{6}He	^{7}Li	^{8}He	^{9}Be	^{12}C
modSSC	✓	✓	◎	✓	◎	◎
SSC/TNI			◎			◎
SRG/N3LO				✓		◎

◎ Underway ◎ Started Yr 2

^{12}C in an external well



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

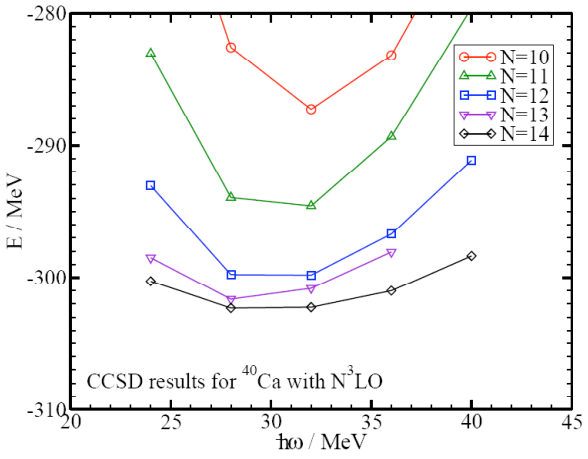
Important ties to Computational Science: Pieper/Lusk (ADLB), Ng/Vary (MFD), ...

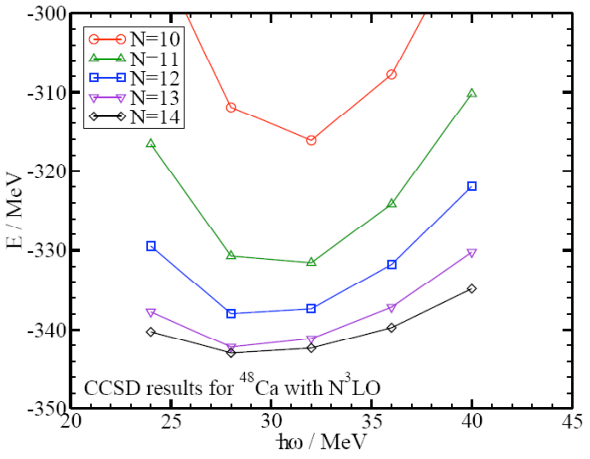
Ab-initio calculations in medium mass nuclei

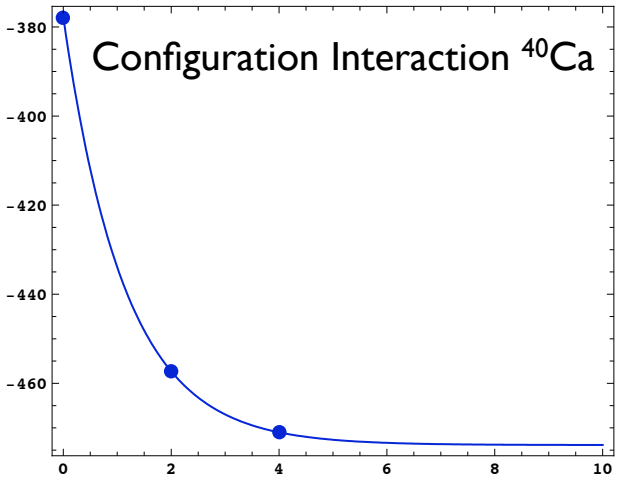
Present Status:

- 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







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-inito

Medium Nuclei: A from 16 to 56

nn interactions - ab initio

ab initio / DFT