UNEDF SCIDAC
ab-initio progress and year 2 plans

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

Neutron Matter/External Pot.
- ab initio / DFT

Emphasizing Connections to DFT / Computational Science
Light Nuclei / Progress

RMS radii need refinement, particularly for weakly bound nuclei

E\_gs\ = \ -26.5(5) \ MeV

E\_gs\ = \ -29.0(4) \ MeV

\textbf{6Li}

\textbf{6He}

\textbf{8He}

\textbf{Benchmark calculations with modified SSCC V8'}

\textbf{Good (0.4 MeV) agreement for energies}

\textbf{RMS radii need refinement, particularly for weakly bound nuclei}
Light Nuclei  GFMC/NCSM

Energy converged to ~0.4 MeV (out of 30–40)
Reasonable understanding of one-body densities

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<th>$^6\text{Li}$</th>
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Physics Issues:
- open shell, weakly bound nuclei
- reliability of evolution from ‘bare’ to lower-momentum interactions
- response to external potentials, one-body density matrix

Few-months time scale
Year 2
Medium Mass Nuclei (A = 16...56)

Reasonable agreement NCSM/CC for Oxygen w/ Vlowk
CC below NCSM for Ca, both well below experimental results

Year 2: CC – Ca isotopes w/ initial TNI
isospin dependence of density functional,
one-body density matrices, ...
Neutron Matter / Drops

EOS/Pairing Gap

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, ...
**Computational Highlights:**

**ADLB**

Scaling results on BG/L
- 256 processors (2 ADLB servers)
  - Speedup of 250; efficiency 97.7%
- 1024 processors (2 ADLB servers)
  - Speedup of 1011; efficiency 98.7%

Should be valuable for many UNEDF codes

**MFD Scaling**

10-B with Nmax = 6 using 3-body interactions on LLNL's Atlas
D = 12,060,706

**CC/pthreads**

MFD Scaling Results
- Speedup: T(Np=1/128)/T(Np)
- Np/128
- MB states
- Eval H
- 500 Lanczos
- SMWF xform
- Observables
- Total

Computational Tuning (with K. Roche)
- Key algorithmic problem: matrix-matrix multiplies
- Use the multi-core capability of the petascale computer (Jaguar will be quad core in Dec)
- Tuned libraries for C=A*B (with p-threads)
- Best-case (square matrices)…trick will be to do things for odd-shaped beasts in CC (year 2).
- Implement in underlying CC algorithm

Should be valuable for many UNEDF codes.
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