Year-3 Deliverables from Continuation Report

- Extend DME and validate against ab initio calculations.
  - low-\(k\) interactions: evolve, test, export evolved 3D 3NF;
  - improve and test nuclear matter on which DME relies;
  - upgrade and validate the DME implementation;
  - compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.

- Develop and test a refit Skyrme functional including universal long-range DME parts.

- Develop orbital-based nuclear DFT (1D models \(\rightarrow\) 3D).

Affiliated Ab Initio DFT Efforts

- Development of non-empirical pairing using \(V_{\text{low } k}\)
Jacob’s Ladder: Coulomb DFT [J. Perdew et al.]

“And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . .” [Genesis 28:12]

HEAVEN $\implies$ Chemical Accuracy
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HEAVEN $\rightarrow$ Chemical Accuracy

1. Local spin density approximation (LSDA) with $\rho_{\uparrow}(r)$ and $\rho_{\downarrow}(r)$ as ingredients.
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HEAVEN $\rightarrow$ Chemical Accuracy

3. Meta-GGA adds (some subset of) $\nabla^2 \rho_\uparrow(r)$, $\nabla^2 \rho_\downarrow(r)$, $\tau_\uparrow(r)$, and $\tau_\downarrow(r)$.
[Note: $\tau[\rho]$ is nonlocal; $\tau[\phi^K_S]$ is semi-local.]

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“Non-empirical” functionals $\rightarrow$ constraints, not fits!
Jacob's Ladder: Nuclear DFT [arXiv:0906.1463]

“And he [Jacob] dreamed, and behold a ladder set up on the earth, and the top of it reached to heaven . . .” [Genesis 28:12]

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2. Generalized Skyrme with $\nabla^n \rho(\mathbf{r})$, $\rho^\alpha(\mathbf{r})$, . . .

1. Conventional Skyrme EDF’s [e.g. SLY4].

- Each rung has sub-rungs!
- Parallel development of 2. – 5. (load balancing??)
- Add constraints (e.g., ab initio neutron drops)
UNEDF Interconnections for Ab Initio Functionals

Ab Initio WF Methods
- CC: UT/ORNL (Hagen et al.)
- TRIUMF (Bacca)
- NCFC: ISU (Maris, Vary)
- LLNL (Navratil et al.)

Ab Initio Functional + Nuclear Matter
- OSU (Drut, Furnstahl, Platter)
- MSU (Bogner, Gebremariam)
- also Saclay/Lyon, TRIUMF

DFT Applications
- UT/ORNL (Schunck, Stoitsov)
- UW (Bertsch, Baroni)
- Saclay (Duguet, Lesinski, ...)

Interactions
- Chiral EFT
- Bonn/Julich (Epelbaum, Nogga)
- Idaho/Salamanca (Entem, Machleidt)
- Vlowk/SRG
- OSU (Jurgenson)
- MSU (Bogner)
- TRIUMF (Schwenk, Bacca, Hebeler)

Participant color key:
- UNEDF
- International collaborator
- Outside UNEDF
**UNEDF Interconnections for Ab Initio Functionals**

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**Tests of DME:**
- Energies, densities with same H
- Vary 3NF, external potential parameters
- Cutoff dependence as diagnostic

**Tests of nuclear matter:**
- New fits, self–energies, ...
- Improved 3NF for DME
- Generalized DME
- DFT from OEP/OPM

**Systematics along isotope chains, odd–even**
- Tests: spin–orbit splittings, time–odd terms, ...
- Non–empirical pairing functional

**Long–range pion contributions**
- from NN and NNN DME
- plus fit residual Skyrme in HFB code

**Wider range of nuclei**
- Full 3NF vs. dd 2NF
- Ab Initio densities
- External potentials

**Interactions**
- Chiral EFT
  - Bonn/Julich (Epelbaum, Nogga)
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- TRIUMF (Schwenk, Bacca, Hebeler)

**N3LO 3NF**
- Explicit Delta’s
- New 3NF fits
- SRG 3NF evolution

**In–medium SRG**

**Participant color key:**
- UNEDF
- International collaborator
- Outside UNEDF
Progress on $V_{\text{low } k}$/SRG Interactions (since Aug. 2008)

OSU + MSU + TRIUMF + LLNL

$V_{\text{low } k}$:


SRG:

SRG/$V_{\text{low } k}$ NN code available; ho matrix elements; new NNN fits

Year 2–3 plan: SRG evolution of NNN (first 1D, then 3D)

Or: In-medium SRG (Bogner), density-dependent dependent NN (TRIUMF)
3D SRG Evolution with $T_{\text{rel}}$ in a Jacobi HO Basis

E. Jurgenson, P. Navratil, rjf, arXiv:0905.1873

- Evolve in any basis [momentum space in progress by L. Platter]
- Here: use anti-symmetric Jacobi HO basis from NCSM
- directly obtain SRG matrix elements in HO basis
- separate 3-body evolution not needed

Compare 2-body only to full $2 + 3$-body evolution:

![Graphs showing ground-state energy for $^3H$ and $^4He$](image)

Ground-State Energy [MeV]

- $^3H$ $N^3LO (500 \text{ MeV})$
- $^4He$ $N^3LO (500 \text{ MeV})$

- NN-only
- NN + NNN-induced
- +NNN-initial

Expt.
3D SRG Evolution with $T_{\text{rel}}$ in a Jacobi HO Basis

E. Jurgenson, P. Navratil, rjf, arXiv:0905.1873

- Good convergence properties independent of 3-body:

- HO matrix elements (to be) available for NCFC, CC, . . .
- Challenge: efficient (on-the-fly) conversion to m-scheme
Nuclear Matter Status [Bogner et al., arXiv:0903.3363]

- Use a chiral EFT to a given order (e.g., E/M N^3LO below); soften with RG (evolve to $\Lambda \approx 2 \text{ fm}^{-1}$ for ordinary nuclei)
- NN interactions fully, NNN interactions (3NF) approximately
- Need CC calculation of nuclear matter to validate!

Generate density functional using NV DME in $k$-space.
Year 2: Adaptation to Skyrme HFB Code (HFBRAD)

\[ \mathcal{E}_{\text{Skyrme}} = \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2) |\nabla \rho|^2 + \cdots \]

\[ \implies \mathcal{E}_{\text{DME}} = \frac{\tau}{2M} + A[\rho] + B[\rho] \tau + C[\rho] |\nabla \rho|^2 + \cdots \]

Kohn–Sham Potentials

Skyrme energy functional
\( t_0, t_1, t_2, \ldots \)

HFB solver

Orbitals and Occupation #’s

\[ J_0(r) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(r)} \iff \left[ -\frac{\nabla^2}{2m} - J_0(x) \right] \psi_\alpha = \varepsilon_\alpha \psi_\alpha \implies \rho(x) = \sum_\alpha n_\alpha |\psi_\alpha(x)|^2 \]
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\[ \implies E_{DME} = \frac{\tau}{2M} + A[\rho] + B[\rho] \tau + C[\rho] |\nabla \rho|^2 + \cdots \]

Kohn–Sham Potentials

DME
energy
functional
A[\rho], B[\rho], ...

HFB
solver

Orbitals and Occupation #'s

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Validation of HFBRAD_DME Implementation

- Reproduces Skyrme results (with good accuracy)
- Possible issues: Sprung et al. test; $dC[\rho]/d\rho$ terms
- Try fine-tuned nuclear matter with low-momentum NN/NNN

$V_{\text{srg}} \lambda = 2.0 \text{ fm}^{-1} (N^3 \text{LO})$

Do densities look like nuclei from Skyrme EDF's? (Yes)
DME Nuclear Matter and Bulk Nuclei

- Use latest (unadjusted) nuclear matter calculations in DME
- Problem: DME approximations cost 1–1.5 MeV/nucleon binding even in nuclear matter

Correct trends for nuclei (Coester line), but way underbound

CC comparison calculations delayed because of 3NF
DFT Validation Against Ab Initio Calculations

“Coester Lines”
- Compare systematics, e.g., by varying 3NF coupling in Hamiltonian

External Potentials
- DFT from response of energy to perturbation of densities ⇒ Apply external fields

Plan: Revisit $c_E$ trends, neutron drops
Revisit Dependence on Contact 3NF (Preliminary!)

- Approximate the 3NF contribution by averaging 3rd particle at fixed $k_F \Rightarrow$ effective NN (K. Hebeler)

- Applied to coupled cluster by S. Bacca $\Rightarrow$ fast!

- Slope vs. $c_E$ gives $\langle 3NF \rangle$

- Here: normalize to $c_E = -1$
What is the OEP?

- Density Functional Theory (Hohenberg-Kohn)
  “A density functional exists…”

- Kohn-Sham approach
  “The density functional can be optimized by solving a Schrödinger-like problem…”

- If the functional is explicitly density-dependent we know how to do this:
  \[ v_{KS}(\mathbf{r}) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(\mathbf{r})} \]

- But what happens if the functional depends explicitly on the KS orbitals and only implicitly on the density?
  (E.g. Hartree-Fock functional (!))
The DFT ladder in quantum chemistry

- **LDA**  “Take the density-dependent energy of the uniform system and replace $n$ with $n(x)$…”
  - Very easy to implement
  - Not very accurate

- **GGA**  “Take the LDA and add gradient corrections…”
  - Great improvement over LDA
  - Has some difficult problems: Absence of negative ions, van der Waals forces, strong correlations...

- **OEP**  “Allow for explicit orbital dependence …”
  - Harder to implement, computationally more expensive
  - Allows for exact exchange, solves many of the GGA problems
The OEP equation

How do we determine $v_{KS}(\mathbf{r})$? Apply chain rule!

$$v_{KS}(\mathbf{r}) = \frac{\delta E_{\text{int}}[\varphi_i, \varepsilon_i]}{\delta \rho(\mathbf{r})} = \int d\mathbf{r}' \frac{\delta v_{KS}(\mathbf{r}')}{\delta \rho(\mathbf{r})} \sum_j \left\{ \int d\mathbf{r}'' \frac{\delta \varphi_j^{\dagger}(\mathbf{r}'')}{\delta v_{KS}(\mathbf{r}')} \frac{\delta E_{\text{int}}}{\delta \varphi_j^{\dagger}(\mathbf{r}'')} + \text{c.c.} + \frac{\delta \varepsilon_j}{\delta v_{KS}(\mathbf{r}')} \frac{\partial E_{\text{int}}}{\partial \varepsilon_j} \right\}$$

Talman & Shadwick (1976):

“What is the best multiplicative potential that minimizes the energy?”

Minimization with subsidiary condition!
The OEP equation

**OEP integral equation**

\[
\int dx' \ Q(x, x') u_{xc}(x') = \Lambda(x)
\]

\[
Q(x, x') = \sum_{j=1}^{N} \varphi_j^*(x') G_j(x', x) \varphi_j(x) + c.c.
\]

\[
\Lambda(x) = \sum_{j=1}^{N} \int dx' \ \varphi_j^*(x') u_{xc,j}(x') G_j(x', x) \varphi_j(x) + c.c.
\]

**Green's function**

\[
G_j(x', x) = \sum_{k \neq j} \frac{\varphi_k(x') \varphi_k^*(x)}{\varepsilon_j - \varepsilon_k}
\]

**Auxiliary potential**

\[
u_{xc,j}(x') = \frac{1}{\varphi_j^*(x')} \frac{\delta E_{int}}{\delta \varphi_j(x')}
\]

Sum over occupied and unoccupied states!
The KLI approximation

- Take the OEP equation and replace...

\[ G_j(x', x) = \sum_{k \neq j} \frac{\varphi_k(x')\varphi_k^*(x)}{\varepsilon_j - \varepsilon_k} \]

\[ G_j^{KLI}(x', x) = \frac{1}{\varepsilon_j - \varepsilon_j^0} \sum_{k \neq j} \varphi_k(x')\varphi_k^*(x) \]

\[ = \frac{1}{\varepsilon_j - \varepsilon_j^0} [\delta(x - x') - \varphi_j(x')\varphi_j(x)] \]

Is this a good approximation?
In practice it gives excellent results in the exchange-only limit.

- KLI equation

\[ \psi_{xc}^{KLI}(r) = V_{SL}(r) + \sum_i \frac{n_i(r)}{n(r)} (\langle i | \psi_{xc}^{KLI} | i \rangle - \langle i | \psi_{xc,i} | i \rangle) \]

\[ V_{SL}(r) = \sum_i \frac{n_i(r)}{n(r)} u_{xc,i}(r) \quad \text{Slater potential} \]

▲ Sum only over occupied states!
▲ Can be solved iteratively or directly!
The KLI approximation

- Performance comparison

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<th>$E_{\text{tot}}$ KLI</th>
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One-Dimensional Laboratory for OEP

- J. Drut, L. Platter, rjf
- Simple short-range repulsion and long-range attraction
- Warm-up for realistic problem
- With trap or self-bound
- Compare approximations (e.g., Hartree-Fock vs. KLI vs. DME vs. full OEP)
Non-Empirical Pairing Functional for Nuclei
T. Duguet (Saclay); T. Lesinski (UT/ORNL), K. Bennaceur, J. Meyer (Lyon)

- Spherical code BSLHFB (T.L.)
  - spherical Bessel function basis
  - finite-range / non-local pairing interactions in EDF
  - separable $V_{\text{low } k}(\Lambda)$ expansion

- Pairing at lowest order in NN (nuclear + Coulomb); no fits!
  - use $V_{\text{low } k}$ at $\Lambda \approx 2 \text{ fm}^{-1}$ as NN pairing interaction
  - Use SLY4 Skyrme for ph EDF with fixed $m_0^*/m = 0.7$

- Studied $m^*(k, k_F)$ for cutoffs $\Lambda$ (K. Hebeler, T.D., T.L., A. Schwenk)
  - see arXiv:0904.3152
  - consistent ph/pp scales needed
  - $V_{\text{low } k}$ ok with $m^*_\text{Skyrme}(k_F)$
Consider matrix elements $V_{\Lambda=1.8/6}(k_F^n, p)$

Write gap equation schematically as

$$\hat{\Delta}(k_F^n) \equiv \int dq \ Y(k_F^n, q)$$

Effect of $m_T^*(k_F^T) = \text{constant}$ - 'pe' values here

- Good approx for soft $\Lambda$ around $k_F^n$
- Bad approx for hard $\Lambda$ at relevant $p \gtrsim 2 \, \text{fm}^{-1}$

Gap generated

- Around the Fermi surface for soft $\Lambda$
- Mainly at large momenta for hard $\Lambda$
Pairing gaps from $\nu^{pp} = V_{NN} + V_{\text{Coul}}$


- $\Delta^{(3)}_{\text{exp}}(\text{odd})$ versus $\Delta_{\text{LCS}}(\text{even})$

- Pairing gaps $\Delta^q$ are consistently close to experimental data
- Coulomb decreases $\Delta^p$ by $\sim 40\%$ to bring them close to experiment
Contribution from Higher Partial Waves

S. Baroni et al., “Partial wave contributions to pairing in nuclei” (soon)

- Several $L_{rel}$ contribute to $J = 0$ pairing with $J = J_{rel} + L_{cm}$
- Time-reversal restricts to $^3P_1$ and $^1D_2$

Non-zero but limited repulsive effects from $^3P_1$ to the OEMS

More pronounced effects on QP excitation spectrum
Comparing theoretical and experimental "pairing gaps"

The good method $\Delta_{\text{expt}}^{(3)}(N)$ vs $\Delta_{\text{theory}}^{(3)}(N)$

The actual method $\Delta_{\text{expt}}^{(3)}(N)$ vs $\Delta_{\text{theory}}^{(3)}(N)$

$\Delta_{\text{exp}}^{(3)}(\text{odd})$ versus $\Delta_{\text{LCS}}^{(\text{even})} = \text{Gap at } \epsilon_F \text{ in even } N \text{ nucleus}$
Pairing gaps $^{1S_0}$ and interplay with shell structure


- $\Delta^{(3)}_{\text{exp}}(N)$ versus $\Delta^{(3)}_{\text{th}}(N)$ (self-consistent qp filling approx)

- $\Delta^{(3)}_{\text{th}}(\text{odd}) \approx [\Delta_{\text{LCS}}(\text{even}) + \Delta_{\text{LCS}}(\text{odd})]/2$  [T. Duguet et al. PRC65 (2002)]

- Deepening around $N \approx 115$ arises from blocking of $\Delta_{\text{LCS}}(\text{odd})$

- $\Delta^{(3)}$ well described close to $N = 82$ without LN, proj. or pairing vib.
Pairing gaps ($^1S_0$) and interplay with shell structure


- $\Delta^{(3)}_{\text{exp}}(N)$ versus $\Delta^{(3)}_{\text{th}}(N)$ (self-consistent qp filling approx)

- Neutron (proton) gaps consistent with (slightly lower than) experiment
- Access detailed interplay with shell structure

Other: Include chiral N$^2$LO 3NF [T. Lesinski] using 3rd particle averaging [K. Hebeler]; include p-h fluctuations [Baroni, Pastore et al.]
Ab Initio Nuclear DFT Progress Report

Year-3 Deliverables from Continuation Report

- Extend DME and validate against ab initio calculations.
  - low-\(k\) interactions: ✓ evolve, ✓ test, ❌ export evolved 3D 3NF;
  - ✓ improve and test nuclear matter on which DME relies;
  - ✓ upgrade and validate the DME implementation;
  - ❌ compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.

- ✓ Develop and test a refit Skyrme functional including universal long-range DME parts.

- ✓ Develop orbital-based nuclear DFT (1D models ➞ 3D).

Affiliated Ab Initio DFT Efforts

- ✓ Development of non-empirical pairing using \(V_{low\ k}\)
Articles and Preprints Citing SCIDAC Support

- Published or Posted since Pack Forest 2008


Plans for **Rest of Year 3 and Year 4 . . .** (Part 1)

- **NNN fits and tests**
  - NNN project to interface $V_{\text{low }k}$ chiral EFT NNN with FCI
  - Test new fits with CC and FCI in larger nuclei (e.g., $\lambda/\Lambda$ dependence)

- **Evolving NNN 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 NNN
  - Validate 3NF fits vs. evolved 3NF

- **Nuclear matter calculational extensions**
  - Full 2nd order calculation with fit NNN (w/TRIUMF)
  - Asymmetric nuclear matter (just coding to finish)
  - Solve uniform matter with in-medium SRG
  - Explore coupled cluster for nuclear matter (UT/ORNL)
Plans for **Rest of Year 3 and Year 4 . . . (Part 1)**

- **Nuclear matter studies**
  - Complete and publish the G-matrix and BBG study
    - 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 $N^3LO$ chiral EFT at Hartree-Fock

- **Validating (or invalidating) DME from $V_{\text{low } k}/\text{SRG}$**
  - Compare energies, $\rho$’s to CC, NCFC with same Hamiltonian
    - Vary contact 3NF strength, full 3NF-fitted $V_{\text{low } k}/\text{SRG}$
  - Compare in external potentials with NCFC, GFMC/AFMC
    - neutron drops

- **Beyond DME**
  - Continue 1D (3D) development of orbital based nuclear DFT
  - KLI approximations vs. full OEP
  - Model tests against DME; full comparison
  - Symmetry breaking, long-range correlations . . .