Ab Initio Functionals
Summary Report

Dick Furnstahl

Department of Physics
Ohio State University

June, 2010
Vlowk/SRG NN+NNN (Jurgenson)

+ operators (Anderson)
Neutron/Nuclear matter (Hebeler)

Vlowk, SRG NN + fit NNN

Neutron/Nuclear matter (Hebeler)
DME development (Bogner)
In-medium SRG (Bogner, Hergert)
DME-based EDF
(Stoitsov, Kortelainen)
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}\text{Ca}$ DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}\text{Ca}$ DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
4\textsuperscript{He} Convergence

- Rapid and smooth convergence
- Induced 4NFs contribute about 30-60 keV
- Smaller than discrepancy of bare with experiment from omitted N3LO 3NF and 4NF
- Monitor induced 4NFs closely with increasing A, due to their strong density dependence

PRL 103, 082501 [arXiv: 0905.1873]
$^6$Li: using the slater-determinant basis

- 6Li, 7Li, and the rest of the p-shell nuclei require a new procedure
  - Push the truncations to 300/36
  - Variational: find the minimum
  - At $N_{\text{max}} = 8$, min is at $\hbar\Omega = 20$
  - Input files here are 13 Gb
    (32 Gb for other p-shells)
$^6$Li: NN and NN+NNN calculations

- Increased $N_{\text{max}}$-A2 to 300 and $N_{\text{max}}$-A3 to 36
- Simple extrapolations show significant spread in $\lambda$
- Induced 4NF? Missing 3NF?
- Width b/n mid and right are different: A3 truncation
- Spectral structure is preserved nicely
- $2^+;1$ and $3^+$ not converging as fast, but more sensitive to higher J
- More evidence that $A_{3n_{max}}$ should be higher

\[ \begin{align*}
\text{Li} & \quad \text{Energy (MeV)} \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -10 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -12 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -14 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -16 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -18 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -20 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -22 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -24 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -26 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -28 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -30 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -32 \\
\hline
\hline
\hline
\text{E}_{\text{max}} & -34 \\
\hline
\hline
\hline
\end{align*} \]
# Plan for Rest of Year 4 and Year 5

## Deliverables

### Recap
- SRG improves convergence
- Variational and model space independent
- Induced forces are of natural size – no larger than the error due to missing initial ANFs
- Still waiting on more precise calculations ($A_3-N_{\text{max}}=40$) to determine their significance at $A \geq 6$

### Outlook
- Monitor hierarchy of induced higher-body forces in p-shell nuclei (MFDn)
- Collaborate to achieve coupled cluster results with 3NF inputs
- Apply these results to reactions (NCSM+RGM)
SRG Operators  (Eric Anderson et al.)

Operator Evolution & Extraction Process

SRG Evolution

\[ U_s = \sum_{\alpha} |\psi_\alpha(s)\rangle \langle \psi_\alpha(0)| \]

\[ U_s^{(1)} \quad 1\text{-Particle Basis} \]
\[ U_s^{(2)} \quad 2\text{-Particle Basis} \]
\[ U_s^{(3)} \quad 3\text{-Particle Basis} \]
\[ \vdots \]

Evolution in n-Particle space determines n-Body component of operator for all A

Original Operator

\[ \hat{O} = \hat{O}^{(1)} + \hat{O}^{(2)} + \cdots \]

Embed in 2-Particle Basis

\[ U_s^{(2)} \hat{O} U_s^{(2)} \]

\[ \hat{O}_s^{(1)} \]

Embed in 3-Particle Basis

\[ U_s^{(3)} \hat{O} U_s^{(3)} \]

\[ \hat{O}_s^{(1)} + \hat{O}_s^{(2)} + \cdots \]

Embed in A-Particle Basis

1-B Operator

2-B Operator

3-B Operator
Factorization in Few-Body Nuclei

- **Variational Monte Carlo Calculation**
  → Using AV14 NN potential

- **Possible explanation of scaling behavior**
  → Results from dominance of NN potential and short-range correlations (Frankfurt, et al.)

- **1D few-body HO space calculation**
  → System of $A$ bosons interacting via a model potential

- **Alternative explanation of scaling behavior**
  → Results from factorization

\[ \psi_\lambda(k') [I_{\alpha\alpha} K_\lambda(k') K_\lambda(k)] \psi_\lambda(k) \]

\[ N(p)/A \]


\[ N_{\text{max}} = 36 \]
Conclusion/Outlook

Recent Progress:
- Consistently evolved nuclear operators with SRG in deuteron & model 1D few-body calculations
- Extraction & embedding process for few-body operators formulated and tested
- Explored alternative generators for oscillator basis
- Factorization demonstrated for few-body model calculation

Computational Issues:
- SRG evolution in n-particle basis
  - Exponential growth of matrix size

Plan:
- Establish bounds on growth of many-body operators
- Do calculations in 3D in harmonic oscillator basis
- Explore factorization of other operators (e.g., electroweak)
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}$Ca DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
Improved NNN Treatment  (Kai Hebeler et al.)

Many-body perturbation theory

central quantity of interest: energy per particle \( E/N \)

\[
H(\Lambda) = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \ldots .
\]

- for low momentum interactions no resummation of diagrams necessary
- self-consistent single-particle propagators \( \rightarrow \) thermodynamic consistency
Symmetric nuclear matter

Improvements:

• full treatment of double exchange terms
• self-consistent single-particle self-energies
• correction of combinatorial factors

Bogner, Furnstahl, Schwenk, Nogga; arXiv:0903.3366
Symmetric nuclear matter

- $3N$ forces crucial for saturation
- Cutoff dependence at 2nd order significantly reduced
- Couplings $c_D$ and $c_E$ fitted to $E_{3H} = -8.482$ MeV and $r_{4He} = 1.95 - 1.96$ fm
- 3rd order pp and hh contributions small

Future: Still need coupled-cluster calculations (or VMC?)
Uncertainties due to coupling constants and RG scheme

**Entem/Machleidt (EM):**

\[
\begin{align*}
  c_1 &= -0.81 \text{ GeV}^{-1} \\
  c_3 &= -3.20 \text{ GeV}^{-1} \\
  c_4 &= +5.40 \text{ GeV}^{-1}
\end{align*}
\]

**Rentmeester et al. (RM):**

\[
\begin{align*}
  c_1 &= -0.76 \text{ GeV}^{-1} \\
  c_3 &= -4.78 \text{ GeV}^{-1} \\
  c_4 &= +3.96 \text{ GeV}^{-1}
\end{align*}
\]

- Uncertainty of about 3.5 MeV in E/A at saturation density
- Reasonable saturation properties
- Improved constraints of \( C_i \) couplings necessary!

Fine-tuning needed for quantitative ab initio DME input
Ab Initio Nuclear DFT Deliverables
Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward \(^{40}\text{Ca}\) DME comparisons
- Further development of \(\pi\)-DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-\(k\) interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and \(\text{ph}\) channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
**Alternative many-body method** (Bogner, Hergert)

**In-medium SRG for Nuclear matter**

- Normal order $H$ w.r.t. non-int. fermi sea
- Choose SRG generator to eliminate “off-diagonal” pieces
  
  \[
  \frac{dH(s)}{ds} = [\eta(s), H(s)]
  \]
  \[
  \eta = [\hat{f}, \hat{\Gamma}]
  \]

  \[
  \lim_{s \to \infty} \Gamma_{od}(s) = 0
  \]
  \[
  \langle 12|\Gamma_{od}|34 \rangle = 0 \text{ if } f_{12} = f_{34}
  \]

- Truncate to 2-body normal-ordered operators “IM-SRG(2)”
  - dominant parts of induced many-body forces included implicitly

\[
H(\infty) = E_{vac}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4} \sum [\Gamma_d(\infty)]_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k)
\]

- $E_{vac}(\infty) \rightarrow E_{gs}$
- $f_k(\infty) \rightarrow \epsilon_k$ (fully dressed s.p.e.)
- $\Gamma_d(\infty) \rightarrow f(k', k)$ (Landau q.p. interaction)

Microscopic realization of SM ideas: dominant MF + weak $A$-dependent $NN_{\text{eff}}$
Alternative many-body method  (Bogner, Hergert)

Correlations “adiabatically” summed into $H(\lambda)$

$P_{N^3}$LO(500)

-$\kappa_F = 1.35 \text{ fm}^{-1}$

PNM*

Weak cutoff dependence over large range $\Rightarrow$ dominant 3,4,...-body terms evolved implicitly

SNM*

$\kappa_F = 1.4 \text{ fm}^{-1}$

*Neglects ph-channel. See Heiko Hergert’s talk.
Application to closed-shell nuclei (Tsukiyama et al.)

IM-SRG(2) diagonalization of closed-shell systems

Comparable to coupled-cluster in closed shell nuclei.

Similar scaling with number of orbitals \( \sim N^6 \)

Neutron droplet comparisons in rest of year 4
In-Medium SRG: Year 4–5 Plans

- Include initial NNN interactions (\(N\)-ordered 0,1,2–body parts) for the single-reference state calculations
- IM-SRG for infinite matter
  - Continue work on including particle-hole channel (hard!!)
  - Normal-order with respect to HFB ground state
- Derive valence shell model effective Hamiltonians and operators
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}$Ca DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
OEP Development (Drut, Platter, rjf)

The OEP equation

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

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

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

Auxiliary potential

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

Green's function

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

Sum over occupied and unoccupied states!
OEP Development  (Drut, Platter, rjf)

The OEP equation

- OEP integral equation

\[ \int dx' \ Q(x, x') v_{xc}(x') = \Lambda(x) \]
Solving the OEP equation

Two problems:

- Constructing the Green’s function explicitly may be expensive
- The OEP equation is singular

\[ \sum_{k=1}^{N} \psi_k^*(x) \varphi_k(x) + c.c. = 0 \]

\[ (\hat{h}_{KS} - \varepsilon_i) \psi_i^*(x) = - \left[ \Delta_i(x) - \bar{\Delta}_i \right] \varphi_i(x) \]

\[ \Delta_i(x) = v_{xc}(x) - u_{xc,i}(x) \]

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

- Implemented full OEP solution in 1D (Kümmel-Perdew algorithm)
  - Allows for orbital-dependent functionals
  - Solves formal and practical problems of GGAs
  - Allows for exact exchange, RPA, Pairing, etc...

- Tested 1D proof-of-concept against Hartree-Fock

- Derived OEP-HFB equations (first time)

- 3D code under development (framework in place, now debugging)

- Minnesota potential & compare with HF, HF-DME, NCSM, GFMC

- RPA?

- QRPA?
Ab Initio Nuclear DFT Deliverables
Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}\text{Ca}$ DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
DME Development (Gebremariam et al.)
Density Matrix Expansion Revisited (Negele and Vautherin)

Expand of DM in local operators w/factorized non-locality

\[ \langle \Phi | \psi^\dagger (\mathbf{R} - \frac{1}{2} \mathbf{r}) \psi (\mathbf{R} + \frac{1}{2} \mathbf{r}) | \Phi \rangle = \sum_n \Pi_n (k_F r) \langle \mathcal{O}_n (\mathbf{R}) \rangle \]

\[ \langle \mathcal{O}_n (\mathbf{R}) \rangle = [\rho (\mathbf{R}), \nabla^2 \rho (\mathbf{R}), \tau (\mathbf{R}), \mathbf{J} (\mathbf{R}), \ldots] \]

Dependence on local densities/currents now manifest

\[ \langle V_2 \rangle \sim \sum_{n,m} \int d\mathbf{R} \mathcal{O}_n (\mathbf{R}) \mathcal{O}_m (\mathbf{R}) \int d\mathbf{r} \Pi_n (k_F r) \Pi_m (k_F r) V_2 (r) \]

\[ \approx \sum_t \int d\mathbf{R} \left\{ C_{t}^{\rho \rho} \rho_t^2 + C_{t}^{\rho \tau} \rho_t \tau_t + C_{t}^{\rho \Delta \rho} \rho_t \Delta \rho_t + C_{t}^{J J} J_t^2 + C_{t}^{J \nabla \rho} J_t \nabla \rho_t \ldots \right\} \]

\[ C^{ij} [u] \xi_i \xi_j , \quad u \equiv \frac{k_F (R)}{m_\pi} \]

\[ C^{ij} [u] = C_{1}^{ij} [u] + C_{2}^{ij} [u] \ln (1 + 4u^2) + C_{3}^{ij} [u] \arctan (2u), \]

\[ C^{ij} [u] = \text{rational polynomial} \]
Prescriptions for $\Pi_n$-functions

**Phase space averaging (PSA-DME)** (Gebremariam et al. arXiv:0910.4979)

\[ \rho(\vec{r}_1, \vec{r}_2) = e^{i\vec{r}_1 \cdot \vec{k}} e^{\frac{i}{2} \cdot (\vec{\nabla}_1 - \vec{\nabla}_2) - i\vec{r}_2 \cdot \vec{k}} \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}} \]

Average the non-locality operator over local momentum distribution $g(\vec{R}, k)$ and expand exponentiated gradients

\[ \rho(\vec{r}_1, \vec{r}_2) \approx \int d^3 k \ g(\vec{R}, k) e^{i\vec{k} \cdot \vec{r}} \sum_{n=0}^{2} \frac{1}{n!} \left\{ \vec{r} \cdot \left( \frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2} - i\vec{k} \right) \right\}^n \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}} \]

Easy to build in physics associated with surface effects in finite fermi systems (**non-isotropic** $g(\vec{R}, k)$)

Crucial to accurately describe spin-vector part of OBDM
Look at $\int d\mathbf{r} d\mathbf{R} V_{1\pi}(r) \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1)$:

- Inclusion of finite fermi phase space effects crucial for **quantitative** agreement
- completely parameter-free

Can now apply modified DME with confidence to spin-unsaturated systems
New development: DME for chiral NNN force (N2LO)

- Expect interesting spin-orbit/tensor couplings from TPE

\[
V_c(q_1, q_2, q_3) \sim \frac{\sigma_1 \cdot q_1 \sigma_2 \cdot q_2}{(q_1^2 + m_\pi^2)(q_2^2 + m_\pi^2)} F^{\alpha\beta}_{123} \tau_1^\alpha \tau_2^\beta + \text{perms}
\]

\[
F^{\alpha\beta}_{123} \equiv \delta_{\alpha\beta} \left[ -4 \frac{c_1 m_\pi^2}{f_\pi^2} + 2 \frac{c_3}{f_\pi^2} q_1 \cdot q_2 \right] + \frac{c_4}{f_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_3^\gamma \sigma_3 \cdot (q_1 \times q_2)
\]

Empirical EDFs (Skyrme, Gogny,...) spin-orbit coupling is density independent \(\Rightarrow\) appropriate for NN spin-orbit forces (short range)

This is a mismatch since microscopic NNN interactions are long-range (DME \(\Rightarrow\) density dependent \(J \cdot \nabla \rho\) couplings)
\[ C^{ijk} \left[ u \right] \xi_i \xi_j \xi_k , \quad u \equiv \frac{k_F(R)}{m_\pi} \quad \text{(note: } u \text{ is NOT small)} \]

\[ C^{ijk} \left[ u \right] = C_1^{ijk} \left[ u \right] + C_2^{ijk} \left[ u \right] \ln(1 + 4u^2) + C_3^{ijk} \left[ u \right] \arctan(2u), \]

\[ C^{ijk}_{\alpha} \left[ u \right] = \text{rational polynomial} \]
DME Year 4 Deliverables

• DME $E_x[\rho]$ from chiral EFT NN + NNN thru NNLO delivered to ORNL EDF group
  – Mathematica package + Python scripts available to public
  – Original NV-DME or PSA-DME options (others easy to implement)
  – Implemented in HFTHO and HFBRAD and 1st optimizations begun by ORNL group (Stoitsov, Kortelainen)

• Use improved DME to validate against ab-initio
  – 1st results obtained for neutron droplets w/Minnesota NN potential
  – Beyond HF and more realistic NN + NNN rest of Year 4 and 5

• Year 5 roadmap
  – revisit comparison to ab initio for nuclei w/realistic NN + NNN (DME improvements + exact Hartree)
  – microscopic constraints on short-range non-analytic density dependencies ($\rho^{2+\gamma}$ etc.)
  – comparison to OEP for $E_x$
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}$Ca DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
Calculations with DME-based EDF (Stoitsov et al.)

Towards Ab Initio Nuclear Energy Density Functional Underlining Philosophy

Exact Two-Body Density Matrix

$$\rho^{(2)}(x_1, x_2; x'_1, x'_2) = \langle \Psi | a^+(x_1) a^+(x_2) a(x'_1) a(x'_2) | \Psi \rangle$$

$$\rho^{(2)}(s) = \int \rho^{(2)}(R + s/2, R - s/2) dR$$

Two-Body Density Matrix in Hartree-Fock Approximation

$$\rho^{(2)}_{HF}(x_1, x_2; x'_1, x'_2) = \langle \Phi | a^+(x_1) a^+(x_2) a(x'_1) a(x'_2) | \Phi \rangle$$

$$\rho^{(2)}_{HF}(s) = \int \rho^{(2)}_{HF}(R + s/2, R - s/2) dR$$

$$E = E_{ct} + E_{\pi} \quad \longrightarrow \quad E[\rho] = E_{ct}[\rho] + E_{\pi}[\rho]$$

Contact part as it is but optimized

DME expansion in HF approximation
DME Functional
NN and NNN amplitudes

\[ g_t^m(u) = g_t^m(u)|_{LO} + g_t^m(u)|_{NLO} + g_t^m(u)|_{N^2LO} \]
\[ h_{tt'}^m(u) = \alpha_0^h + \beta_0^h \log(1 + 4u^2) + \beta_1^h (\log(1 + 4u^2))^2 \]
\[ + \gamma_0^h \arctan(u) + \gamma_1^h (\arctan(2u))^2 \]
\[ + \gamma_2^h \log(1 + 4u^2) \arctan(2u) \]
\[ g(u)|_{LO} = \alpha_0^g + \beta_0^g \log(1 + 4u^2) + \gamma_0^g \arctan(2u) \]
\[ g(u)|_{NLO} = \alpha_1^g + \beta_1^g (\log(1 + 2u^2 + 2u\sqrt{1 + u^2}))^2 \]
\[ + \gamma_1^g \sqrt{1 + u^2} \log(1 + 2u^2 + 2u\sqrt{1 + u^2}) \]
\[ g(u)|_{N^2LO} = \alpha_2^g + \beta_2^g \log(1 + u^2) + \gamma_2 \arctan(u) \]

\[ \alpha_k = \alpha_k(u), \beta_k = \beta_k(u), \gamma_k = \gamma_k(u) \]

Rational polynomials of \( u \)
\[ u = \frac{k_F(r)}{m_\pi} \]

Mathematica Notebooks
Complete analytical expressions in Mathematica
*.nb format

B. Gebremariam, T. Duguet and S.K. Bogner
(submitted)

(see the talk by S. Bogner)

FORTRAN 90 module
Can be ported to any DFT solver
Already working with HFBRAD and HFBTHO

M. Kortelainen and M. Stoitsov
(in preparation)

(see the talk by M. Kortelinen)
<table>
<thead>
<tr>
<th>Parameters</th>
<th>SLY4</th>
<th>SLY4'</th>
<th>LO</th>
<th>NLO</th>
<th>N2LO</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{00}^\rho )</td>
<td>-933.342</td>
<td>-727.093</td>
<td>-757.689</td>
<td>-607.108</td>
<td></td>
</tr>
<tr>
<td>( C_{10}^\rho )</td>
<td>830.052</td>
<td>474.871</td>
<td>477.931</td>
<td>316.939</td>
<td></td>
</tr>
<tr>
<td>( C_{02}^\rho )</td>
<td>861.062</td>
<td>612.104</td>
<td>628.504</td>
<td>-1082.854</td>
<td></td>
</tr>
<tr>
<td>( C_{12}^\rho )</td>
<td>-1064.273</td>
<td>-705.739</td>
<td>-694.665</td>
<td>-4369.425</td>
<td></td>
</tr>
<tr>
<td>( C_{0}^\rho )</td>
<td>57.129</td>
<td>33.885</td>
<td>18.471</td>
<td>322.4</td>
<td></td>
</tr>
<tr>
<td>( C_{1}^\rho )</td>
<td>24.657</td>
<td>32.405</td>
<td>92.233</td>
<td>-156.901</td>
<td></td>
</tr>
<tr>
<td>( \gamma )</td>
<td>0.16667</td>
<td>0.30622</td>
<td>0.287419</td>
<td>1.06429</td>
<td></td>
</tr>
</tbody>
</table>

**Volume Parameters**

**Surface Parameters**

| \( C_{0}^{\rho \Delta \rho} \) | -76.287  | -76.180  | -67.437  | -63.996  | -197.132  |
| \( C_{1}^{\rho \Delta \rho} \) | 15.951   | 24.823   | 21.551   | -9.276   | -12.503   |
| \( C_{0}^{\rho \nabla J} \) | -92.250  | -92.959  | -95.451  | -95.463  | -193.188  |
| \( C_{1}^{\rho \nabla J} \) | -30.75   | -82.356  | -65.906  | -60.800  | 37.790    |

**Pairing Parameters**

| \( V_n \) | -258.992  | -232.135  | -241.203  | -241.484  | -272.164  |
| \( V_p \) | -258.992  | -244.050  | -252.818  | -252.222  | -286.965  |

**SVD Optimization Results**

| \( \chi^2 \) | 12.5002  | 2.1235   | 1.837    | 1.7662   | 1.7884    |
| RMSD(\( E \)) | 7.008    | 2.6931   | 2.5539   | 2.5143   | 2.590     |
| RMSD(\( \Delta_n \)) | 0.1297   | 0.0828   | 0.0587   | 0.0554   | 0.0476    |
| RMSD(\( \Delta_p \)) | 0.094    | 0.0988   | 0.0902   | 0.0866   | 0.0706    |

*Volume parameters fitted to INM SLY4, SLY4', LO, NLO, N2LO
Surface and pairing parameters fitted to finite nuclei (SVD optimization)

HFBTHO solver (HFB+LN)

- binding energies of 72 nuclei
- 30 spherical and 42 deformed
- 4 neutron OEM differences
- 4 proton OEM differences

The same set of data as UNDEFpre

*(see the talk by N. Schunck)*
Effects on single-particle levels?

![Graph showing energy levels for Pb neutrons and Pb protons with labels for different states like 3d$_{3/2}$, 2g$_{7/2}$, 4s$_{1/2}$, etc., and comparisons between experimental (Exp), Skyrme (Sk.), LO, and NLON2LO calculations.]
Effects on deformations?

Deformation Energy (MeV)

$^{100}\text{Zr}$

Deformation $\beta_2$

- SLY4'
- LO
- NLO
- $N^2$LO
Nuclear DFT Calculations With DME Energy Density Functional

Conclusions

- DME contributions modify the functional to such extent that it cannot be applied without optimization
- DME functional performs in almost the same way (or slightly better) as the standard Skyrme functional with respect to the optimized binding energies and OEM differences
- Infinite nuclear matter can have reasonable EOS, including an incompressibility $K^{NM} = 230$ MeV, with a density dependence power of the order of one
- The new, microscopically motivated, density dependence leads to some modifications of the results as, e.g., in the deformability of the functional, which are expected to further improve the ability of the functional to capture physics in the areas where the standard Skyrme functional is known that has deficiencies

Restrictions to be removed

- The Hartree contribution has been treated in LDA
- Tensor contributions have been discarded nevertheless they naturally appear in the DME functional

Improvements

- Further improvements of the DME techniques - could bring more precise fine tuning
- Other interactions could be an option to investigate
Ab Initio Nuclear DFT Deliverables

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}$Ca DME comparisons
- Further development of $\pi$–DME functionals; include pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: test and export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
Neutron droplets

Preliminary results – DME plot from Markus Kortelainen
Density for 8 neutrons in a HO trap with Minnesota NN interaction

Qualitative agreement between NCFC and DME calculations
Neutron droplets

Preliminary results – DME plot from Markus Kortelainen
Density for 8 neutrons in a HO trap with Minnesota NN interaction

![Graph showing density vs. radius for different Hamiltonians](image)

- qualitative agreement between NCFC and DME calculations
DME–Ab Initio Comparisons: Year 4–5 Plans

- On-going neutron droplet comparisons
  - Make systematic comparisons with simplified interaction
  - Comparisons with ab initio low-momentum NN-only
- Compare (symmetric) nuclei in traps (same progression)
- Revisit comparisons with improved DME and exact Hartree
  - Generalizations of DME beyond HF
- Compare with NNN included (NCFC and CC)


Preprints in preparation (post by CPR deadline)

- “Microscopically-constrained Fock energy density functionals from chiral effective field theory. II. Three-nucleon interactions,” B. Gebremariam, S.K. Bogner, and T. Duguet
- “Nuclear matter from chiral low-momentum interactions,” S.K. Bogner, R.J. Furnstahl, K. Hebeler, A. Nogga, and A. Schwenk
- First SRG operator paper (Anderson et al.)
- First OEP paper (Drut, Furnstahl, Platter)
- First DME-based EDF paper (Stoitsov et al.)
Ab Initio Functional Year-4 Deliverable Scorecard

Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward $^{40}\text{Ca}$ DME comparisons
- Further development of $\pi$–DME functionals; pairing
- Continue development and testing of orbital-based DFT

Other deliverables from CPR

- Low-$k$ interactions: evolve, test, export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Upgrade and validate the DME implementation
- Develop and test a refit Skyrme functional including universal long-range DME parts
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.