MSU Year 4 Status Report

I) Density Matrix Expansions
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Biruk Gebremariam (graduated May 2010)
Juan Burgos (new student)
Thomas Duguet**

II) In-medium SRG
Scott Bogner
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**External
Microscopically-guided functionals
- $V_{NN} + V_{NNN} + \text{MBPT} + \text{DME}$ to guide next-generation EDFs

In-medium similarity renormalization group (IM-SRG)
- new ab-initio method
- effective interactions
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 $E_x$
DME-related papers completed in Year 4

1. “Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions”
B. Gebremariam, S. K. Bogner and T. Duguet

2. “Symbolic Integration Of A Product Of Two Spherical Bessel Functions With An Additional Exponential And Polynomial Factor”
B. Gebremariam, T. Duguet and S. K. Bogner

3. “Symbolic computation of the Hartree-Fock energy from a chiral EFT three-nucleon interaction at N^2LO”
B. Gebremariam, S. K. Bogner and T. Duguet

4. “An improved density matrix expansion for spin-unsaturated nuclei,”
B. Gebremariam, T. Duguet and S. K. Bogner,

and 1 Ph.D. thesis (Biruk Gebremariam)
What could be missing in phenomenological EDFs?

- Density dependencies too simplistic
- Isovector components not well constrained
- What’s the connection to many-body forces?

Turn to microscopic many body theory for guidance, aided by the simplifications enabled by soft RG-evolved interactions

Simplest idea: Map non-local exchange energy into local EDF (non-trivial density-dependence)
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

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

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

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

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

\[ C^{ij} [u] = \text{rational polynomial} \]
Similarly for $<V_{\text{NNN}}>\) (but trilinear and many more terms...) \(\)

\[
\varepsilon^{C_{R4,2x}} = \int d\bar{r} \left\{ C^{\rho_0^3}_{\rho_0^2} \rho_0^3(\bar{r}) + C^{\rho_0^2\rho_1^1}_{\rho_0^2} \rho_0(\bar{r}) \rho_1^2(\bar{r}) + C^{\rho_0^1\rho_1^2}_{\rho_0^1} \rho_0(\bar{r}) \rho_1(\bar{r}) \rho_1^1(\bar{r}) \right. \\
+ C^{\rho_0^2\Delta\rho_0}_{\rho_0^2} \rho_0^2(\bar{r}) \Delta\rho_0(\bar{r}) + C^{\rho_0^1\Delta\rho_1}_{\rho_0^1} \rho_0(\bar{r}) \rho_1(\bar{r}) \Delta\rho_1(\bar{r}) + C^{\rho_0^1\Delta\rho_2}_{\rho_0^1} \rho_0^1(\bar{r}) \rho_2^1(\bar{r}) \\
+ C^{\rho_0^2\rho_1^1}_{\rho_0^2} \rho_1^2(\bar{r}) \rho_0^1(\bar{r}) \Delta\rho_0(\bar{r}) + C^{\rho_0^1\rho_1^2}_{\rho_0^1} \rho_0(\bar{r}) \rho_1^2(\bar{r}) + C^{\rho_0^2\rho_1^2}_{\rho_0^2} \rho_0^2(\bar{r}) \rho_1^2(\bar{r}) \\
+ C^{\rho_0^2J_0_{\rho_0}^2}_{\rho_0^2} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_1^2\rho_0^1J_0}_{\rho_0^1} \rho_1(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1\rho_0^1J_0}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) \\
+ C^{\rho_0^2J_0_{\rho_1}^2}_{\rho_0^2} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_0}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_1}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) \\
\left. + C^{\rho_0^2J_0_{\rho_1}^2}_{\rho_0^2} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_1^2\rho_0^1J_0}_{\rho_0^1} \rho_1(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1\rho_0^1J_0}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) \right. \\
+ C^{\rho_0^2J_0_{\rho_1}^2}_{\rho_0^2} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_0}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_1}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) \\
+ C^{\rho_0^2J_0_{\rho_1}^2}_{\rho_0^2} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_0}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) + C^{\rho_0^1J_0_{\rho_1}^2}_{\rho_0^1} \rho_0(\bar{r}) \vec{J}_0(\bar{r}) \cdot \vec{J}_0(\bar{r}) \right\}. \]

\(C^{ijk}[u]\xi_i\xi_j\xi_k, \quad u \equiv \frac{k_F(R)}{m_\pi} \quad \text{(note: } u \text{ is NOT small)} \)

\[
C^{ijk}[u] = C^{ijk}_1[u] + C^{ijk}_2[u] \ln(1 + 4u^2) + C^{ijk}_3[u] \arctan(2u),
\]

\[
C^{ijk}_\alpha[u] = \text{rational polynomial}
\]
New development: DME for chiral NNN force (N2LO)

- Expect interesting spin-orbit/tensor couplings from TPE

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

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

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

This is a mismatch since microscopic NNN interactions are long-range (DME ==> density dependent J\cdot\nabla\rho couplings)
Prescriptions for $\Pi_n$-functions

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

$$\rho(\vec{r}_1, \vec{r}_2) = e^{i\vec{r} \cdot \vec{k}} e^{\frac{i}{2} (\nabla_1 - \nabla_2) - i \vec{r} \cdot \vec{k}} \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

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

$$\rho(\vec{r}_1, \vec{r}_2) \approx \int d^3 \vec{k} \ g(\vec{R}, \vec{k}) e^{i\vec{k} \cdot \vec{r}} \sum_{n=0}^{2} \frac{1}{n!} \left\{ \vec{r} \cdot \left( \frac{\nabla_1 - \nabla_2}{2} - i \vec{k} \right) \right\}^n \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

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

**Crucial to accurately describe spin-vector part of OBDM**
Prescriptions for $\Pi_n$-functions

Negele and Vautherin (NV-DME)
Truncated Bessel expansion of non-locality operator
Sufficient for spin-unsaturated nuclei only

Why it fails: no phase space averaging (not even over INM) done for spin-vector part
Improved Vector PSA-DME

anisotropy of $g(R,k)$ in the spatial surface

(Bulgac et al.)
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
Including Long Range Chiral EFT in Skyrme-like EDFs

\[ V_{EFT} = V_{ct}(\Lambda) + V_{1\pi} + V_{2\pi} + \cdots \]

Each HF DME coupling function splits into 2 terms

1) Skyrme-like coupling constants (contact terms)
2) Nontrivial coupling functions from “universal” pion physics

\[ C_t^{\rho\tau} \Rightarrow C_t^{\rho\tau}(\Lambda; V_{ct}) + C_t^{\rho\tau}[k_F(R); V_\pi] \]

From contact terms in EFT/RG V's  
From pion exchanges

Suggests a microscopically-improved Skyrme phenomenology

Add pion-exchange couplings to existing Skyrme EDF and refit Skyrme constants (mimics higher-order ladder contributions)

Analogous to separation of long- and short-distance Coulomb (J. Drut’s talk)
Including DME pion couplings in Skyrme

See Mario/Markus’s talk for details of the implementation and restricted “pre-optimization” fits.

1) Implemented into HFTHO and HFBRAD
2) Stable enough for optimization
3) Bulk properties ok (as expected)
4) Small but stable improvement over Skyrme

No show stoppers yet!

* 1st paper by ORNL group + MSU & OSU coming soon
Part 2: In-medium SRG

In-medium similarity renormalization group (IM-SRG)
- new ab-initio method
- effective interactions

See arXiv:1006.3639
Unitary transformation via flow equations:

\[
\frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda] \quad \text{with} \quad \eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^+(\lambda)
\]

Engineer \( \eta \) to do different things as \( \lambda \to 0 \)

\[
\eta(\lambda) = [G_\lambda, H_\lambda]
\]

\( G_\lambda = T \Rightarrow H_\lambda \) driven towards diagonal in \( k \) – space

\( G_\lambda = PH_\lambda P + QH_\lambda Q \Rightarrow H_\lambda \) driven to block–diagonal

increases “perturbativeness”, accelerates basis expansions, ...

need to evolve NNN (at least) to keep \( \lambda \) independent

\( A > 2 \) observables (E. Jurgenson’s talk)
Normal Ordered Hamiltonians

\[ H = \sum t_i a_i^\dagger a_i + \frac{1}{4} \sum V_{ijkl}^{(2)} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{36} \sum V_{ijklmn}^{(3)} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \]

Normal-order w.r.t. some reference state \( \Phi \) (e.g., HF):

\[ H = E_{vac} + \sum f_i N(a_i^\dagger a_i) + \frac{1}{4} \sum \Gamma_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k) + \frac{1}{36} \sum W_{ijklmn} N(a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l) \]

\[ E_{vac} = \langle \Phi | H | \Phi \rangle \]

\[ f_i = t_{ii} + \sum_{h} \langle ih | V_2 | ih \rangle n_h + \frac{1}{2} \sum_{hh'} \langle ihh' | V_3 | ihh' \rangle n_h n_{h'} \]

\[ \Gamma_{ijkl} = \langle ij | V_2 | kl \rangle + \sum_{h} \langle ijh | V_3 | klh \rangle n_h \]

\[ W_{ijklmn} = \langle ijk | V_3 | lmn \rangle \]

\[ \langle \Phi | N(\cdots) | \Phi \rangle = 0 \]

0-, 1-, 2-body terms contain some 3NF effects thru density dependence \( \Rightarrow \) Efficient truncation scheme for evolution of 3N?
In-medium SRG for Nuclear matter

- Normal order $H$ w.r.t. non-int. fermi sea
- Choose SRG generator to eliminate “off-diagonal” pieces
  \[
  \frac{dH(s)}{ds} = [\eta(s), H(s)]
  \]
  \[\eta = [\hat{f}, \hat{\Gamma}]\]
  \[\lim_{s \to \infty} \Gamma_{od}(s) = 0\]
  \[\langle 12|\Gamma_{od}|34 \rangle = 0 \text{ if } f_{12} = f_{34}\]
  \[\lambda \equiv s^{-1/4}\]

- 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$_{\text{eff}}$
Correlations “adiabatically” summed into $H(\lambda)$

PNM*

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

*Neglects ph-channel. See Heiko Hergert’s talk.
In-medium SRG to diagonalize closed-shell nuclei

Define “offdiagonal” as terms that don’t annihilate the reference HF state

\[
\begin{align*}
\Gamma^{od}(s) &= \sum_{pp'h'h'} \Gamma_{pp'h'h'}(s)\{a_p^\dagger a_{p'}^\dagger a_h a_{h'}\} + h.c. , \\
\eta(s) &= [H(s), H(s)] \\
f^{od}(s) &= \sum_{ph} f_{ph}(s)\{a_p^\dagger a_h\} + h.c. , \\
\end{align*}
\]

HF reference state decouples from higher npnh states

\[
\lim_{s \to \infty} \langle \phi | H(s) | \phi \rangle = E_{gs}
\]

\[
QH(\infty)P = 0, \quad PH(\infty)Q = 0,
\]

where \( P = |\Phi\rangle \langle \Phi| \) and \( Q = 1 - P \).
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
Can also use IM-SRG(2) to “soften” convergence of MBPT well before total decoupling achieved.

Note the ~ cutoff-independent CC results using H(s). Further indication that our N-ordered truncation is robust.
Some observations

1) pp channel + 2 ph channels treated on equal footing (like Parquet theory but without the technical problems of energy-dependence, poles, etc.)

2) Intrinsically non-perturbative, and issues of small energy denominators, poles, etc. bypassed.

3) no unlinked diagrams (size extensive, etc.)

4) “3rd-order exact” and similar scaling to coupled cluster (deeper connection?)

5) Extensions to open shell possible (derive valence Heff)
Year 4 and 5 roadmap for IM-SRG

1) Eliminate quasi-particle number changing interactions

\[ \eta = [Q, H(s)] \quad Q = \sum_{i} sgn(\epsilon_i - \epsilon_F) \{ a_i^\dagger a_i \} \]

non-perturbatively derive valence shell-model Heff/Oeff
Year 4 and 5 roadmap for IM-SRG

2) Decouple highly-virtual s.p. orbitals

\[ \eta = [Q, H(s)] , \quad Q = \sum_i \theta(\epsilon_i - (\epsilon_F + \Lambda)) \{a_i^\dagger a_i\} \]

Evolved H(\infty) doesn’t mix many-body states that differ in the number of s.p. orbits above the chosen cutoff

use to truncate # of basis states for ab-initio calculation of low-lying states
Year 4 and 5 roadmap for IM-SRG

3) Decouple highly-virtual and deeply bound s.p. orbitals

\[ \eta = [Q, H(s)] , \quad Q = \sum_i \theta(|\epsilon_i - \epsilon_F| - \Lambda) \{a_i^\dagger a_i\} \]

Evolved H(\infty) doesn’t mix many-body states that differ in the # of s.p. orbits lying within the cutoff centered on the fermi level

reduce d.o.f. to just a few active orbitals close to the fermi level (i.e., shell model)
Year 4 and 5 roadmap for IM-SRG

4) IM-SRG for infinite matter (See Heiko’s talk)

- include particle-hole channel (hard!!)
  - is it worth the effort? Folklore about ph-contributions to bulk...

- Use HFB groundstate to N-order w.r.t.
  - bypass technical problems of Nambu-Gorkov Green’s functions?