Microscopically Based Energy Functionals

S.K. Bogner (NSCL/MSU)
Dream Scenario: From QCD to Nuclei

Microscopic DFT

MB Methods + DME

\( V_{\text{lowk}} \)

(2,3...N interactions)

RG evolution

Chiral EFT

(2N...N interactions)

LEC’s for \( L_{\text{EFT}} \)

Lattice QCD

- Density Functional Theory \( A > 100 \)
- Coupled Cluster, Shell Model \( A < 100 \)
- Exact methods \( A \leq 12 \)
- GFMC, NCSM
- Lattice QCD
- Chiral EFT interactions
  (low-energy theory of QCD)
- QCD Vacuum
- QCD Lagrangian

Proton Number

Neutron Number
SciDAC 2 Project Building a Universal Nuclear Energy Density Functional

See [http://undef.org](http://undef.org) for details
UNEDF Project Goals

• Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications.”

• Scope is all nuclei
  ==> DFT the method of choice

• Order of magnitude improvement over present capabilities
  ==> precision calculations of, e.g., masses

• Utilize the best available microscopic physics
  ==> chiral EFT NN and NNN interactions, ab-initio MBT

• Maximize predictive power will well-quantified theoretical uncertainties
Years 2 & 3: Personnel, Tasks, and Interconnections

**Interactions**
- Chiral EFT
- Bonn/Julich (Epelbaum, Nogga)
- Idaho/Salamanca (Entem, Machleidt)

**Ab Initio WF Methods**
- CC: UT/ORNL (Dean, Hagen, Papenbrock)
- FCI: ISU (Maris, Vary)
  - LLNL (Navratil)

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

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

Participant color key:
- **UNEDF**
- International collaborator outside UNEDF
Years 2 & 3: Personnel, Tasks, and Interconnections

**Ab Initio WF Methods**
- CC: UT/ORNL (Dean, Hagen, Papenbrock)
- FCI: ISU (Maris, Vary)
- LLNL (Navratil)

**Ab Initio Functional + Nuclear Matter**
- 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 OPM

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

**Participant color key:**
- UNEDF
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**Interactions**
- Chiral EFT
- Bonn/Julich (Epelbaum, Nogga)
- Idaho/Salamanca (Entem, Machleidt)
- Vlowk/SRG
- OSU, MSU
- TRIUMF (Schwenk)

**N3LO 3NF**
- Explicit Delta’s
- New 3NF fits
- SRG 3NF evolution
Limitations of Existing Energy Functionals (Predictability)

- Uncontrolled extrapolations towards the drip-line
- Theoretical error-bars?
Limitations of Existing Energy Functionals (Predictability)

- Pairing gaps not under control for increasing (N−Z)
What’s missing in phenomenological EDF’s

- Density dependencies might be too simplistic
- Isovector components not well constrained
- No systematic organization of terms in the EDF
- No way to estimate theoretical uncertainties
- Over-determined parameters
- What’s the connection to many-body forces?
- Pairing part of the EDF not treated on same footing

Turn to microscopic many body theory for guidance
Nuclear forces from Chiral EFT

Separation of scales: low momenta $Q \ll \Lambda_b$ breakdown scale

- Explains empirical hierarchy $\text{NN} > 3\text{N} > 4\text{N}$

- Formal Consistency
  - $\text{NN}$ and $3\text{NN}$ forces
  - $\pi\pi$ and $\pi\text{N}$, electroweak operators
  - QCD, systematic expansion

- Error estimates from truncation order, lower bound from $\Lambda$ variation

Weinberg, van Kolck, Epelbaum, Meissner, Machleidt, …
Resolution dependence of nuclear interactions

with high-energy probes: quarks+gluons

cf. scale/scheme dependence of parton distribution functions

Lattice QCD

Effective theory for NN, many-N interactions, operators depend on resolution scale $\Lambda$

$$H(\Lambda) = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \ldots$$

$\Lambda_{\text{chiral}}$ momenta $Q \sim \lambda^{-1} \sim m_\pi$: chiral effective field theory

nucleons interacting via pion exchanges + contact interactions

typical Fermi momenta in nuclei $\sim m_\pi$

$\Lambda_{\text{pionless}}$

$Q \ll m_\pi = 140 \text{ MeV}$: pion not resolved

pionless effective field theory

large scattering lengths + corrections

applicable to loosely-bound, dilute systems, reactions at astro energies

Freedom to vary the resolution via RG to simplify certain features…
“Scheme-Dependent” Sources of Non-perturbative Physics

- short-ranged repulsive core
- strong tensor force

BUT typical momentum in a large nucleus only ≈ 1 fm\(^{-1}\) (200 MeV)!
2 Types of Renormalization Group Transformations

- "$V_{\text{low } k}$" $\Rightarrow$ lowers a cutoff $\Lambda$ in $k', k$

  ![Image of renormalization group transformations]

- SRG $\Rightarrow$ drives $H$ towards the diagonal ($\lambda = \text{width about diagonal}$)

  ![Image of renormalization group transformations]

Both decouple the high momentum modes leaving low $E_{\text{NN}}$ observables unchanged.
Integrating out high-momentum modes ("$V_{\text{low } k}$").

$-k' \quad +k' \quad -k' \quad +k'$

$T$ \quad $V_{\Lambda}$

$q \leq \Lambda$

$V_{\Lambda}$

UV cutoff $\Lambda$

- Demand $\frac{d}{d\Lambda} T = 0$

$\Rightarrow$ RGE's for "running" of $V_{\Lambda}$ w/ $\Lambda$

- Integrate RGE's to smaller $\Lambda$

$\Rightarrow$ decouples high $k$ modes

- Low momentum universality

$\Rightarrow$ evolved interactions ("$V_{\text{low } k}$") coalesce to $\approx$ universal curve
The Similarity Renormalization Group
[Wegner, Glazek and Wilson]

• Unitary transformation on an initial $H = T + V$

$$H_s = U(s)H U^\dagger(s) \equiv T + V_s \quad s = \text{continuous flow parameter}$$

• Differentiating with respect to $s$:

$$\frac{dH_s}{ds} = [\eta(s), H_s] \quad \text{with} \quad \eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

• Engineer $\eta(s)$ to do different things as $s \to \infty$

$$\eta(s) = [G_s, H_s]$$

$G_s = T \Rightarrow H_s \text{ driven towards the diagonal in } k - \text{ space}$

$G_s = PH_sP + QH_sQ \Rightarrow H_s \text{ driven towards block diagonal form}$
Run to Lower $\lambda$ via SRG $\implies$ Universality

Note: $\lambda = s^{-1/4}$
Run to Lower $\lambda$ via SRG $\implies \approx$ Universality

Note: $\lambda = s^{-1/4}$
Observations on 3N forces

Arise whenever eliminate DOF (relativity, nucleon excitations, high momentum intermediate states)

Omitting 3NF's => observables depend on $\Lambda$. 
Why Bother lowering $\Lambda$ if 3NF’s grow?

$<3N>$ gets bigger for low $\Lambda$ BUT

- Approximate treatments of 3NF “work” better
  - e.g., normal ordering (D. Dean’s talk)
  - perturbative, HF dominates

Ratio $<3N>/<2N>$ not unnaturally large

Chiral: $\langle V_{3N} \rangle \sim (Q/\Lambda)^3 \langle V_{NN} \rangle$

Hard work for a small contribution (large $\Lambda$) versus less work for a larger contribution (small $\Lambda$)?
**Approximate RG Evolution of 3NF**

Leading chiral EFT 3NF appears in $N^2\text{LO}$

\[ c_1 = -0.9^{+0.2}_{-0.5}, \quad c_3 = -4.7^{+1.2}_{-1.0}, \quad c_4 = 3.5^{+0.5}_{-0.2} \]

Note: significant decrease of $c_3$ and $c_4$ in $N^3\text{LO}$

- Chiral EFT is a complete operator basis
- Approximate RG running by refitting D and E at each $\Lambda$
- Equivalent to truncating RGE to leading operators

Consistency checks of the approximation:

- Weak $\Lambda$-dependence in NM (renormalization is working)
- $<3N>/<2N>$ agrees w/power counting estimates
Progress on “honest” 3NF RG evolutions

4-boson model problem

NM using in-medium SRG

Anderson and Furnstahl 2008
SRG in H.O. basis

S.K. Bogner, in prep
In-medium SRG w/normal-ordering
New low-momentum NNN fits and Nuclear Matter

Smooth cutoff $V_{\text{low }k}$ from $N^3\text{LO}(500)$

$N^2\text{LO} 3\text{NF fit to } A = 3, 4$
B.E. and $^4\text{He}$ radii

self-bound w/ saturation

Perturbative expansion about HF becomes sensible

NOTE: 3NF drives saturation NOT the tensor force
New low-momentum NNN fits and Nuclear Matter

Knobs to estimate
Theoretical error bars:

Λ-dependence =>
theoretical error bands
(lower limit)

Assess the impact of large uncertainties in the $c_i$'s
appearing in 2- and 3-body TPEP (to do)

Vary the order of the underlying EFT (to do)

Sensitivity to many-body approximations

Energy/nucleon [MeV]

$k_F$ [fm$^{-1}$]
New low-momentum NNN fits and Nuclear Matter

Ladder sum $\approx$ 2nd-order
Excellent saturation, NO fine-tuning to nuclear matter

But...

1) $V_{\text{NNN}} \Rightarrow V_{2N}(r)$
2) HF propagators
3) Beyond 2-hole lines?
4) Angle-averaging
5) Particle-hole channel
6) ...

Coupled-cluster calculations of nuclear matter, $^{16}\text{O}$ and $^{40}\text{Ca}$ would be a huge help!
Guidance from NM for fixing EFT couplings

Supports suggestion of Navratil et al. to use $^4$He radii to constrain fits of 3NF couplings ($c_E$ and $c_D$)

NM to constrain $c_3$ and $c_4$?
Local Functionals from Many-Body Theory

- Dominant MBPT contributions to bulk properties take the form

\[
\langle V \rangle \sim \text{Tr}_1 \text{Tr}_2 \int d\mathbf{R} \, dr_{12} \, dr_{34} \rho(r_1, r_3) K(r_{12}, r_{34}) \rho(r_2, r_4) + \text{NNN} \cdots
\]

\[K\] is either free-space interaction (HF) or resummed in-medium vertex (BHF)

- Written in terms on non-local quantities
  - density matrices and s.p. propagators
  - finite range and non-local resummed vertices K

Connection to \( E = E[\rho] \) is not obvious!
Density Matrix Expansion Revisited (Negele and Vautherin)

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

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

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

• Fall off in \( r \) controlled by local \( k_F \)
  
  => expand and resum so LO term exact in uniform limit
  
  => NOT a simple short-distance expansion in \( r \)

\[
\rho (\mathbf{R} + \frac{1}{2} \mathbf{r}, \mathbf{R} - \frac{1}{2} \mathbf{r}) = \frac{3j_1 (k_F r)}{k_F r} \rho (\mathbf{R}) + \frac{35j_3 (k_F r)}{2k_F^3 r} \left( \frac{1}{4} \nabla^2 \rho (\mathbf{R}) - \tau (\mathbf{R}) + \frac{3}{5} k_F^2 \rho (\mathbf{R}) \right) + \cdots
\]

• Dependence on local densities now manifest
Skyrme-like EDF’s from the DME

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

Skyrme

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

DME

- coupling **constants** --> coupling **functions**
  - finite range effects encoded as \( \rho \)-dependence in \( ABC \)
  - microscopic isovector, spin-orbit terms
  - well-suited for existing SkyHF codes

Kohn–Sham Potentials

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

HFB solver

Orbitals and Occupation #’s
Skyrme-like EDF's from the DME

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Kohn–Sham Potentials

DME energy functional
\( A[\rho], B[\rho], \ldots \)

HFB solver

• Don’t touch the HFB solver
• Trivial to upgrade as each new coupling becomes available
• Implemented in HFBRAD

Orbitals and Occupation #’s
Including Long Range Chiral EFT in Skyrme-like EDFs

Derived the most general (N≠Z, spin-unsaturated) EDF from chiral EFT thru \( N^2 \)LO at HF level [SKB and B. Gebremariam]

\[
\mathcal{E}^{\rho\rho} \equiv \sum_q \int \! dx \left[ A^{\rho\rho} \rho_q \rho_q + A^{\rho\Delta} \rho_q \Delta_q + A^{\nabla \rho \nabla \rho} \nabla \rho_q \cdot \nabla \rho_q + A^{\rho T} \left( \rho_q \tau_q - j_q \cdot j_q \right) 
+ A^{s s \cdot s_q} s_q \cdot s_q + A^{s \Delta \cdot s_q} s_q \cdot \Delta_q + A^{s \nabla \Delta \cdot s_q} \nabla s_q \cdot \nabla s_q 
+ A^{\rho \Delta J} \left( \rho_q \nabla \cdot J_q + j_q \cdot \nabla \times s_q \right) + A^{\nabla \cdot s_q \cdot s_q} \left( \nabla \cdot s_q \right) \left( \nabla \cdot s_q \right) 
+ A^{J J} \left( \sum_{\mu \nu} J_{q,\mu \nu} J_{q,\mu \nu} - s_q \cdot T_q \right) + A^J \left( \sum_{\mu} J_{q,\mu} \right) \left( \sum_{\mu} J_{q,\mu} \right) + \sum_{\mu \nu} J_{q,\mu \nu} J_{q,\mu \nu} - 2 s_q \cdot F_q \right]
\]

Each coupling function splits into 2 terms

1) \( \Lambda \)-dependent Skyrme-like coupling constants
2) \( \Lambda \)-independent coupling functions from pion physics with non-trivial density dependence

\[
A^{\rho \Delta} \rho \Rightarrow A^{\rho \Delta} \rho (\Lambda) + A^{\rho \Delta} \rho [\rho]
\]

From contact terms in EFT/RG V’s

From pion exchanges

Etc…
Long-range pion exchange contributions to the EDF

Longest range $V$ $\iff$ Strongest density dependence in EDF

Novel density-dependencies in EDF from $1\pi$ and $2\pi$ exchanges:

$$\rho^{7/3}, \rho^{4/3}, \rho^{2/3}, \frac{1}{\rho^{2/3}} \log(1 + c\rho^{2/3}), \ldots$$
Effects of NNN on Couplings

Gradient term \((\nabla \rho)^2\)

- Only scalar-isoscalar terms worked out so far
- Consistent with Kaiser et al. results with explicit \(\Delta\)'s

In Progress:
Spin-orbit couplings from \(2\pi\) 3NF

SKB, Furnstahl and Platter, in prep.

Should find interesting density dependencies compared to NN spin-orbit, which is a short-range effect!
Including Long Range Chiral EFT in Skyrme-like EDFs

- Derive coupling functions from $\chi$-EFT pion exchange NN and NNN interactions via the DME

- Refit the Skyrme coupling constants (EFT constraints $\Rightarrow$ naturalness, $\Lambda$-dependence, etc.)

- Look for improved observables and for sensitivities

- Can we “see” the pion as in NN phase shift analyses
Comparison to ab-initio calculations

Start from the same Hamiltonian and compare ab initio solution to the Microscopic DFT calculation based on the DME functional

CC or FCI calculations of nuclei and nuclei in external fields

How important is non-locality and how accurate is the DME?

Are systematics reproduced by DME as we vary parameters (e.g., 3NF couplings, RG cutoff $\Lambda$, order of input EFT, ... ) in $H$?

Is the many-body treatment of nuclear matter sufficient?

Early indications are that non-trivial extensions of the DME are needed
DME for Low-Momentum Interactions

- HO model
- errors $\approx +5$ MeV (NLO), $-10$ MeV (N$^3$LO),
- $\Lambda$-independent errors
- Schematic V’s (1970’s) much worse (larger finite-range direct terms)

Errors ($\langle V \rangle_{\text{DME}} - \langle V \rangle$) in Ca-40

- Negele-Vautherin G-matrix
- Brink-Boeker Force (Sprung et al.)
- $V_{\text{low } k}$ (N$^3$LO)
- $V_{\text{low } k}$ (NLO)

Long-range contributions ($1\pi$, leading $2\pi$)

DME error in $1\pi$ exchange $\approx 4$ MeV (out of 431 MeV)

...But the “success” of this test of the DME is misleading...
Comparison to ab-initio calculations

CC and DFT calculations of $^{16}$O (w/3N contact of varying strength)

Quantitative and qualitative disagreement btw. coupled-cluster and DFT calculation. What is going on?
Possible Reasons for the Poor Agreement

1) DME averages out too much information

- COM P-dependence (spatial non-locality)
- energy-dependence

![Graph showing energy dependence](image)

Errors of 1 MeV/nucleon in infinite NM
Possible Reasons for the Poor Agreement

2) Gradient expansion breaks down when saturation not good

e.g., N3LO NM looks reasonable at lower densities despite poor saturation

Ab-initio results for O16 and Ca40 pretty decent, but DME is poor

Gradients no longer “small” since DME = expansion about NM?

<table>
<thead>
<tr>
<th></th>
<th>O16</th>
<th>Ca40</th>
<th>Ca48</th>
</tr>
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<tr>
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<td>Coupled Cluster</td>
<td>DME</td>
<td>Coupled Cluster</td>
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<tr>
<td>E/A</td>
<td>-6.72</td>
<td>-7.89</td>
<td>-7.72</td>
</tr>
<tr>
<td>$r_{ch}$</td>
<td>2.73</td>
<td>2.47</td>
<td>3.35</td>
</tr>
</tbody>
</table>
Possible Reasons for the Poor Agreement

3) Errors in the Hartree contribution => feedback via self-consistency!

\[ \rho(R + r/2) \rho(R - r/2) \]

Exact \hspace{1cm} DME

Treat Hartree exactly a-la Coulomb? [Negele and Vautherin, Sprung et al.]

- “Ab-initio DFT” should be taken with a grain of salt!
- However, microscopic MBT still useful to build in missing physics (density dependencies) to Skyrme
Work in the near-term

• spin-orbit couplings from N$^2$LO 3NF

• Extension of DME beyond even-even nuclei (time-odd couplings)

• Refits of Skyrme + Long-range coupling functions (ORNL group)

• Extension of DME to pairing channel (B. Gebremariam)

• Generalization of DME to handle non-localities in time (I.e., energy-dependence from beyond HF)

• Refinements of original DME (B. Gebremariam)
Conclusions

- Lowering $\Lambda$ via RG greatly simplifies nuclear few and many-body problems
  - Comparison of DFT to ab initio (same H) now possible
  - use $\Lambda$-dependence as a tool for estimating errors
  - $V_{3N}$ can be treated as perturbation/simple approximations
  - perturbative nuclear matter?
  - Correlations “blurred out” $\Rightarrow$ HF is decent starting point
  - Extension of Skyrme EDF’s via DME (novel density dep.)
  - Theoretical guidance for future fits possible using
    “error bars” generated from $\Lambda$-dependence
Collaborators

• MSU/NSCL: B. Gebremariam
• Ohio State: R. Furnstahl, L. Platter
• Iowa State: J. Vary, P. Maris
• ORNL: G. Hagen, T. Papenbrock
• TRIUMF: A. Schwenk
• Orsay/France: T. Duguet, V. Rotival
Observables Sensitive to 3N Interactions?

- Study systematics along isotopic chains
- Example: kink in radius shift $\langle r^2 \rangle (A) - \langle r^2 \rangle (208)$

![Graph showing isotopic shift $r^2(A)-r^2(208)$ for Pb isotopes]

- Associated phenomenologically with behavior of spin-orbit
  - isoscalar to isovector ratio fixed in original Skyrme
- Clues from chiral EFT contributions? (Kaiser et al.)
Ratio of Isoscalar to Isovector Spin-Orbit

- Ratio fixed at 3:1 for short-range spin-orbit (usual Skyrme)
- Kaiser: DME spin-orbit from chiral two-body (left) and three-body (right)

- Systematic investigation needed
Observables Sensitive to 3N Interactions?

- Recent studies of tensor contributions [e.g., nucl-th/0701047]

- See also Brown et al., PRC 74 (2006)
Naturalness to Constrain Skyrme Couplings

- Old NDA analysis:
  \[ c \left( \frac{\psi^\dagger \psi}{f_\pi^2 \Lambda} \right)^l \left( \frac{\nabla}{\Lambda} \right)^n f_\pi^2 \Lambda^2 \]
  \[ \rho \longleftrightarrow \psi^\dagger \psi \]
  \[ \tau \longleftrightarrow \nabla \psi^\dagger \cdot \nabla \psi \]
  \[ \mathbf{J} \longleftrightarrow \psi^\dagger \nabla \psi \]

- Density expansion?
  \[ \frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda} \leq \frac{1}{4} \]
  for \( 1000 \geq \Lambda \geq 500 \)

\[ k_F = 1.35 \text{ fm}^{-1} \]

Furnstahl and Hackworth 1997
3NF’s for $N^3$LO not necessarily small