Similarity Renormalization Group and Evolution of Many-Body Forces

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Outline

- Overview of Similarity Renormalization Group (SRG)
- Decoupling between high- and low-energy degrees of freedom
- Evolving three-nucleon forces (3NFs in 3D!!)
- One-Dimensional Model
- Future Work and Conclusions
Renormalization Group $\Rightarrow$ focus on relevant dof’s
Which picture should I use?
Nuclear Interactions in Momentum Space

- Fourier transform in partial waves (Bessel transform)

\[ V_{L=0}(k, k') = \int d^3r j_0(kr)V(r)j_0(k'r) = \langle k | V_{L=0} | k' \rangle \]

- Repulsive core \( \Rightarrow \) big high-\( k \) (\( \geq 2 \text{ fm}^{-1} \)) components
- EFTs are softer - but still have high-\( k \) components
Although momentum is continuous in principle, in practice represented as discrete (gaussian quadrature) grid:

\[
\langle k | V | k' \rangle + \sum_{k'} \frac{\langle k | V | k' \rangle \langle k' | V | k \rangle}{(k^2 - k'^2)/m} + \cdots \Rightarrow V_{jj} + \sum_{ij} V_{ij} V_{ji} \frac{1}{(k_j^2 - k_j'^2)/m} + \cdots
\]

100 × 100 Resolution is sufficient for many significant figures
Try a Low-Pass Filter

- Start with a potential (AV18 - $^1S_0$)
- Cut at $\Lambda$ (2.2 fm$^{-1}$)
- Compute observables ($\delta_0(E)$)
- Compare to uncut
Try a Low-Pass Filter

Start with a potential

\[(AV18 - ^1S_0)\]

Cut at \(\Lambda\)

\[(2.2 \text{ fm}^{-1})\]

Compute observables

\[(\delta_0(E))\]

Compare to uncut
Try a Low-Pass Filter

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- Compute observables \((\delta_0(E))\)
- Compare to uncut
Basic problem: high and low are coupled!

Perturbation theory for $\tan(\delta_0)$

$$\langle k | V | k \rangle + \sum_{k'} \frac{\langle k | V | k' \rangle \langle k' | V | k \rangle}{(k^2 - k'^2)/m} + \ldots$$

Can’t just change high-momentum elements (intermediate virtual states)

Absorb high-energy effects into low-energy physics $\Rightarrow$ “Renormalization Group” (“flow equations”)

Unitary transformation:

$$E_n = \langle \psi_n | U^\dagger \rangle U H U^\dagger \langle U | \psi_n \rangle$$
What is the Similarity Renormalization Group (SRG)?


\[ H_s = U(s)H U^\dagger(s) \equiv T_{\text{rel}} + V_s \]

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

\[ \eta(s) = [T_{\text{rel}}, H_s] \implies \frac{dH_s}{ds} = [[T_{\text{rel}}, H_s], H_s] \]

Projected onto partial-wave momentum space:

\[ \frac{dV_s(k, k')}{ds} = -(\epsilon_k - \epsilon_{k'})^2 V_s(k, k') \]

\[ + \frac{2}{\pi} \int_0^\infty q^2 dq \left( \epsilon_k + \epsilon_{k'} - 2\epsilon_q \right) V_s(k, q) V_s(q, k') \]
What is the Similarity Renormalization Group (SRG)?

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\( ^1S_0 \quad \lambda = 15.0 \text{ fm}^{-1} \)
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\(^1S_0\) \(\lambda = 10.0\) fm\(^{-1}\)
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![Graph showing the similarity renormalization group](image)
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\[ {^1S_0} \quad \lambda = 2.0 \text{ fm}^{-1} \]

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SRG and 3NF
Unitary Transformations $\Longrightarrow$ Preserve Observables

$\delta [\text{deg}]$

- $^1S_0$
- $^1P_1$
- $^3P_0$
- $^3P_1$
- $^3F_3$
- $^3G_4$

$E_{\text{lab}} [\text{MeV}]$

- bare ps
- vsrg ps
Now Low-Pass Filters Work!

- Phase shifts with $V_s(k, k') = 0$ for $k, k' > k_{\text{max}}$
Testing Decoupling Quantitatively

[EDJ, Bogner, Furnstahl, Perry - arXiv:0711.4252]

$\Lambda$

1. run SRG to $\lambda$
2. set tail to zero
   - $V_{s,\Lambda} =$
     $e^{-\left(\frac{k^2}{\Lambda^2}\right)^n} V_s e^{-\left(\frac{k'^2}{\Lambda^2}\right)^n}$
   - $n = 4, 8, 12, ...$
3. relative errors

$^1S_0$ Partial Wave, N$^3$LO (500 MeV) E/M
Decoupling above $\lambda$

$^1S_0$ \quad N$^3$LO

$\lambda = 2.0 \text{ fm}^{-1}$

Decoupling clean and universal for all observables!
Decoupling above $\lambda$

$^1S_0$ N$^3$LO $\lambda = 2.0 \text{ fm}^{-1}$

- Decoupling clean and universal for all observables!
\[ \frac{dH_s}{ds} = [[G_s, H_s], H_s] \]

\[ H_{\infty} = \begin{pmatrix} PH_{\infty} P & 0 \\ 0 & QH_{\infty} Q \end{pmatrix} \implies G_s = \begin{pmatrix} PH_s P & 0 \\ 0 & QH_s Q \end{pmatrix} \]

3S1, kvnn = 10, \( \lambda = 5.0 \) fm\(^{-1}\), \( Z_{\text{lim}} = 0.5 \)

3S1, kvnn = 10, \( \lambda = 1.0 \) fm\(^{-1}\), \( Z_{\text{lim}} = 0.5 \)
Many-Body Forces

- Why do we need many-body forces?
  - 3NFs arise from eliminating dof’s
  - Omitting 3NFs leads to model dependence (Tjon line)
  - 3NF contributions saturate nuclear matter
  - Many-body methods must deal with them (eg. MFD, CC, ...)

- SRG will induce many-body forces!

\[ \frac{dV}{ds} = \left[ \sum a^\dagger a, \sum a^\dagger a^\dagger aa, \sum a^\dagger a^\dagger aa \right] \]

2-body

\[ = \ldots + \sum a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a^\dagger a + \ldots \]

3-body!

- Stop evolution if induced become too unnatural
- RG flows with SRG extend consistently to many-body spaces
- Recent progress: 3NF evolved!!!
Current Realistic NCSM Calculations

- Triton calculations from P. Navratil (arXiv:0707.4680)

- “eff” ≡ Lee-Suzuki: Generated in large space and cut down with LS
- 3NF is N2LO
- $N_{\text{max}} = 40$ converged to within 5keV

- 3NF parameters $c_E$ and $c_D$ are fit to two observables
Evolving NN Forces in NCSM $A=3$ space

MATLAB evolved $N_{\text{max}} = 30$ in only $\approx$ half a day

- **Unitary evolution of initial NN-only forces!**
- $\hbar \omega = 28$ is optimal for initial interaction, $\hbar \omega = 20$ for $\lambda = 2$
- Need to study the trade-off in convergence
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- Same plots but now including an initial 3NF from N2LO
- Collaboration with P. Navratil - up next: size of induced 4NF in $^4$He calculations
Evolving NN forces

- Comparing the SRG to Lee-Suzuki

![Graph showing energy levels for different forces and models](image_url)
1-D model: \( V^{(2)}(x) = \frac{V_1}{\sigma_1 \sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2 \sqrt{\pi}} e^{-x^2/\sigma_2^2} \)


How do we handle many-body forces? Use a discrete basis to avoid "dangerous" delta functions

EDJ and R. J. Furnstahl - [arXiv:0809.4199]
• HO wavefunction examples $\psi_n(k)$ with $\hbar \omega = 4$
• resulting truncated delta function
  $\tilde{\delta}(k - k') = \sum_{n=0}^{N_{\text{max}}} |\psi_n(k)\rangle \langle \psi_n(k')|$
• tradeoff between small $\hbar \omega$ resolution and large $\hbar \omega$ scope
• bigger $N_{\text{max}} \rightarrow$ flatter in $\hbar \omega$
• optimal $\hbar \omega$ will shift with SRG evolution
Embedding: initial potential

- Symmetrized Jacobi Oscillator Basis (here: Bosons)
  - EDJ and R. J. Furnstahl - [arXiv:0809.4199]

\[ V(p, p') \rightarrow V(N_2, N'_2) \rightarrow V(N_3, N'_3) \]

- diagonalize symmetrizer \( \langle N_A | N_{A-1}; n_{A-1} \rangle \); use recursively
- 3D: Use Navratil et al. technology for NCSM
- embedding is everything, SRG coding is trivial
Symmetrized Jacobi Oscillator Basis (here: Bosons)

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\[ V(p, p') \rightarrow V(N_2, N_2') \rightarrow V(N_3, N_3') \]

diagonalize symmetrizer \( \Rightarrow \langle N_A | N_{A-1}; n_{A-1} \rangle \); use recursively

3D: Use Navratil et al. technology for NCSM

embedding is everything, SRG coding is trivial
Some many-body examples

Legend: Embedding, Evolving, BE calculation, Initial 3NF

- $A=3$ (2N only):

$$V_{osc}^{(2)} \xrightarrow{SRG} V_{\lambda,osc}^{(2)} \xrightarrow{\text{embed}} V_{\lambda,3Nosc}^{(2)} \xrightarrow{\text{diag}} \text{BE}_3^{(2N\text{only})}$$

- $A=4$ (2N only):

$$V_{osc}^{(2)} \xrightarrow{SRG} V_{\lambda,osc}^{(2)} \xrightarrow{\text{embed}} V_{\lambda,3Nosc}^{(2)} \xrightarrow{\text{embed}} V_{\lambda,4Nosc}^{(2)} \xrightarrow{\text{diag}} \text{BE}_4^{(2N\text{only})}$$

- $A=4$ (2N+3N only):

$$V_{osc}^{(2)} \xrightarrow{\text{embed}} V_{3Nosc}^{(2)} \xrightarrow{SRG} V_{\lambda,3Nosc}^{(2+3)} \xrightarrow{\text{embed}} V_{\lambda,4Nosc}^{(2+3)} \xrightarrow{\text{diag}} \text{BE}_4^{(2N+3N\text{only})} $$

$$+ V_{3Nosc}^{(3\text{init})} \cdots$$
Induced Many-Body Forces are Small - A=3

\[ V^{(2)}(x) = \frac{V_1}{\sigma_1 \sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2 \sqrt{\pi}} e^{-x^2/\sigma_2^2} \]

- Basis independent: same evolution in momentum or HO basis
- Black: Same evolution pattern for 2-body only as 3D NN-only
Induced Many-Body Forces are Small - $A=3$

\[
V^{(2)}(x) = \frac{V_1}{\sigma_1 \sqrt{\pi}} e^{-x^2/\sigma_1^2} + \frac{V_2}{\sigma_2 \sqrt{\pi}} e^{-x^2/\sigma_2^2}
\]

- Basis independent: same evolution in momentum or HO basis
- Black: Same evolution pattern for 2-body only as 3D NN-only
- Red: Three-body forces induced - Unitary!
Induced Many-Body Forces are Small - $A=4$

$$V^{(2)}(\lambda=\infty) = V_{\alpha}$$

$$V^{(3)}(p, q, p', q') = c_E e^{-((p'^2+q'^2)/\Lambda^2)^n} e^{-((p^2+q^2)/\Lambda^2)^n} \quad (\Lambda = 2 \quad n = 4)$$

$A = 4 \quad N_{\text{max}} = 28$

$c_E = -0.05$
$c_E = 0.00$
$c_E = 0.05$
Induced Many-Body Forces are Small - \( A = 4 \)

\[ V^{(2)}(\lambda = \infty) = V_\alpha \]

\[ c_E = -0.05 \]

\[ c_E = 0.00 \]

\[ c_E = 0.05 \]

\[ V^{(3)}(p, q, p', q') = c_E e^{-((p'^2 + q'^2)/\Lambda^2)^n} e^{-((p^2 + q^2)/\Lambda^2)^n} \quad (\Lambda = 2 \quad n = 4) \]
Induced Many-Body Forces are Small - $A=5$

- Five-body force is negligible
- Hierarchy of induced many-body forces

E.D. Jurgenson SRG and 3NF
\[
\frac{d}{d\lambda} \langle \psi^{(3)}_\lambda | V^{(3)}_\lambda | \psi^{(3)}_\lambda \rangle = \langle \psi^{(3)}_\lambda | [\overline{V}^{(2)}_\lambda, V^{(2)}_\lambda]_c - [\overline{V}^{(3)}_\lambda, V^{(3)}_\lambda] | \psi^{(3)}_\lambda \rangle
\]

- Majority evolution dominated by \([\overline{V}^{(2)}, V^{(2)}], (\overline{V} \equiv [T, V])\)
- Hierarchy of contributions
\[
\frac{d}{d\lambda} \langle \psi_\lambda^{(4)} | V^{(4)}_\lambda | \psi_\lambda^{(4)} \rangle = \langle \psi_\lambda^{(4)} | [\overline{V}^{(2)}_\lambda, V^{(3)}_\lambda]_c + [\overline{V}^{(3)}_\lambda, V^{(2)}_\lambda]_c + [\overline{V}^{(3)}_\lambda, V^{(3)}_\lambda]_c - [\overline{V}^{(4)}_\lambda, V^{(4)}_\lambda] | \psi_\lambda^{(4)} \rangle
\]

- No \([\overline{V}^{(2)}, V^{(2)}]\):
- \[\therefore\] Induced 4-body is small - Hierarchy persists
Fitting Three-Body Force Evolution

- Evolve in two-particle oscillator space → fit 3-body parameters to missing energy
- One term $V^{(3)} = Ce^{-[(k^2+k'^2)/\Lambda^2]^n}$ reduces $\lambda$ dependence to the 80-90% level.

Future work: add a second, short distance 3NF term with a gradient correction to test systematic reduction.
$H_s = U_s^\dagger H_0 U_s \implies U_s = \sum_i |\psi_i(0)\rangle \langle \psi_i(s)|$

- Here unevolved operator $(a^\dagger a)$ with evolved wavefunctions

- More of this to come from E. R. Anderson
Decoupling in the Oscillator Basis

⇒ Evolve with $T_{rel}$ and cut off to study decoupling

SRG space:  2-body only    3-body

- Decoupling not straightforward with $T_{rel}$ SRG
- Decoupling improves until some $\lambda$ and then degrades
- What about other SRG generators?

$A = 3$  $N_{max} = 40$

$V^{(2)}(\lambda = \infty) = V_\alpha$

$V^{(2)}(\lambda = \infty) = V_\alpha$

E.D. Jurgenson SRG and 3NF
Using other SRG Generators

- Matrices in NCSM basis for $T_{\text{rel}}$ and $V$

In this basis $T_{\text{rel}}$ will not drive to diagonal

Harmonic Oscillator Hamiltonian ($H_{\text{ho}} = T_{\text{rel}} + V_{\text{ho}}$) is diagonal in this basis
Evolve with $H_{ho}$

Using $G = H_{ho}$ improves convergence dramatically

- **Compare** $T_{rel}$ on the left with $H_{ho}$ on the right
- **Work in progress**: Spurious bound states contaminate evolution with $H_{ho} \rightarrow$ need further investigation
Recap

- SRG Decouples high- and low-energy DOF
- SRG is very flexible and powerful - can use many shapes to evolve potentials
- One-Dimensional model gives proof-of-principle of many-body hierarchy
- One-Dimensional model provides toolbox to gain intuition quickly - everything is directly applicable to 3D NCSM
- First results now coming in 3NF evolution in the NCSM basis!
Future Work

- One-Dimensional model leaves many opportunities for quick exploration
  - Operator evolution
  - SRG generators ($H_{ho}$, $H_{BD}$, $H_{D}$)
  - Basis issues
  - Fitting procedures
- All of these can be started in 3D now
- Door is opening quickly to other areas (MFD, CC, UNEDF collaboration)
Extra Slides
What is the Similarity Renormalization Group (SRG)?

Unitary transformations: [PRC 75:(2007)061001
arXiv:nucl-th/0611045]

\[
H_s = U(s)H U^\dagger(s) \equiv T_{\text{rel}} + V_s
\]

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

\[
\eta(s) = [T_D, H_s] \implies \frac{dH_s}{ds} = [[T_D, H_s], H_s]
\]

Projected onto partial-wave momentum space:

\[
\frac{dV_s(k, k')}{ds} = -\left(\epsilon_k - \epsilon_{k'}\right)^2 V_s(k, k')
\]

\[
+ \frac{2}{\pi} \int_{0}^{\infty} q^2 dq \left(\epsilon_k + \epsilon_{k'} - 2\epsilon_q\right) V_s(k, q) V_s(q, k')
\]
The Mechanics of Decoupling

\[
\frac{dV_s(k,k')}{ds} = -(\epsilon_k - \epsilon_{k'})^2 V_s(k, k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_s(k, q) V_s(q, k')
\]

\[
V_s = 2.5 \quad + \quad \text{1st term} \quad + \quad \text{2nd term} \quad \rightarrow \quad V_s = 1.5
\]

- Off-diagonal elements
  \[
  \implies V_s(k, k') \propto V_{NN}(k, k') e^{-[(\epsilon_k - \epsilon_{k'})/\lambda^2]^2}
  \]
- Relevant physics flows to low momentum elements
Phase Shifts: Decoupled above $\lambda$ - vary $\lambda$

$^1S_0$ $N^3$LO

$\lambda = 2.0 \text{ fm}^{-1}$

- Relevant physics flows to low momentum $\rightarrow$ Decoupling!
Phase Shifts: Decoupled above $\lambda - \text{vary } n$

$^1S_0$ $N^3LO$

$\lambda = 2.0 \text{ fm}^{-1}$

$V_{\lambda,\Lambda} = e^{-\frac{(k^2/\Lambda^2)^a}{2}} V_{\lambda} e^{-\frac{(k^2/\Lambda^2)^a}{2}}$

- Relevant physics flows to low momentum $\rightarrow$ Decoupling!
Deuteron Observables

- Binding Energy
- Quadrupole Moment
- RMS radius

\[ \lambda = 2.0 \text{ fm}^{-1} \]
dependence on $N_{\text{max}}$

- $^4\text{He}$
- $\lambda = 2.0 \text{ fm}^{-1}$

dependence on $\lambda$

- $^4\text{He}$
- $N_{\text{max}} = 12$

- **SRG improves convergence with basis size in NCSM**
- **NN-only $\Rightarrow$ different $^4\text{He}$ Binding Energies**
\( ^6\text{Li} \) Energy using No Core Shell Model

dependence on \( \lambda \)

\[
\begin{array}{c|c|c|c}
\lambda & \text{Energy [MeV]} & \Lambda [\text{fm}^{-1}] \\
3 \text{ fm}^{-1} & -35 & 0 \\
2 \text{ fm}^{-1} & -30 & 1 \\
1.5 \text{ fm}^{-1} & -25 & 2 \\
\end{array}
\]

dependence on \( n \)

\[
\begin{array}{c|c|c|c}
\lambda & \text{Energy [MeV]} & \Lambda [\text{fm}^{-1}] \\
3 \text{ fm}^{-1} & -35 & 0 \\
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\]

- SRG improves convergence with basis size in NCSM
- NN-only \( \implies \) different \( ^6\text{Li} \) Binding Energies

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SRG and 3NF
See edj et al.: arXiv:0801.1098

\[
\text{Goal} \rightarrow H_{\infty} = \begin{pmatrix} PH_{\infty} P & 0 \\ 0 & QH_{\infty} Q \end{pmatrix}
\]

\[
\text{SRG} \rightarrow \frac{dH_s}{ds} = [\eta_s, H_s] = [[G_s, H_s], H_s]
\]

\[
\text{sharp} \rightarrow G_s = \begin{pmatrix} PH_s P & 0 \\ 0 & QH_s Q \end{pmatrix}
\]

\[
\text{smooth} \rightarrow G_s = fH_sf + (1 - f)H_s(1 - f)
\]

\[
f(k) = e^{-(k^2/\Lambda_{BD}^2)^n}
\]
Block-Diagonal SRG - Smooth \( (n=4) \)

- \( 3S1, k_{\text{vnn}} = 10, \lambda = 3.0 \text{ fm}^{-1}, Z_{\text{lim}} = 0.5 \)
- \( 3S1, k_{\text{vnn}} = 10, \lambda = 2.0 \text{ fm}^{-1}, Z_{\text{lim}} = 0.5 \)
- \( 3S1, k_{\text{vnn}} = 10, \lambda = 1.5 \text{ fm}^{-1}, Z_{\text{lim}} = 0.5 \)
- \( 3S1, k_{\text{vnn}} = 10, \lambda = 1.1 \text{ fm}^{-1}, Z_{\text{lim}} = 0.5 \)
- \( 3S1, k_{\text{vnn}} = 10, \lambda = 1.0 \text{ fm}^{-1}, Z_{\text{lim}} = 0.5 \)
UNEDF Interconnections for Ab Initio Functionals

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

**Wider range of nuclei**
- Full 3NF
- Ab Initio densities
- External potentials

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

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

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

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

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

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

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

Ab Initio WF Methods
CC: UT/ORNL (Dean, Hagen, Papenbrock)
NCFC: ISU (Maris, Vary)
LLNL (Navratił)

Wider range of nuclei
Full 3NF
Ab Initio densities
External potentials

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

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

Tests of nuclear matter:
new fits, self-energies, ...
Improved 3NF for DME
Generalized DME
DFT from OPM

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

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

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

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N3LO 3NF
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