UNEDF SciDAC Collaboration

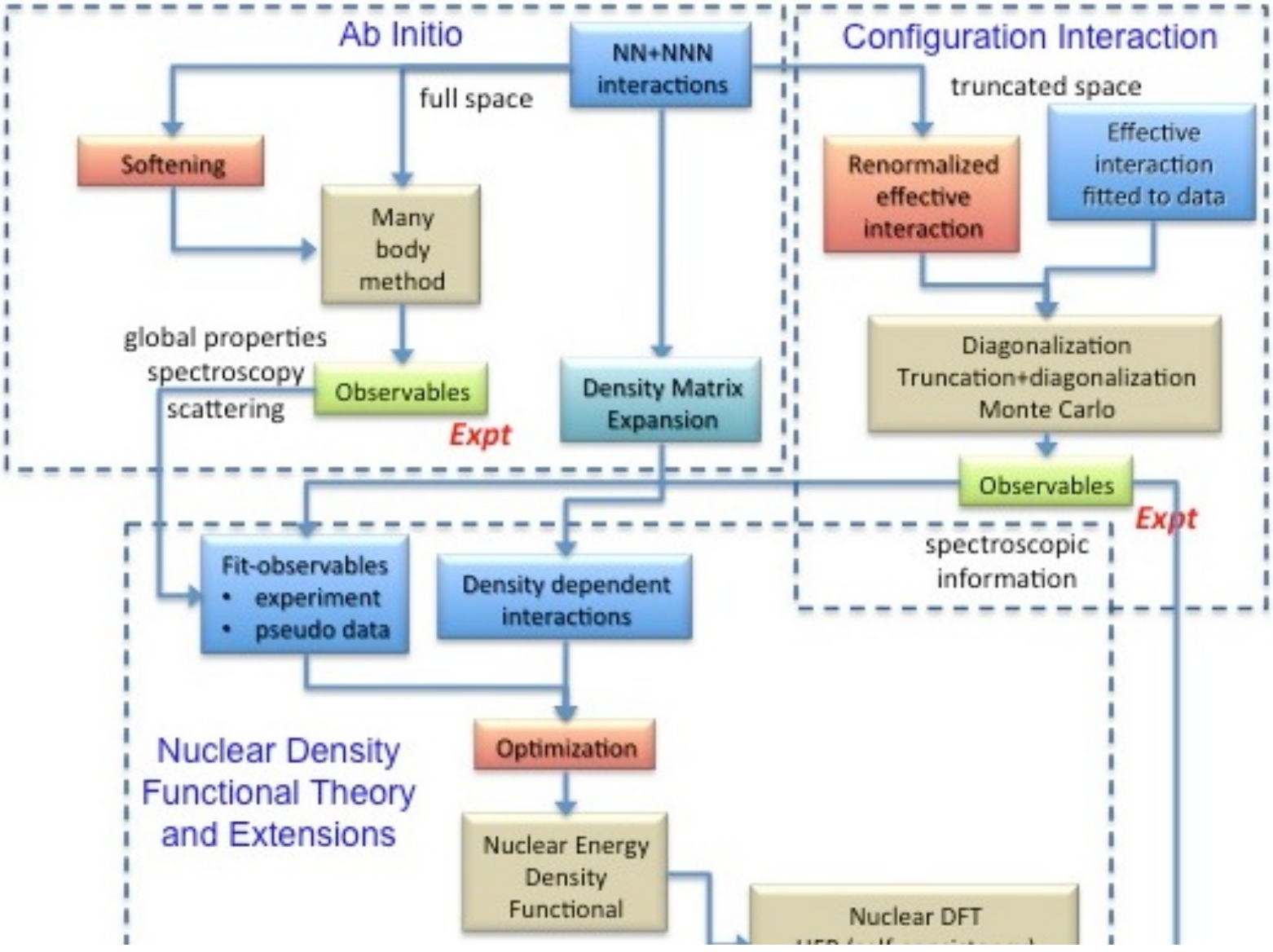
Universal Nuclear Energy Density Functional

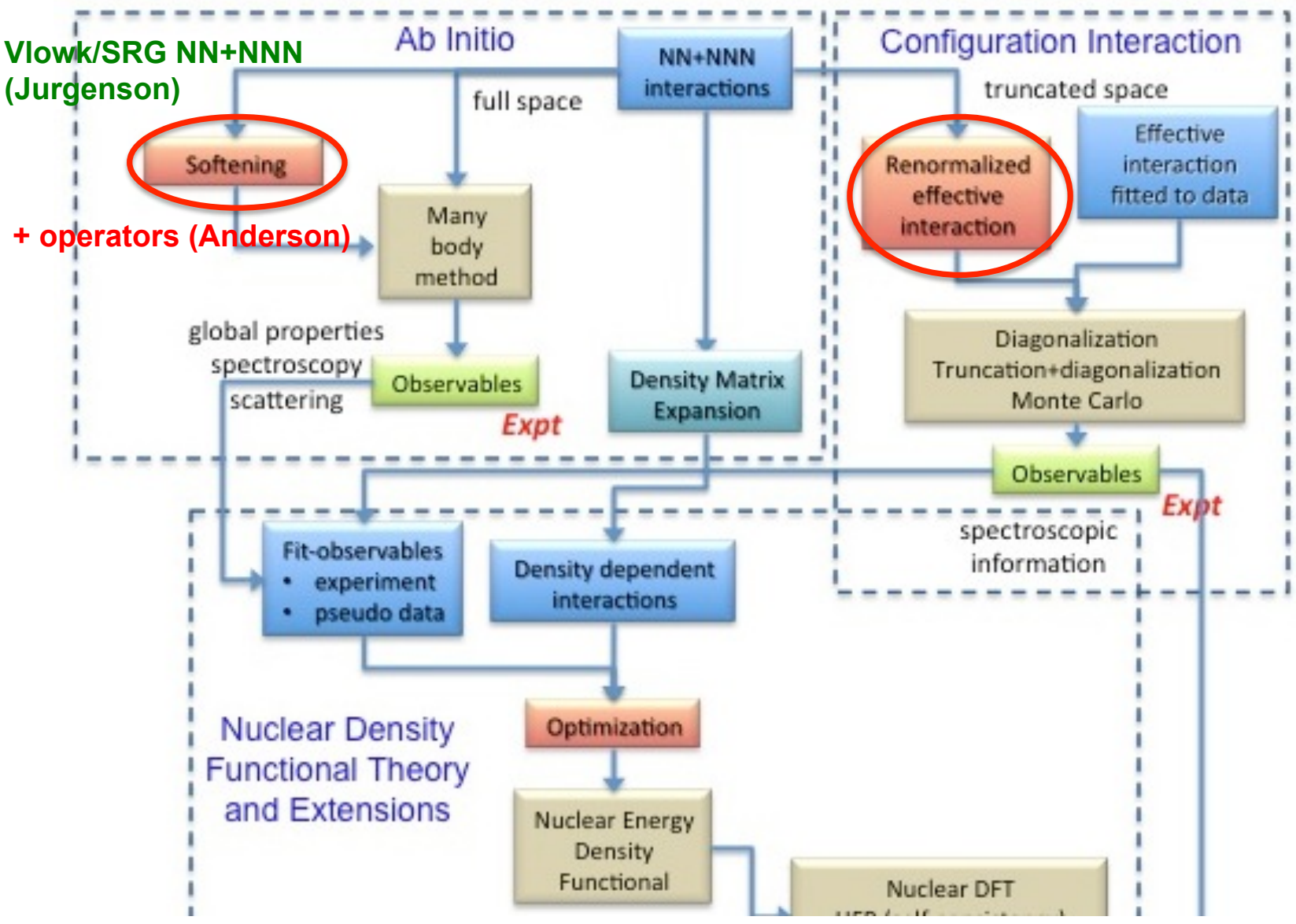
Ab Initio Functionals Summary Report

Dick Furnstahl

Department of Physics
Ohio State University

June, 2010


Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT


Vlowk/SRG NN+NNN
(Jurgenson)
+ operators (Anderson)
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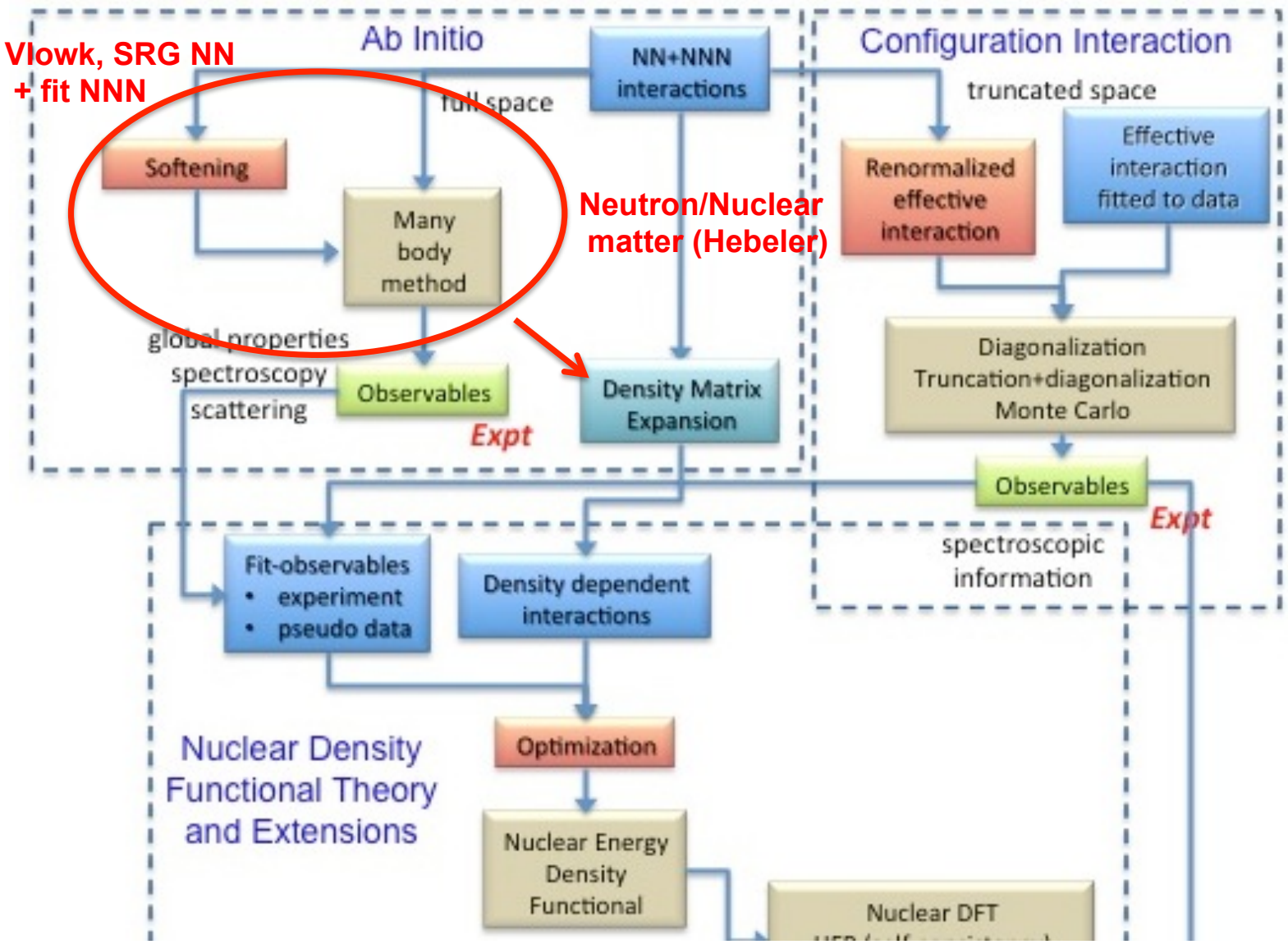
Vlowk, SRG NN
+ fit NNN
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Neutron/Nuclear
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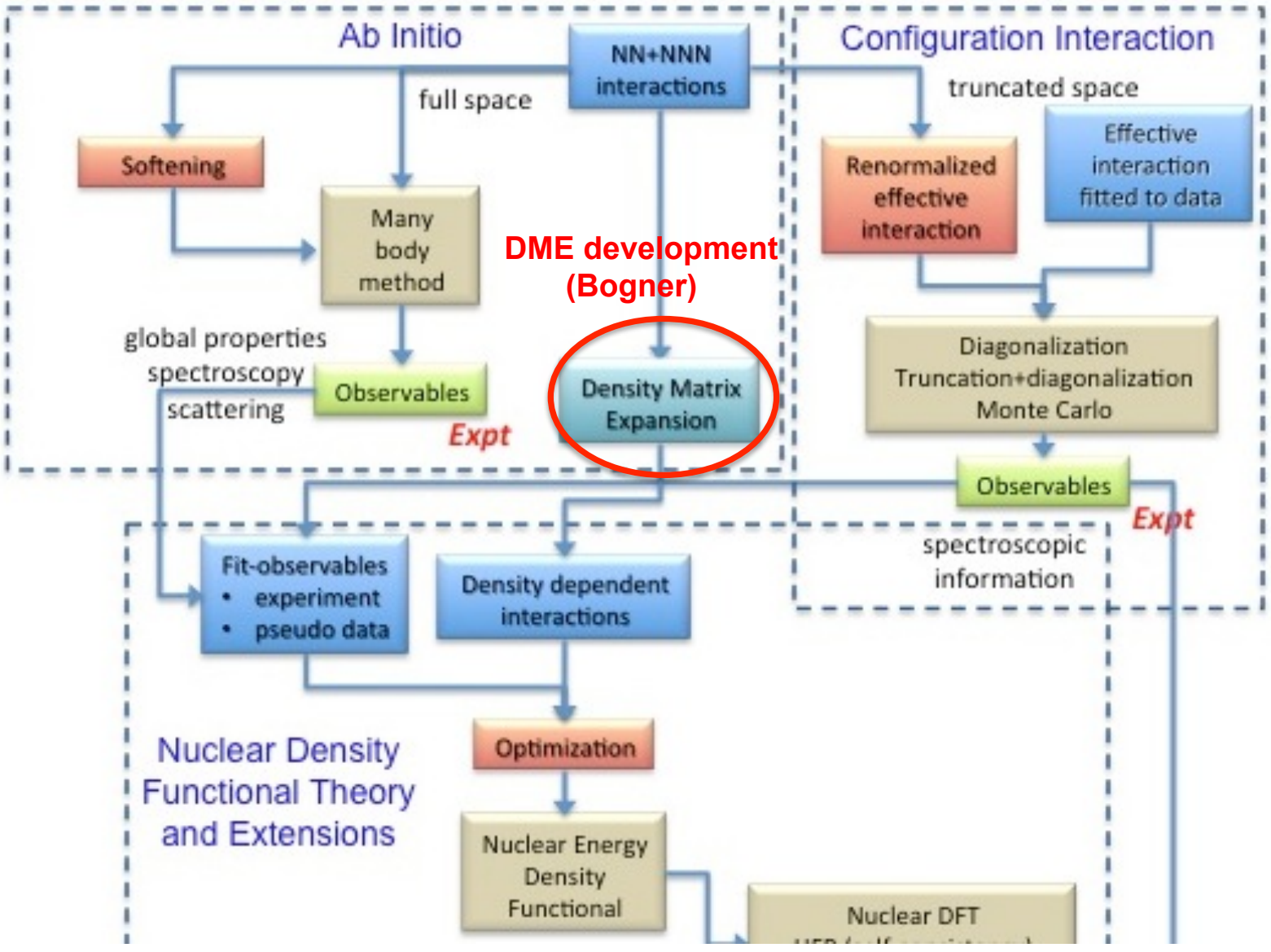
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DME development (Bogner)
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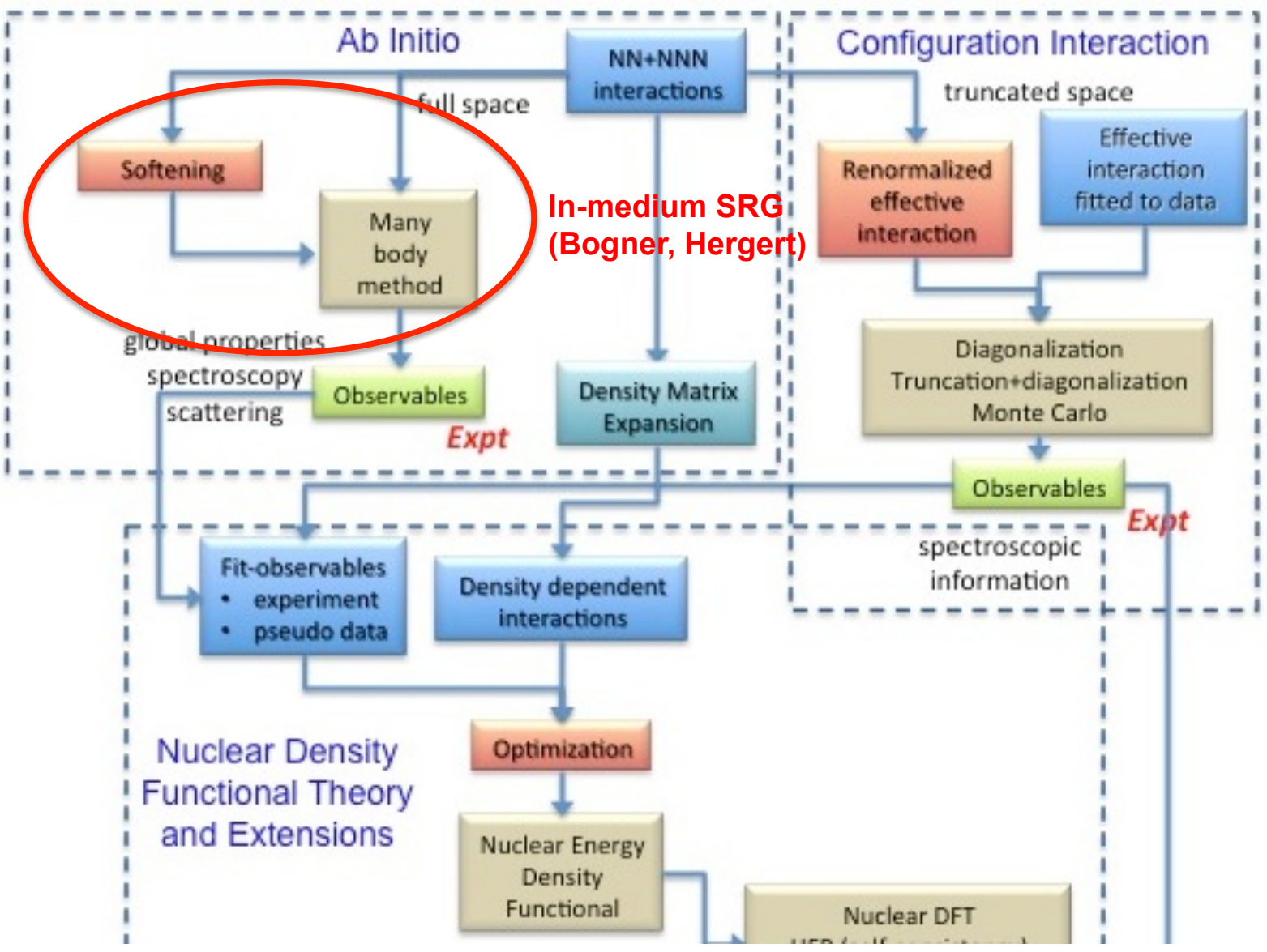
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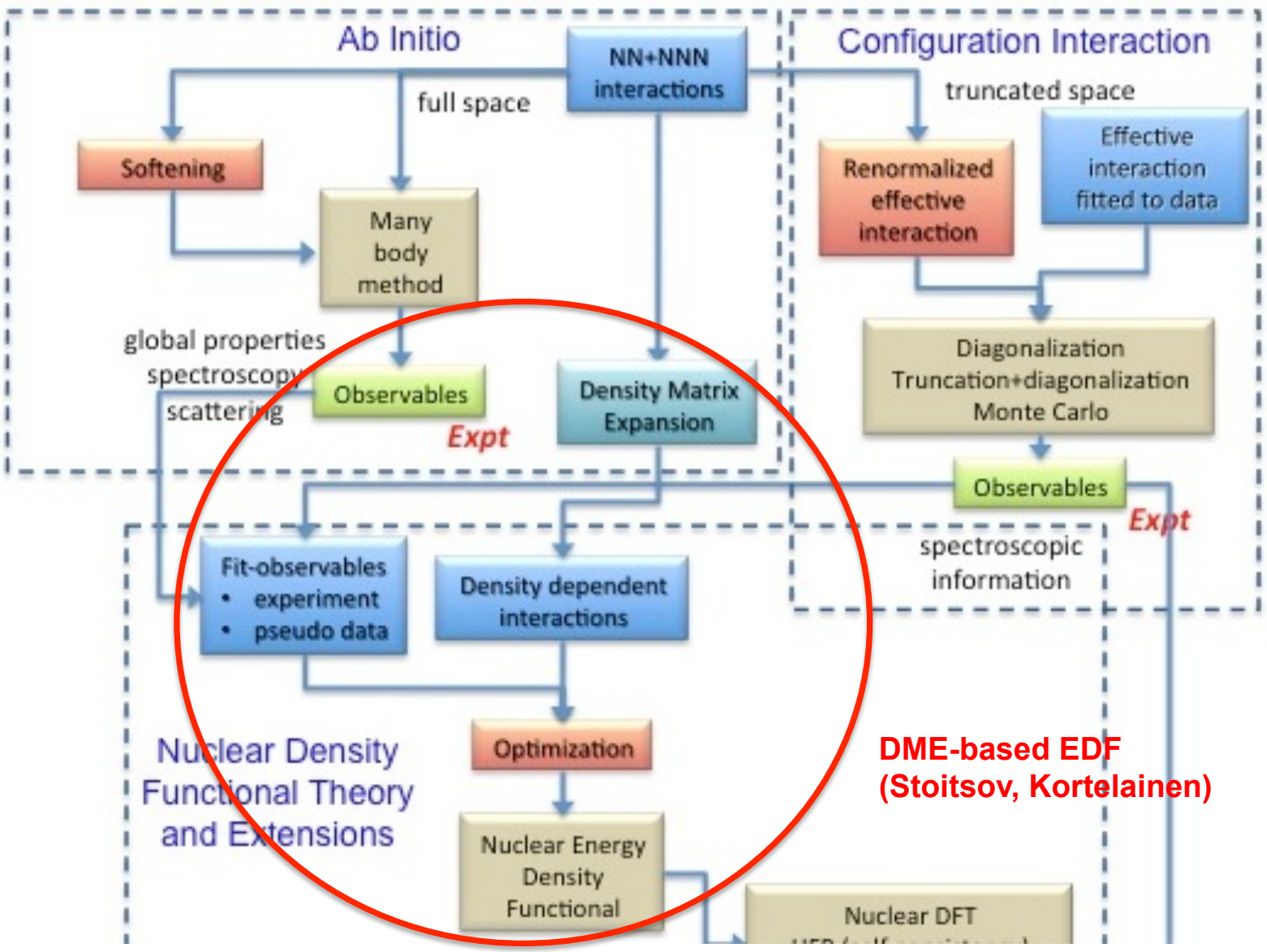
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DME-based EDF
(Stoitsov, Kortelainen)

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}Ca DME comparisons
- Further development of π–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
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- 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.

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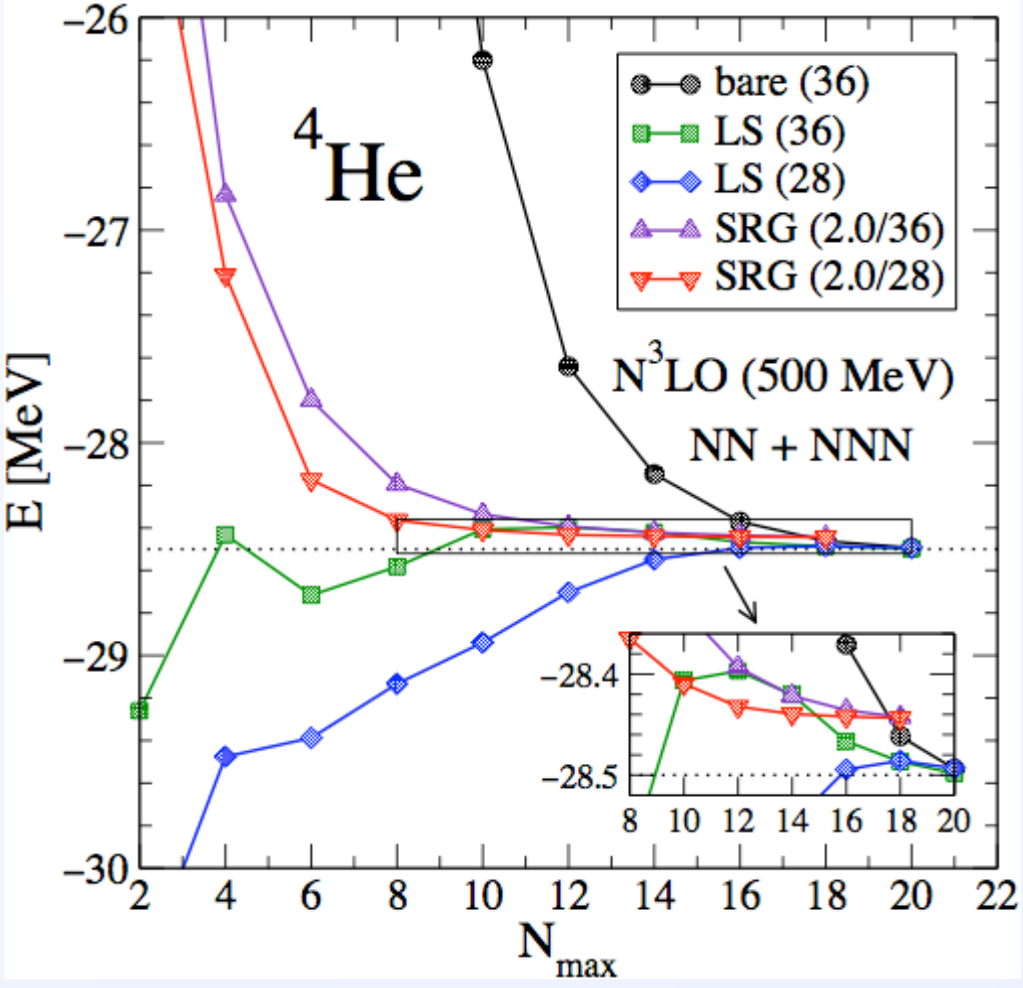
NNN Evolution (Jurgenson with Navratil, rjf)

^{4}He Convergence



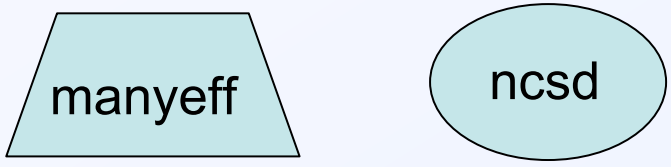
- Rapid and smooth convergence
- Induced 4NFs contribute about 30-60 keV
- Smaller than discrepancy of bare with experiment from omitted N3LO 3NF and 4NF
- Monitor induced 4NFs closely with increasing A, due to their strong density dependence

PRL **103**, 082501 [arXiv: 0905.1873]

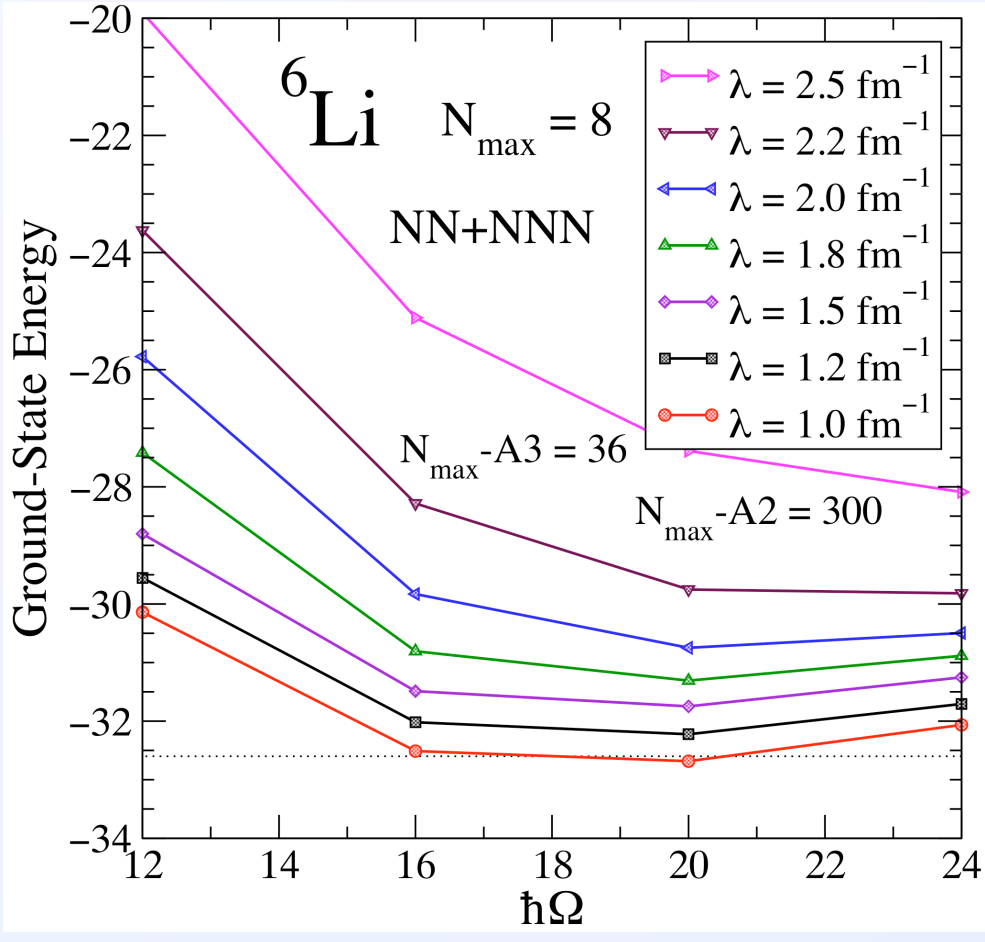
^{6}Li: using the slater-determinant basis

- 6Li, 7Li, and the rest of the p-shell nuclei require a new procedure

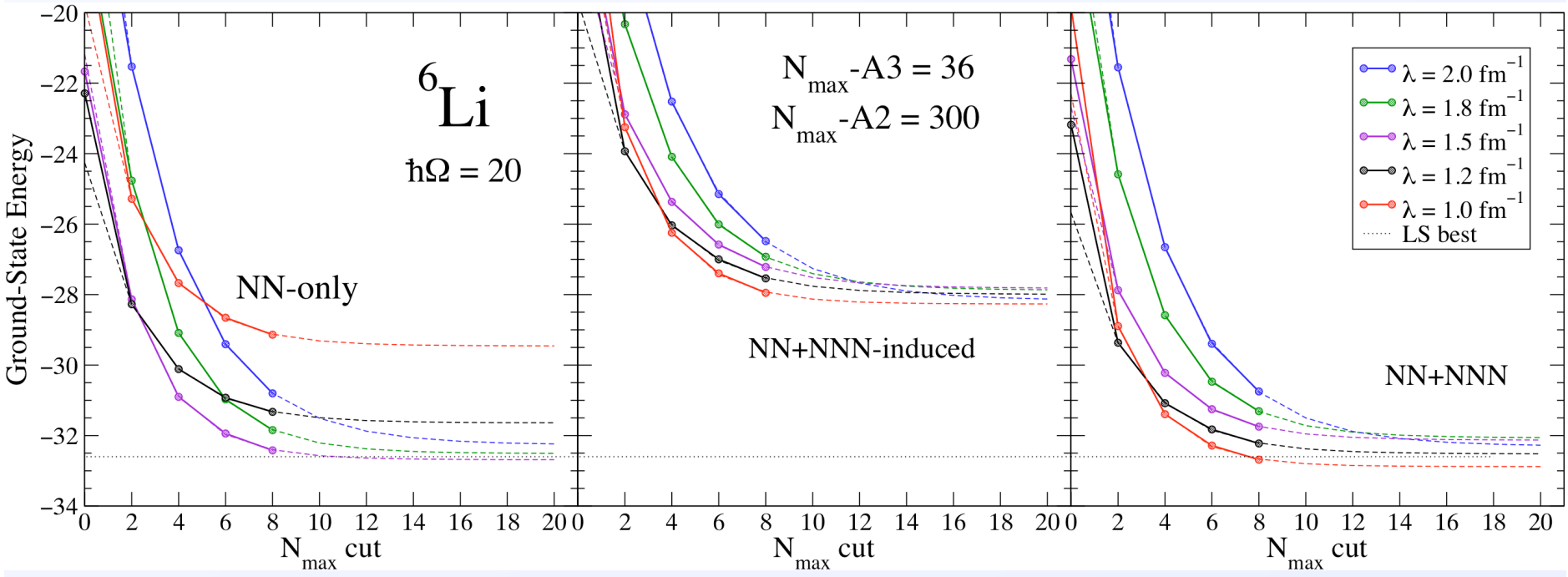
Jacobi ➔ Slater-determinant



- Push the truncations to 300/36
- Variational: find the minimum
- At N_{max} = 8, min is at ħΩ = 20
- Input files here are 13 Gb
  (32 Gb for other p-shells)

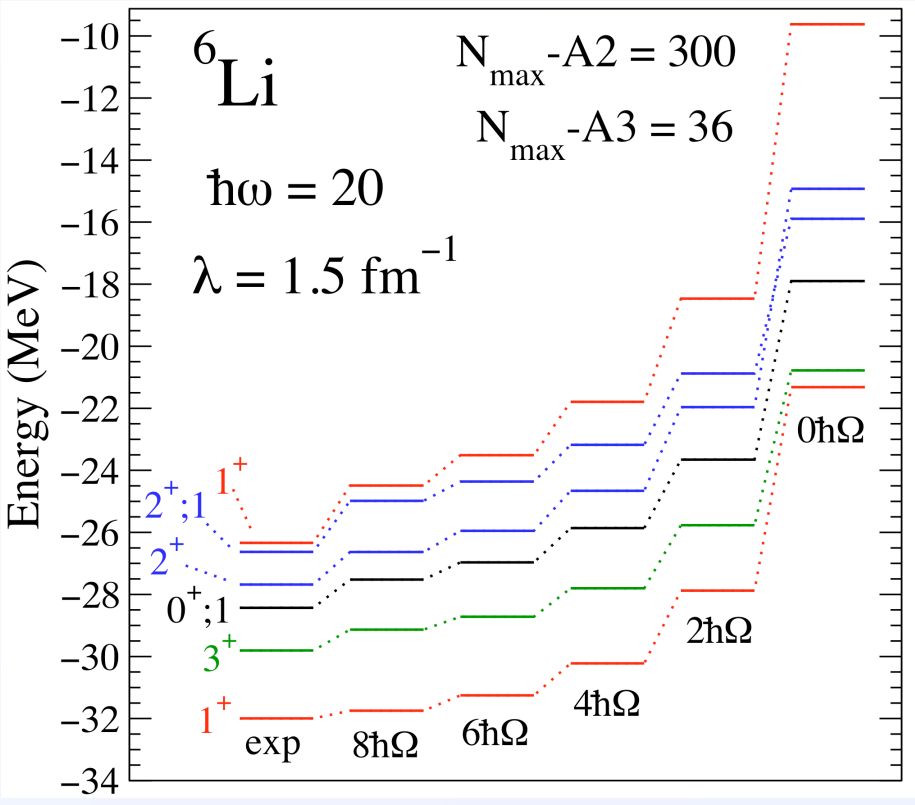


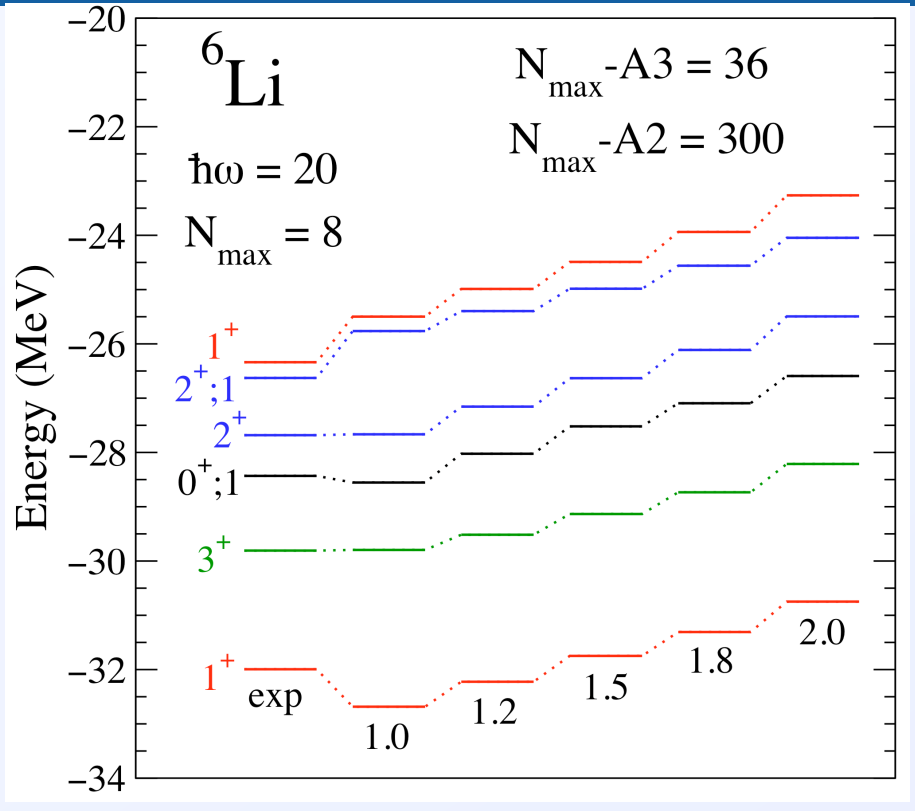
^{6}Li: NN and NN+NNN calculations



- Increased N_{max}-A2 to 300 and N_{max}-A3 to 36
- Simple extrapolations show significant spread in λ
- Induced 4NF? Missing 3NF?
- Width b/n mid and right are different: A3 truncation

^{6}Li: Spectrum





- Spectral structure is preserved nicely
- 2+;1 and 3^{+} not converging as fast, but more sensitive to higher J
- More evidence that A3nmax should be higher

Plan for Rest of Year 4 and Year 5

Deliverables

Recap

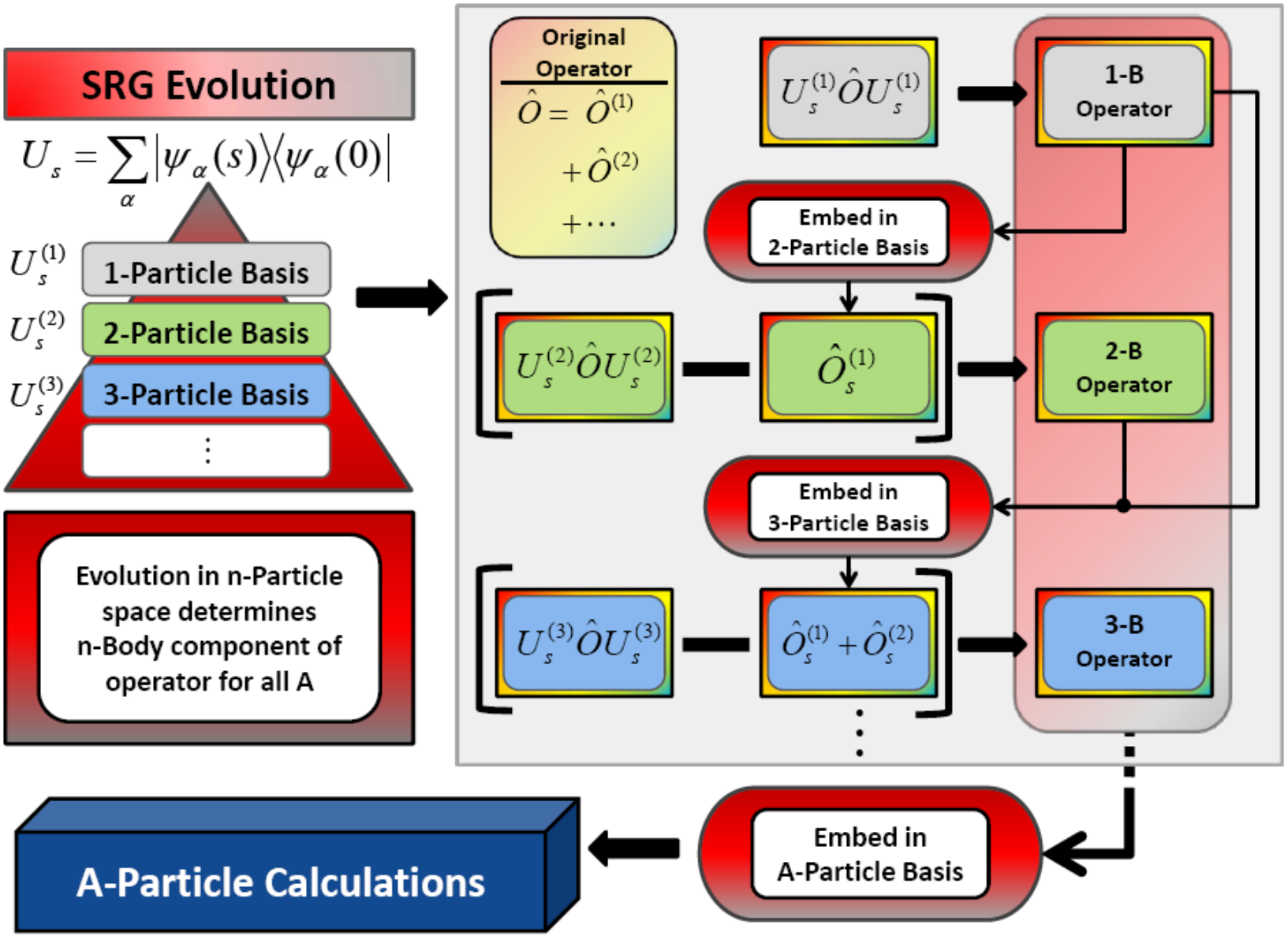
- SRG improves convergence
- Variational and model space independent
- Induced forces are of natural size – no larger than the error due to missing initial ANFs
- Still waiting on more precise calculations (A3-N_{max}=40) to determine their significance at $A \geq 6$

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)

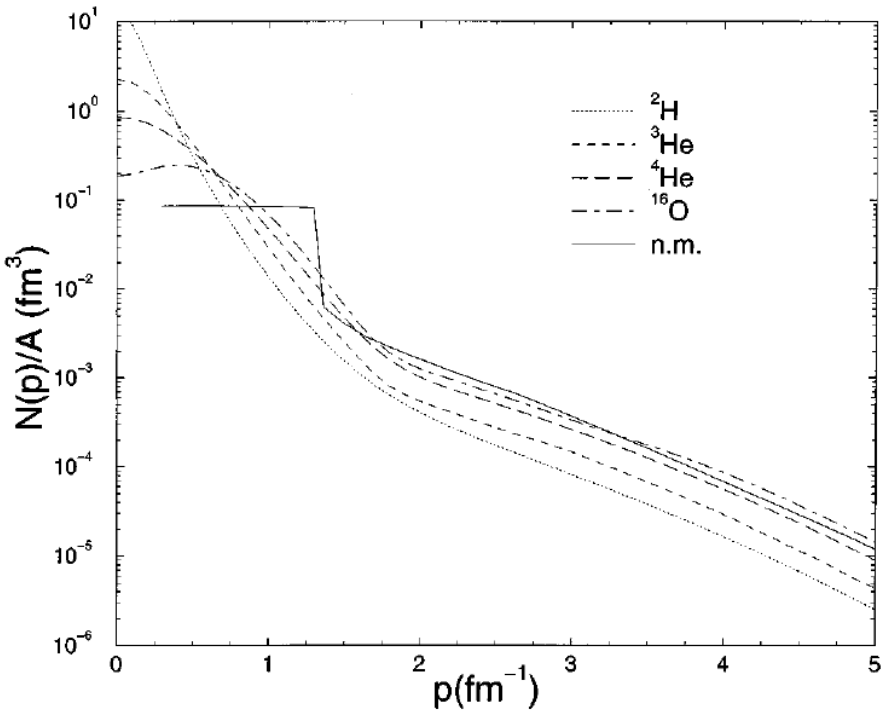
SRG Operators (Eric Anderson et al.)

Operator Evolution & Extraction Process



Factorization in Few-Body Nuclei

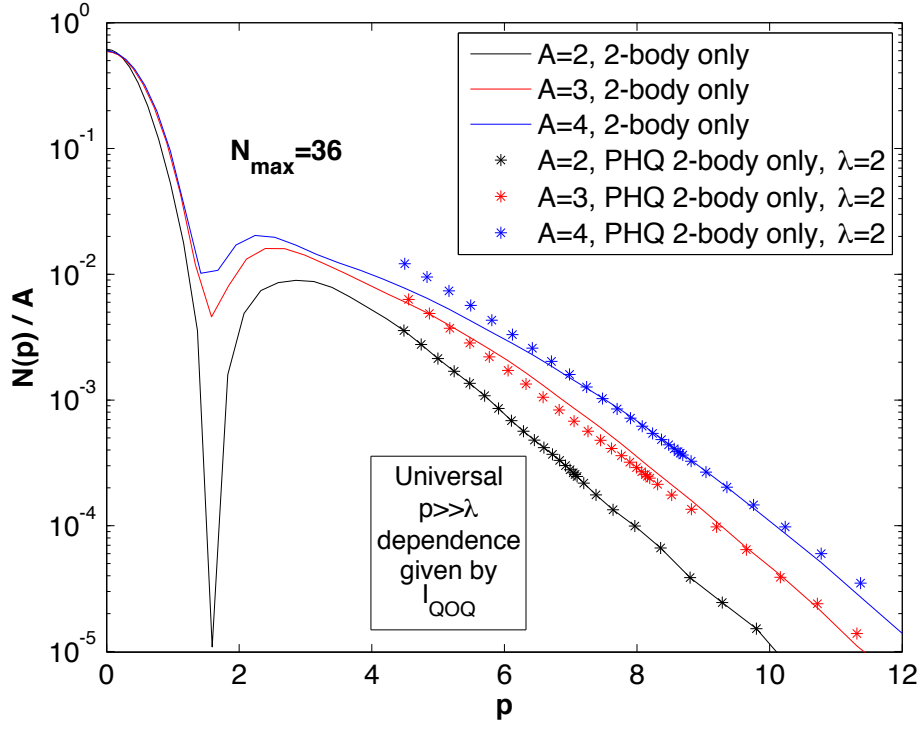
- **Variational Monte Carlo Calculation**
  → Using AV14 NN potential



From Pieper, Wiringa, and Pandharipande (1992).

- 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



→ A Test Bed for 3D NCSM calculations:

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

$$\int_0^\lambda \int_0^\lambda \psi_\lambda^\dagger(k') \left[I_{QOQ} K_\lambda(k') K_\lambda(k) \right] \psi_\lambda(k)$$

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)

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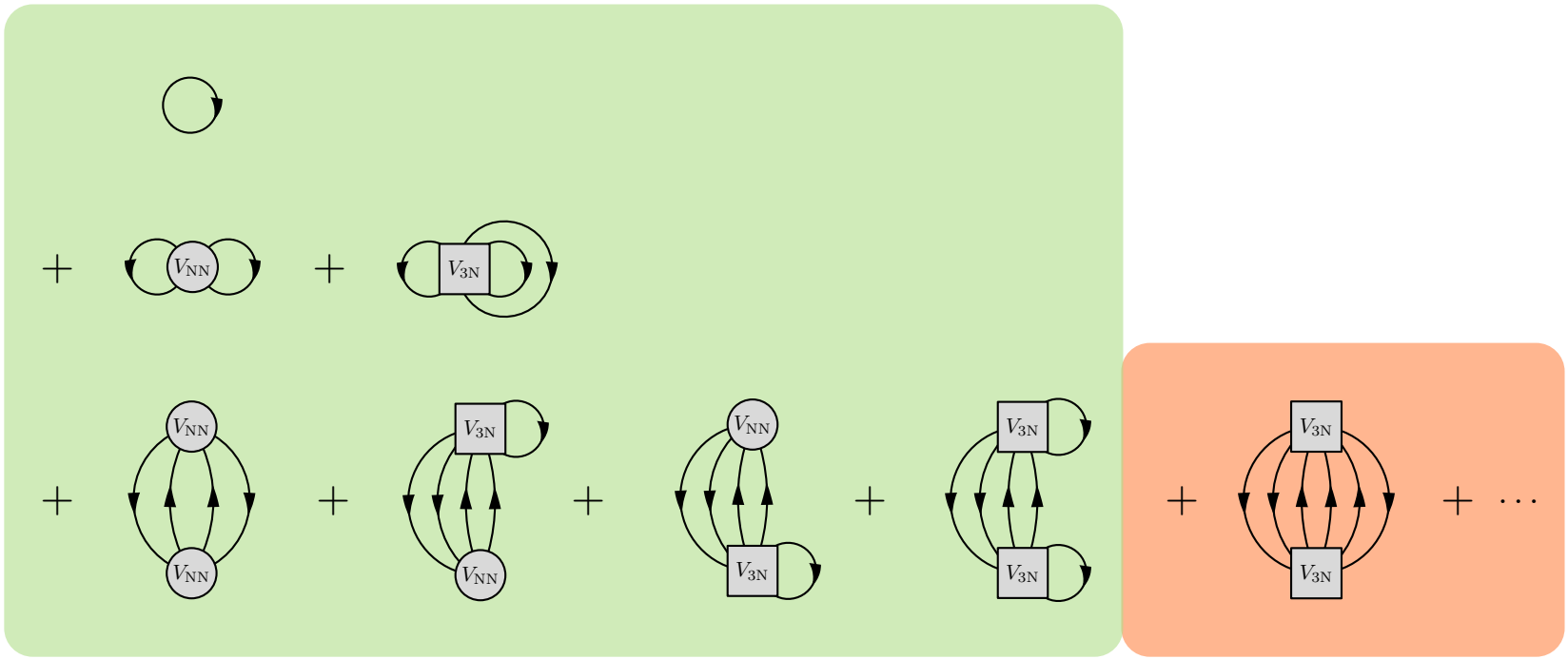
Improved NNN Treatment (Kai Hebeler et al.)

Many-body perturbation theory

central quantity of interest: energy per particle E/N

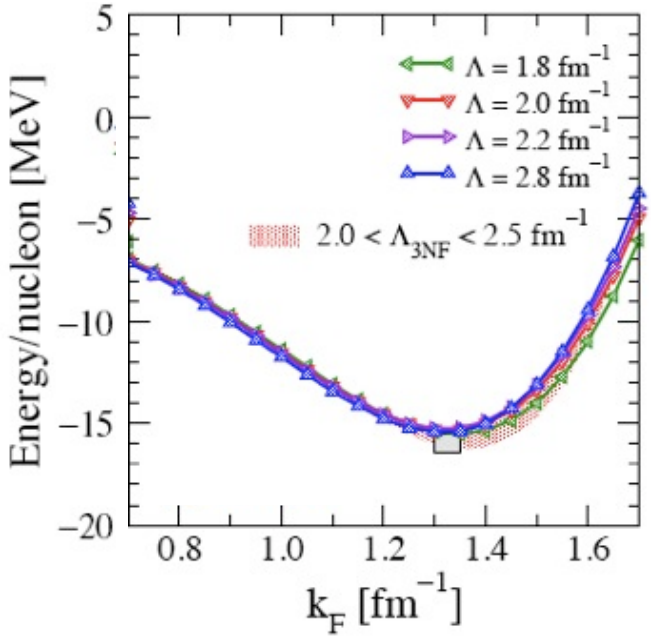
$$H(\Lambda) = T + V_{\mathrm{NN}}(\Lambda) + V_{\mathrm{3N}}(\Lambda) + \dots .$$

$E =$

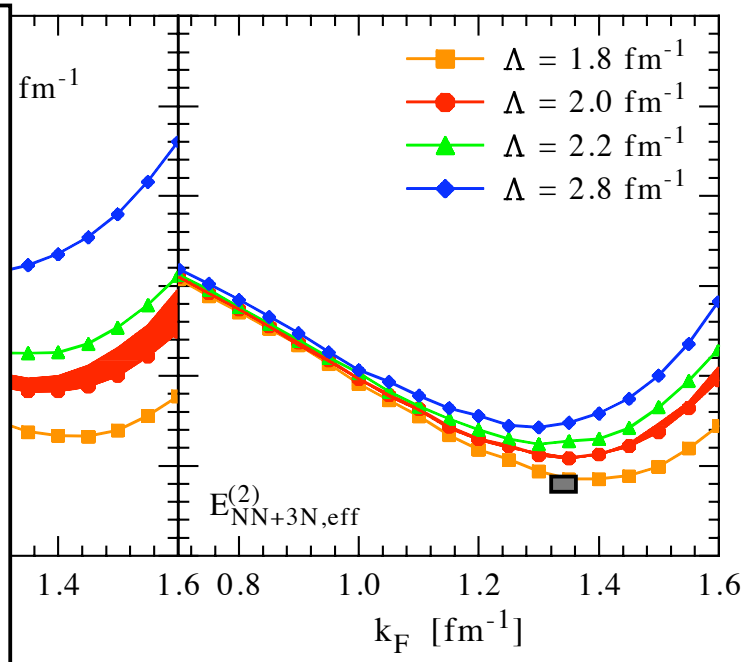


- for low momentum interactions no resummation of diagrams necessary
- self-consistent single-particle propagators ⟶ thermodynamic consistency

Symmetric nuclear matter



Bogner, Furnstahl, Schwenk, Nogga; arXiv:0903.3366



Bogner, Furnstahl, Schwenk, Nogga, KH;i

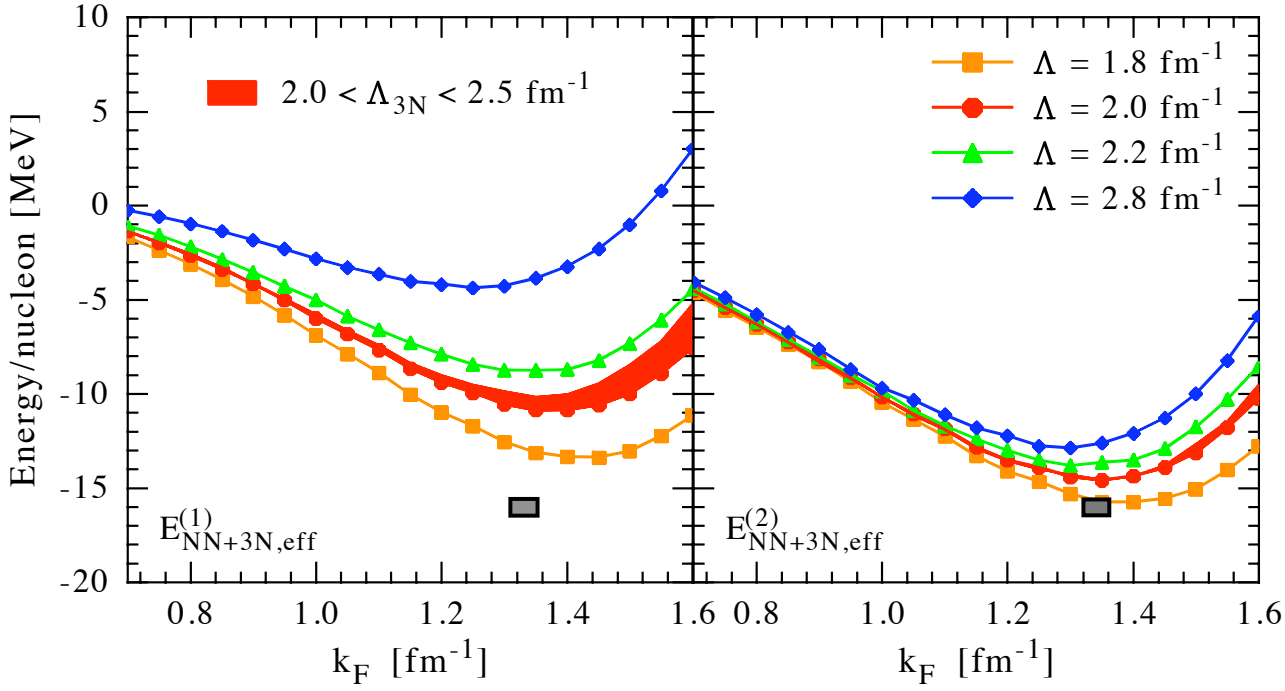
Improvements:

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

educed

MeV and $r_{^4\mathrm{He}} = 1.95 - 1.96\,\mathrm{fm}$

Symmetric nuclear matter

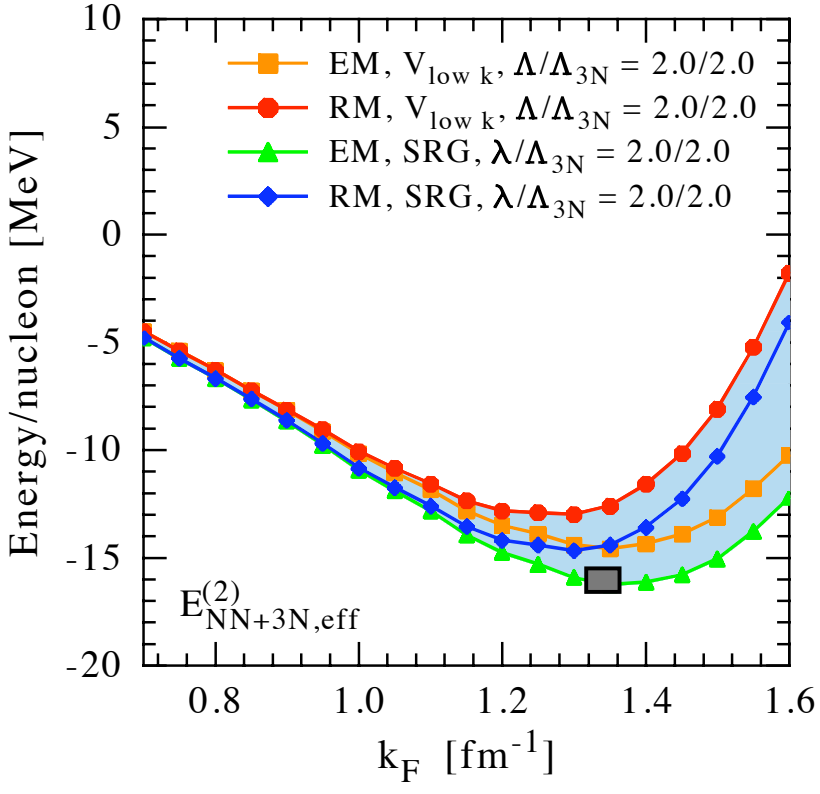


Bogner, Furnstahl, Schwenk, Nogga, KH;in preparation

- 3N forces crucial for saturation
- cutoff dependence at 2nd order significantly reduced
- couplings c_D and c_E fitted to $E_{^3\mathrm{H}} = -8.482\,\mathrm{MeV}$ and $r_{^4\mathrm{He}} = 1.95 - 1.96\,\mathrm{fm}$
- 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): PRC 68, 041001

$$c_1 = -0.81\,\mathrm{GeV}^{-1}$$
$$c_3 = -3.20\,\mathrm{GeV}^{-1}$$
$$c_4 = +5.40\,\mathrm{GeV}^{-1}$$

Rentmeester et al. (RM): PRC 67, 044001

$$c_1 = -0.76\,\mathrm{GeV}^{-1}$$
$$c_3 = -4.78\,\mathrm{GeV}^{-1}$$
$$c_4 = +3.96\,\mathrm{GeV}^{-1}$$

- 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

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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

$$\frac{dH(s)}{ds} = [\eta(s), H(s)] \qquad \eta = [\hat{f}, \hat{\Gamma}]$$

$$\Rightarrow \quad \lim_{s\to\infty} \Gamma_{od}(s) = 0 \qquad \langle 12|\Gamma_{od}|34\rangle = 0 \ \text{ if } \ \mathrm{f}_{12} = \mathrm{f}_{34}$$

$$\lambda \equiv s^{-1/4}$$

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

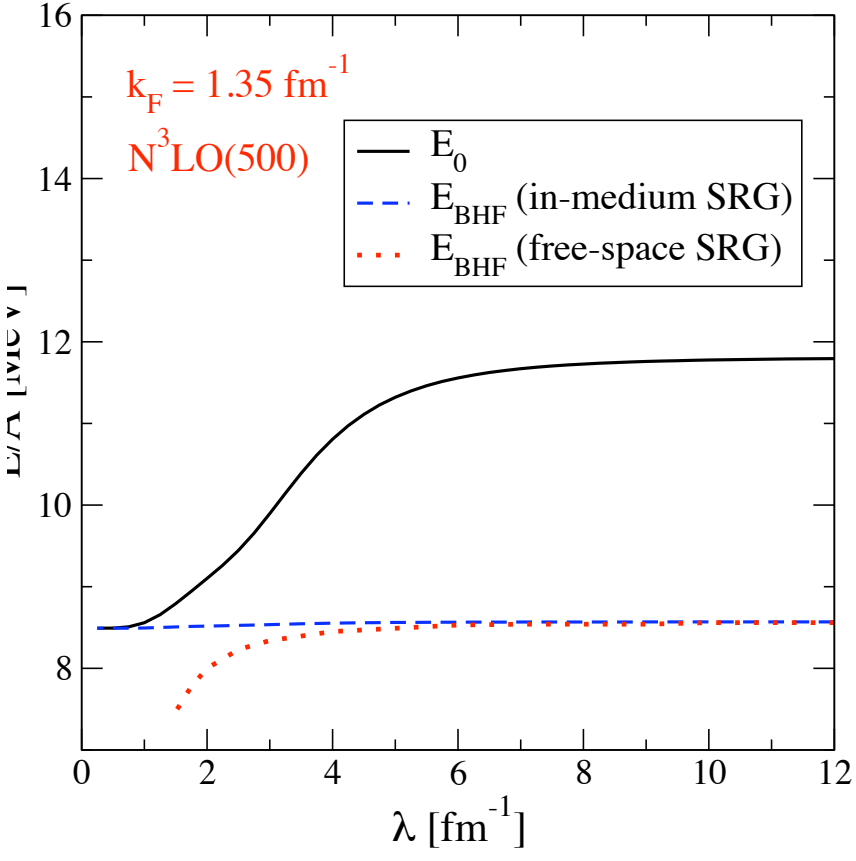
$$H(\infty) = E_{vac}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4}\sum [\Gamma_d(\infty)]_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k)$$

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

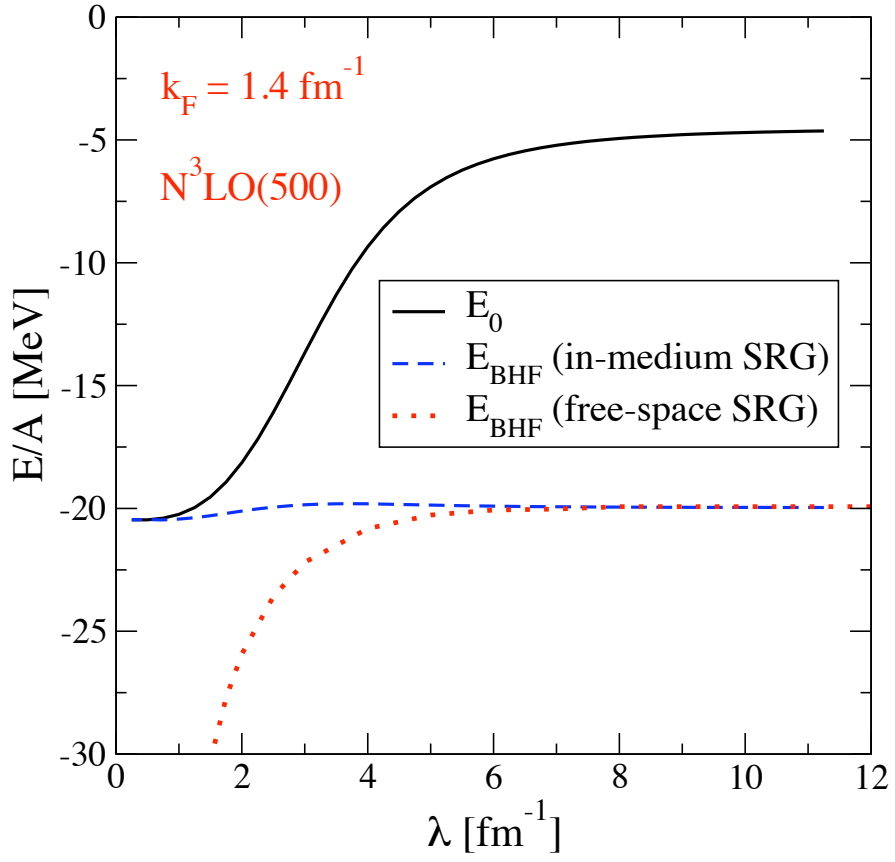
Microscopic realization of SM ideas: dominant MF + weak A-dependent NN_{eff}

Alternative many-body method (Bogner, Hergert)

Correlations "adiabatically" summed into H(λ)



PNM*



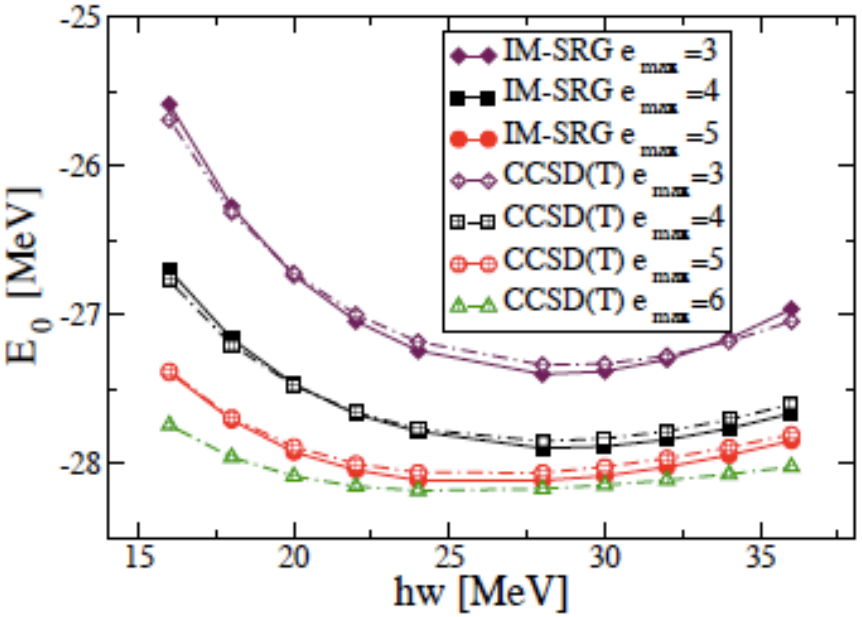
SNM*

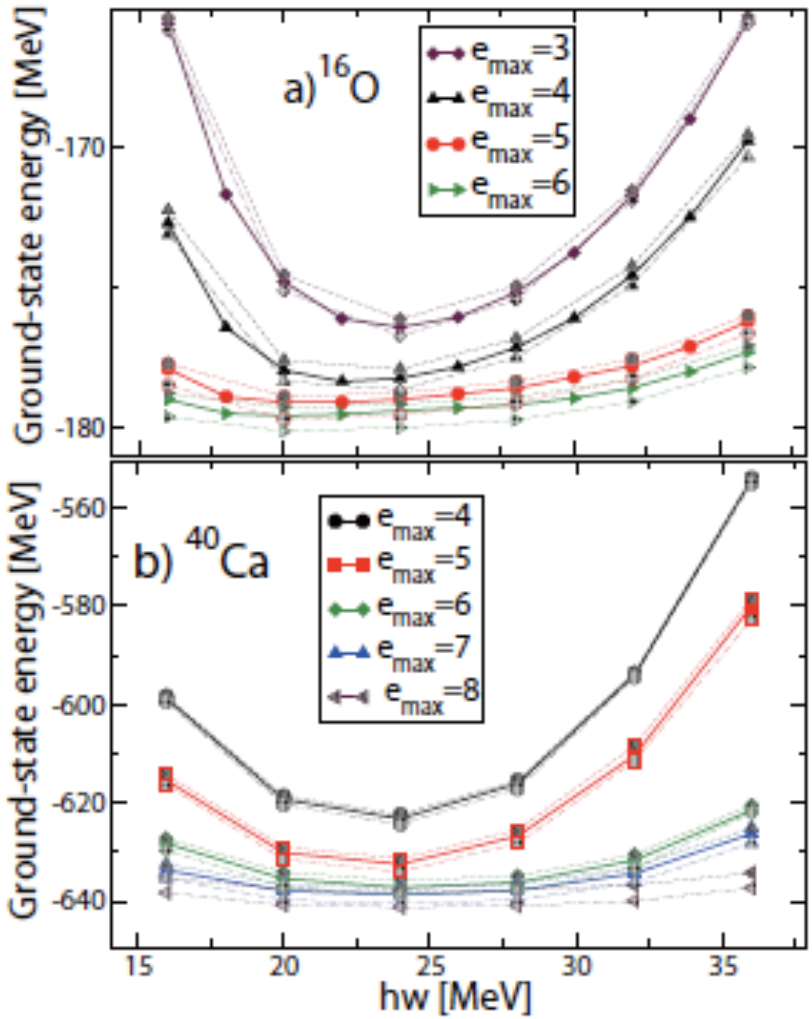
Weak cutoff dependence over large range => dominant 3,4,...-body terms evolved implicitly

*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 ~ 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

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OEP Development (Drut, Platter, rjf)

The OEP equation

- OEP integral equation

$$\int dx'\ Q(x,x')v_{\rm xc}(x') = \Lambda(x)$$

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

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

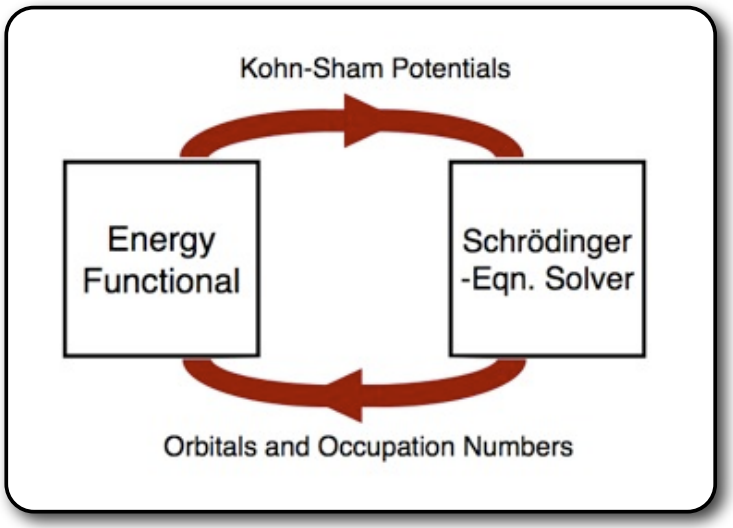
Green's function

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

Sum over occupied **and** unoccupied states!

Auxiliary potential

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



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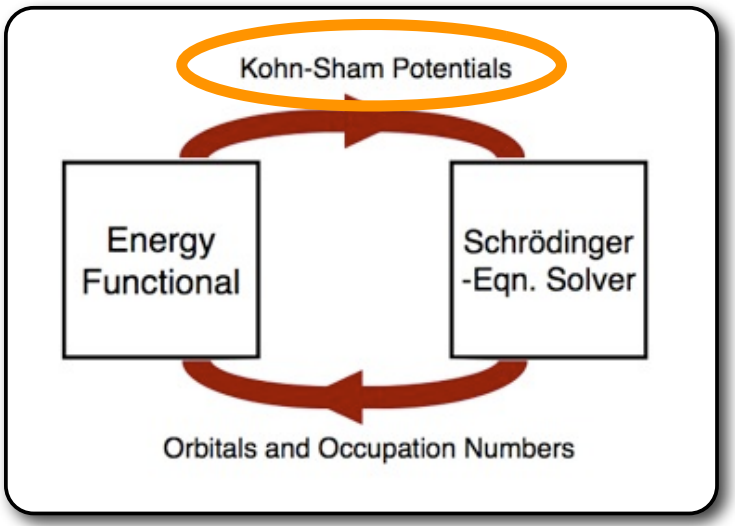

Solving the OEP equation

- Two problems:
  - Constructing the Green's function explicitly may be expensive

Kümmel-Perdew
Iterative solution

  - The OEP equation is **singular**

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

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

$$\Delta_i(x) = v_{\mathrm{xc}}(x) - u_{\mathrm{xc},i}(x) \qquad u_{xc,j}(x') = \frac{1}{\varphi_j^*(x')}\frac{\delta E_{int}}{\delta\varphi_j(x')}$$

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}Ca DME comparisons
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- 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

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

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

NV, PSA, ...

Dependence on local densities/currents now manifest

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

$$\sim\sum_t\int d\mathbf{R}\left\{C_t^{\rho\rho}\rho_t^2+C_t^{\rho\tau}\rho_t\tau_t+C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t+C_t^{JJ}\mathbf{J}_t^2+C_t^{J\nabla\rho}\mathbf{J}_t\nabla\rho_t\cdots\right\}$$

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

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

$$C^{ij}[u]\ =\ \text{rational polynomial}$$

Prescriptions for Π_n-functions

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

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

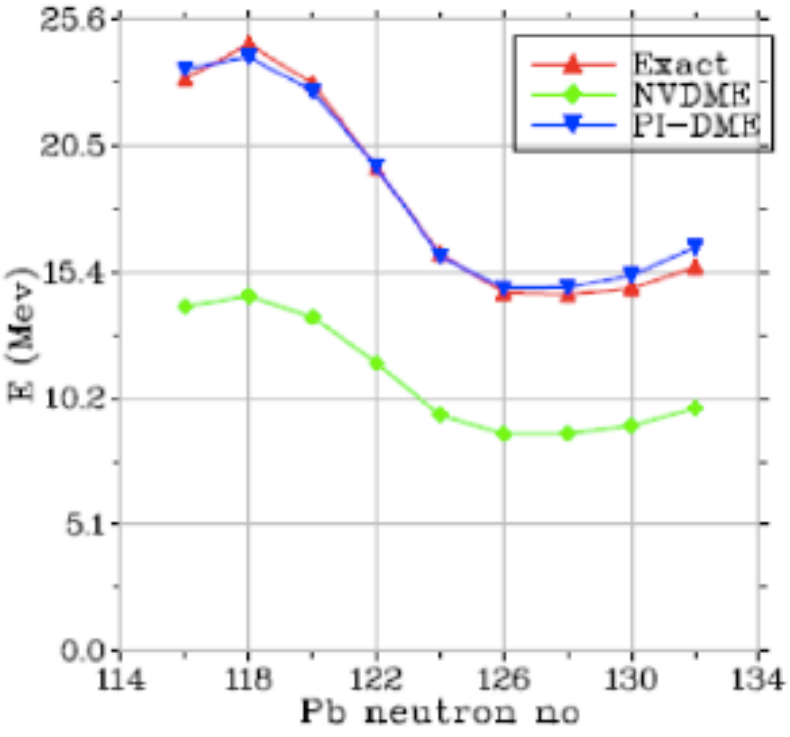
Average the non-locality operator over local momentum distribution g(**R**,**k**) and expand exponentiated gradients

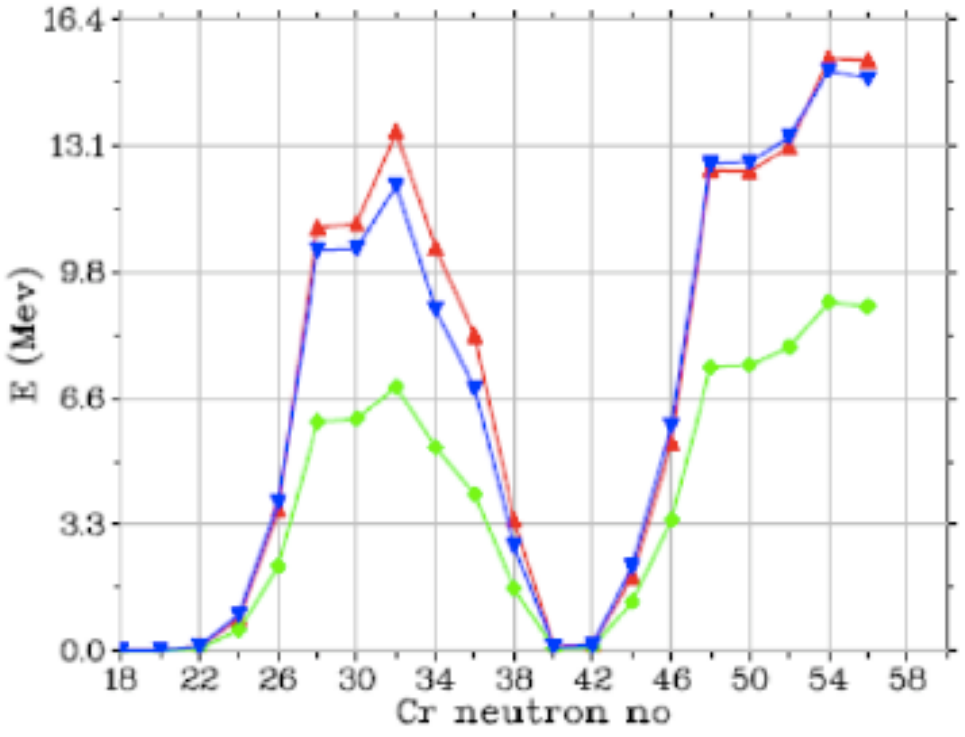
$$\rho(\vec{r}_1,\vec{r}_2) \quad \approx \quad \int d^3\vec{k}\; g(\vec{R},\vec{k})\, e^{i\vec{k}\cdot\vec{r}} \sum_{n=0}^{2} \frac{1}{n!}\left\{\vec{r}\cdot\left(\frac{\nabla_1-\nabla_2}{2}-i\vec{k}\right)\right\}^n \rho(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

Easy to build in physics associated with surface effects in finite fermi systems (non-isotropic g(R,k))

Crucial to accurately describe spin-vector part of OBDM

Look at $\int d\mathbf{r}\, d\mathbf{R}\, V_{1\pi}(r)\, \mathbf{s}_n(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{s}_n(\mathbf{r}_2, \mathbf{r}_1)$:



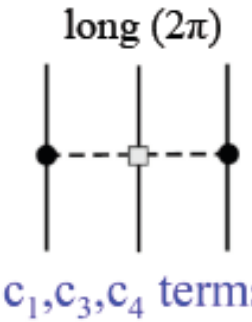


- Inclusion of finite fermi phase space effects crucial for **quantitative** agreement
- completely parameter-free

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



$$V_c(\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3) \sim \frac{\sigma_1\cdot\mathbf{q_1}\sigma_2\cdot\mathbf{q_2}}{(q_1^2+m_\pi^2)(q_2^2+m_\pi^2)}F_{123}^{\alpha\beta}\tau_1^\alpha\tau_2^\beta + perms$$

$$F_{123}^{\alpha\beta} \equiv \delta_{\alpha\beta}\left[-4\frac{c_1 m_\pi^2}{f_\pi^2}+2\frac{c_3}{f_\pi^2}\mathbf{q}_1\cdot\mathbf{q}_2\right] + \frac{c_4}{f_\pi^2}\epsilon^{\alpha\beta\gamma}\tau_3^\gamma\sigma_3\cdot(\mathbf{q}_1\times\mathbf{q}_2)$$

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·∇ρ couplings)

Similarly for <V_{NNN}> (but trilinear and many more terms...)

$$
\begin{aligned}
\mathcal{E}^{CR4,2x} \;=\; \int d\vec{r}\Big\{ & \mathcal{C}_7^{\rho_0^3}\,\rho_0^3(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\rho_1^2}\,\rho_0(\vec{r})\,\rho_1^2(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\rho_1\varsigma_1^1}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\varsigma_1^1(\vec{r}) \\
& + \mathcal{C}_7^{\rho_0^2\Delta\rho_0}\,\rho_0^2(\vec{r})\,\Delta\rho_0(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\rho_1\Delta\rho_1}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\Delta\rho_1(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0^2\varsigma_0^2}\,\rho_0^2(\vec{r})\,\varsigma_0^2(\vec{r}) \\
& + \mathcal{C}_7^{\rho_1^2\varsigma_0^2}\,\rho_1^2(\vec{r})\,\varsigma_0^2(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\rho_1\varsigma_1^2}\,\rho_0(\vec{r})\,\rho_1(\vec{r})\,\varsigma_1^2(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0^2\varsigma_0^1}\,\rho_0^2(\vec{r})\,\varsigma_0^1(\vec{r}) \\
& + \mathcal{C}_7^{\rho_0 J_0^2}\,\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\rho_1 J_0 J_1}\,\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0 J_1^2}\,\rho_0(\vec{r})\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + \mathcal{C}_7^{J_0^2\nabla J_0}\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{J_1^2\nabla J_0}\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{J_0 J_1\nabla J_1}\,\vec{J}_0(\vec{r})\,\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) \\
& + \mathcal{C}_7^{\Delta\rho_0 J_0^2}\,\Delta\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\varsigma_0^2 J_0^2}\,\varsigma_0^2(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\varsigma_0^1 J_0^2}\,\varsigma_0^1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_0(\vec{r}) \\
& + \mathcal{C}_7^{\nabla\rho_0 J_0\nabla J_0}\,\vec{\nabla}\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\nabla J_0\nabla J_0}\,\rho_0(\vec{r})\left[\vec{\nabla}\cdot\vec{J}_0(\vec{r})\right]^2 \;+\; \mathcal{C}_7^{\rho_0 J_0\Delta J_0}\,\rho_0(\vec{r})\,\vec{J}_0(\vec{r})\cdot\Delta\vec{J}_0(\vec{r}) \\
& + \mathcal{C}_7^{\varsigma_1^1 J_0 J_1}\,\varsigma_1^1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\Delta\rho_1 J_0 J_1}\,\Delta\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\varsigma_1^2 J_0 J_1}\,\varsigma_1^2(\vec{r})\,\vec{J}_0(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + \mathcal{C}_7^{\nabla\rho_1 J_1\nabla J_0}\,\vec{\nabla}\rho_1(\vec{r})\cdot\vec{J}_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\rho_1 J_1\Delta J_0}\,\rho_1(\vec{r})\,\vec{J}_1(\vec{r})\cdot\Delta\vec{J}_0(\vec{r}) \;+\; \mathcal{C}_7^{\varsigma_0^2 J_1^2}\,\varsigma_0^2(\vec{r})\,\vec{J}_1(\vec{r})\cdot\vec{J}_1(\vec{r}) \\
& + \mathcal{C}_7^{\nabla\rho_1 J_0\nabla J_1}\,\vec{\nabla}\rho_1(\vec{r})\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\rho_1\nabla J_0\nabla J_1}\,\rho_1(\vec{r})\,\vec{\nabla}\cdot\vec{J}_0(\vec{r})\,\vec{\nabla}\cdot\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0\nabla J_1\nabla J_1}\,\rho_0(\vec{r})\left[\vec{\nabla}\cdot\vec{J}_1(\vec{r})\right]^2 \\
& + \mathcal{C}_7^{\rho_1 J_0\Delta J_1}\,\rho_1(\vec{r})\,\vec{J}_0(\vec{r})\cdot\Delta\vec{J}_1(\vec{r}) \;+\; \mathcal{C}_7^{\rho_0 J_1\Delta J_1}\,\rho_0(\vec{r})\,\vec{J}_1(\vec{r})\cdot\Delta\vec{J}_1(\vec{r})\Big\}. \qquad (91)
\end{aligned}
$$

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

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

$$C_\alpha^{ijk}[u] = \text{rational polynomial}$$

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

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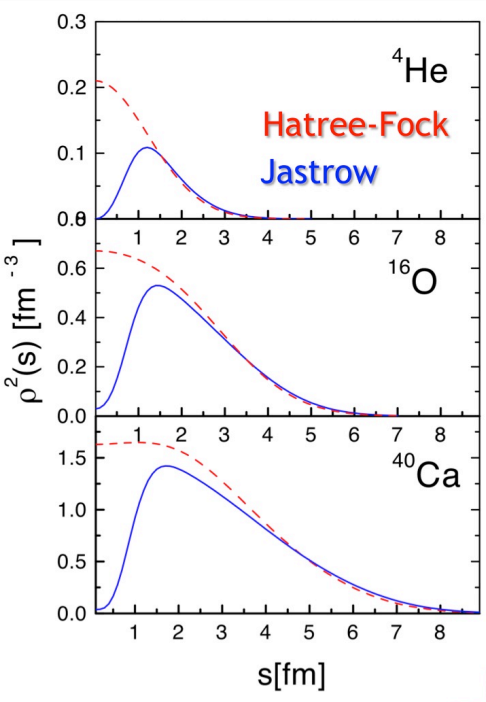
Calculations with DME-based EDF (Stoitsov et al.)

Towards Ab Initio Nuclear Energy Density Functional
Underlining Philosophy



Exact Two-Body Density Matrix

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

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

Two-Body Density Matrix in Hartree-Fock Approximation

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

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

Contact part as it is but optimized

DME expansion in HF approximation

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

Exact Energy

DME Functional

DME Functional
NN and NNN amplitudes

❖ NN

$$g_t^m(u) = g_t^m(u)|_{LO} + g_t^m(u)|_{NLO} + g_t^m(u)|_{N^2LO}$$

$$g(u)|_{LO} = \alpha_0^g + \beta_0^g \log\left(1+4u^2\right) + \gamma_0^g \arctan\left(2u\right)$$

$$g(u)|_{NLO} = \alpha_1^g + \beta_1^g \left(\log\left(1+2u^2+2u\sqrt{1+u^2}\right)\right)^2 + \gamma_1^g \sqrt{1+u^2} \log\left(1+2u^2+2u\sqrt{1+u^2}\right)$$

$$g(u)|_{N^2LO} = \alpha_2^g + \beta_2^g \log\left(1+u^2\right) + \gamma_2 \arctan\left(u\right)$$

❖ NNN

$$h_{tt'}^m(u) = \alpha_0^h + \beta_0^h \log\left(1+4u^2\right) + \beta_1^h \left(\log\left(1+4u^2\right)\right)^2 + \gamma_0^h \arctan\left(u\right) + \gamma_1^h \left(\arctan\left(2u\right)\right)^2 + \gamma_2^h \log\left(1+4u^2\right) \arctan\left(2u\right)$$

$\alpha_k = \alpha_k(u)$, $\beta_k = \beta_k(u)$, $\gamma_k = \gamma_k(u)$

rational polynomials of u

$$u = \frac{k_F(\mathbf{r})}{m_\pi}$$

➢ 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)

Parameters	SLY4	SLY4′	LO	NLO	N2LO
			Volume Parameters		
$C_{00}^{\rho^2}$	-933.342		-727.093	-757.689	-607.108
$C_{10}^{\rho^2}$	830.052		474.871	477.931	316.939
$C_{0D}^{\rho^2}$	861.062		612.104	628.504	-1082.854
$C_{1D}^{\rho^2}$	-1064.273		-705.739	-694.665	-4369.425
$C_{0}^{\rho\tau}$	57.129		33.885	18.471	322.4
$C_{1}^{\rho\tau}$	24.657		32.405	92.233	-156.901
γ	0.16667		0.30622	0.287419	1.06429
			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		
χ^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

EFT Set A

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)

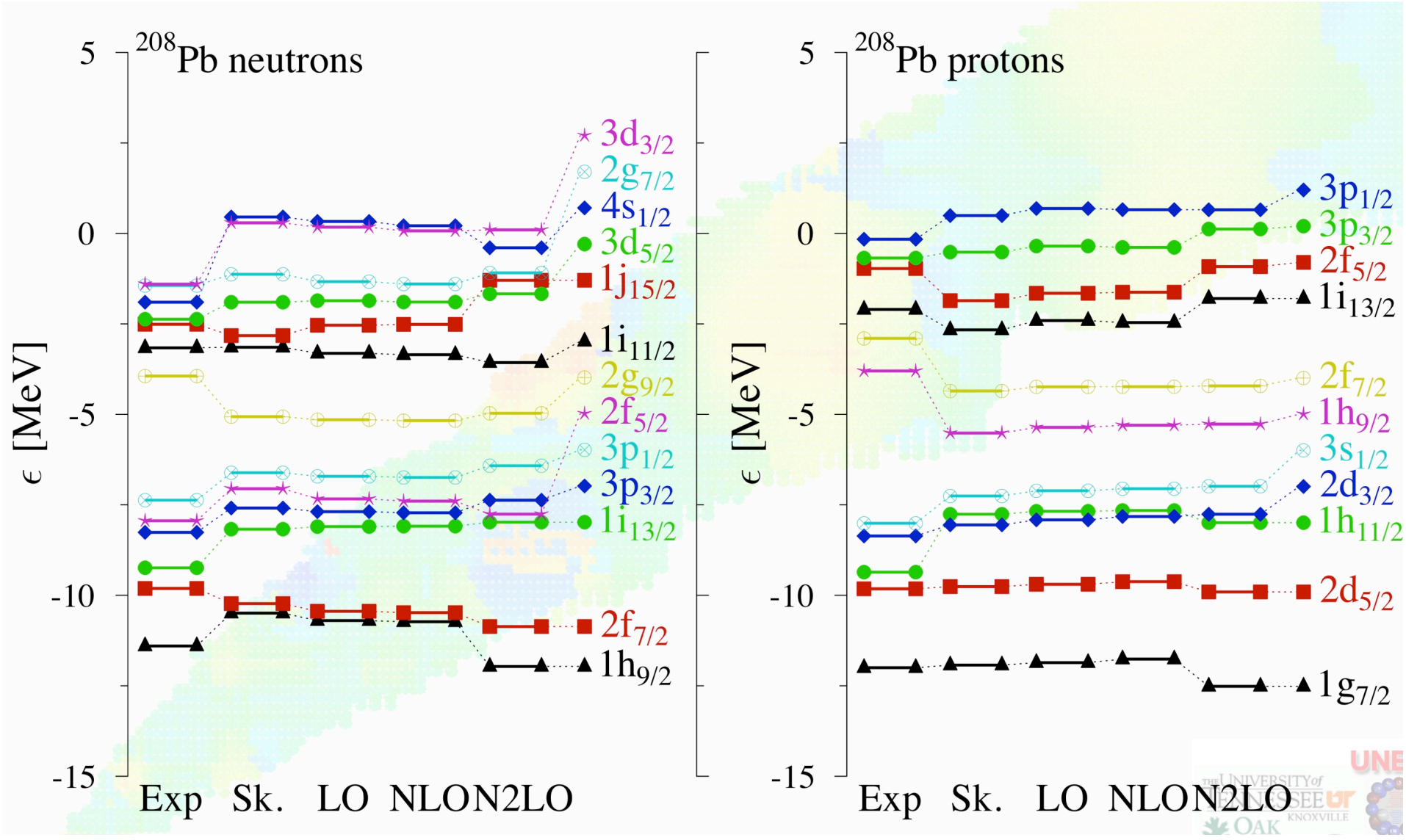
UNEDF

THE UNIVERSITY of TENNESSEE KNOXVILLE

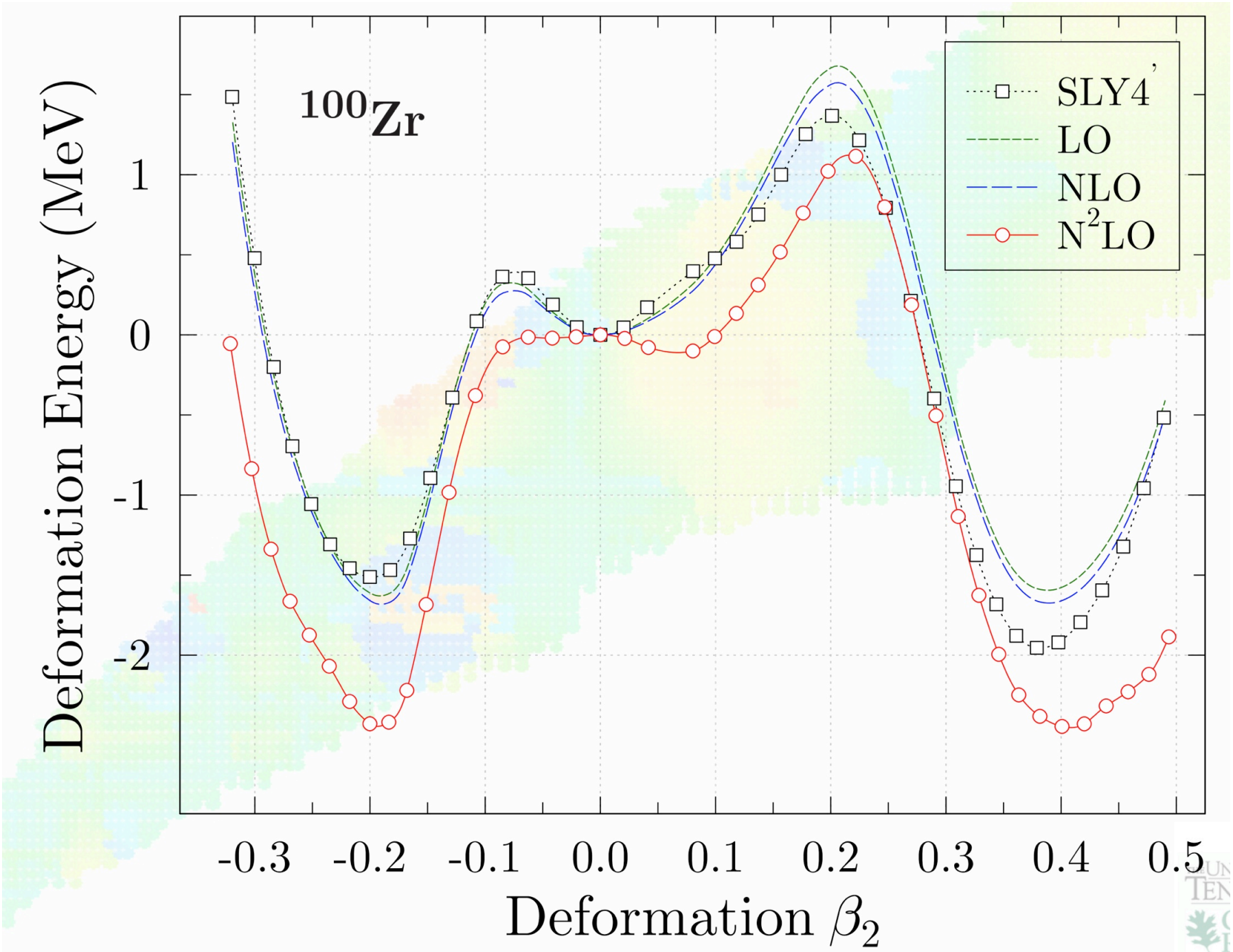
OAK RIDGE National Laboratory

SciDAC

Effects on single-particle levels?



Effects on deformations?



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

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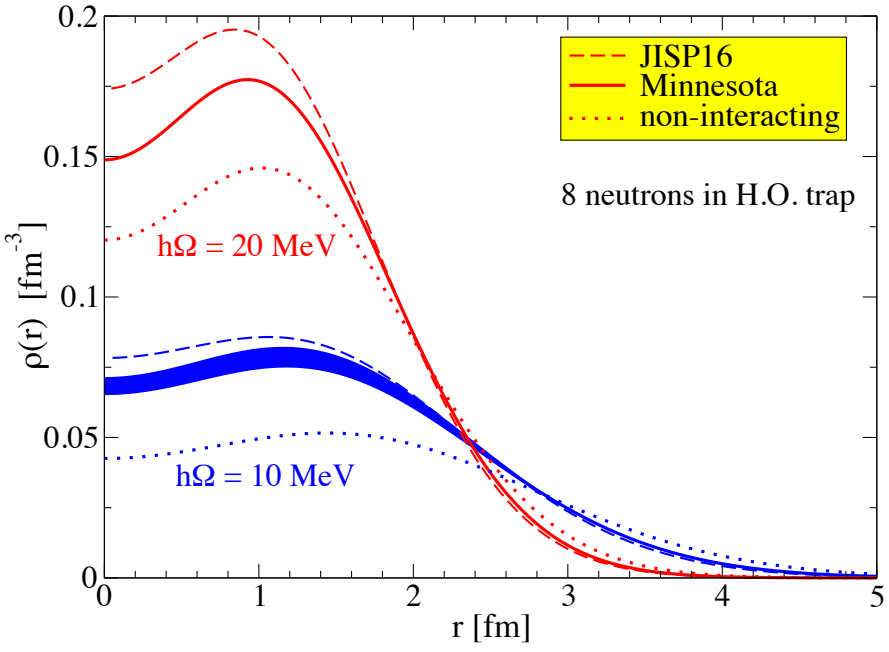
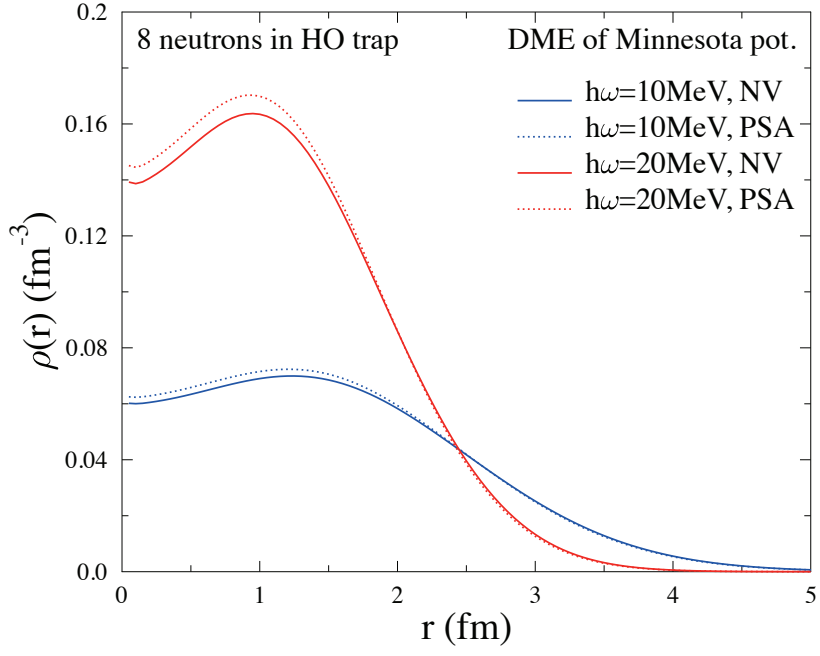
DME–NCFC Comparisons (P. Maris et al.)

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

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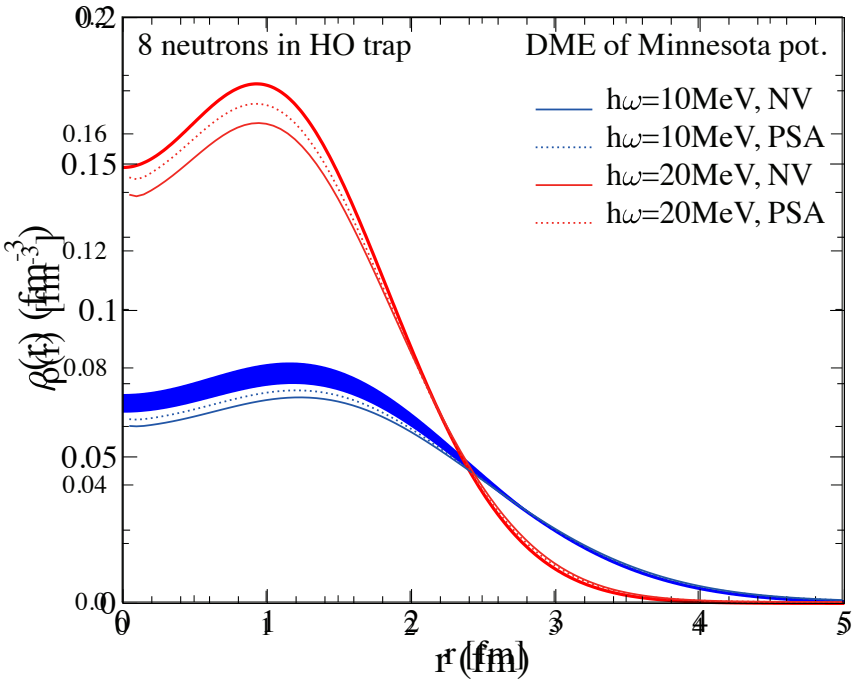

- qualitative agreement between NCFC and DME calculations

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)

Articles and Preprints Citing SCIDAC Support

✓ Published or Posted since Pack Forest 2009

- "Evolution of nuclear many-body forces with the similarity renormalization group," E.D. Jurgenson, P. Navratil and R.J. Furnstahl, Phys. Rev. Lett. **103**, 0820501 (2009)
- "Toward ab initio density functional theory for nuclei," J.E. Drut, R.J. Furnstahl, and L. Platter, Prog. Part. Nucl. Sci. **64**, 120 (2010)
- "From low-momentum interactions to nuclear structure," S.K. Bogner, R.J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Sci.
- "Is chiral symmetry manifested in nuclear structure?," R.J. Furnstahl and A. Schwenk, J. Phys. G **37**, 064004 (2010)
- "How should one formulate, extract, and interpret 'non-observables' for nuclei?," R.J. Furnstahl and A. Schwenk, J. Phys. G **37**, 064005 (2010)
- "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, Comp. Phys. Comm. **181**, 1136 (2010).

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- "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, Comp. Phys. Comm. **181**, 1167 (2010).
- "An improved density matrix expansion for spin-unsaturated nuclei," B. Gebremariam, T. Duguet, and S.K. Bogner, arXiv:0910.4979.
- "Natural units for nuclear energy density functional theory," M. Kortelainen, R.J. Furnstahl, W. Nazarewicz, and M.V. Stoitsov, arXiv:1005.2552, submitted to PRC.
- "Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions," B. Gebremariam, S.K. Bogner, and T. Duguet, arXiv:1003.5210.
- "In-medium similarity renormalization group for nuclei," K. Tsukiyama, S.K. Bogner, and A. Schwenk, arXiv:1006.3639.

Articles and Preprints Citing SCIDAC Support

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}Ca DME comparisons
- ✓ Further development of π–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.