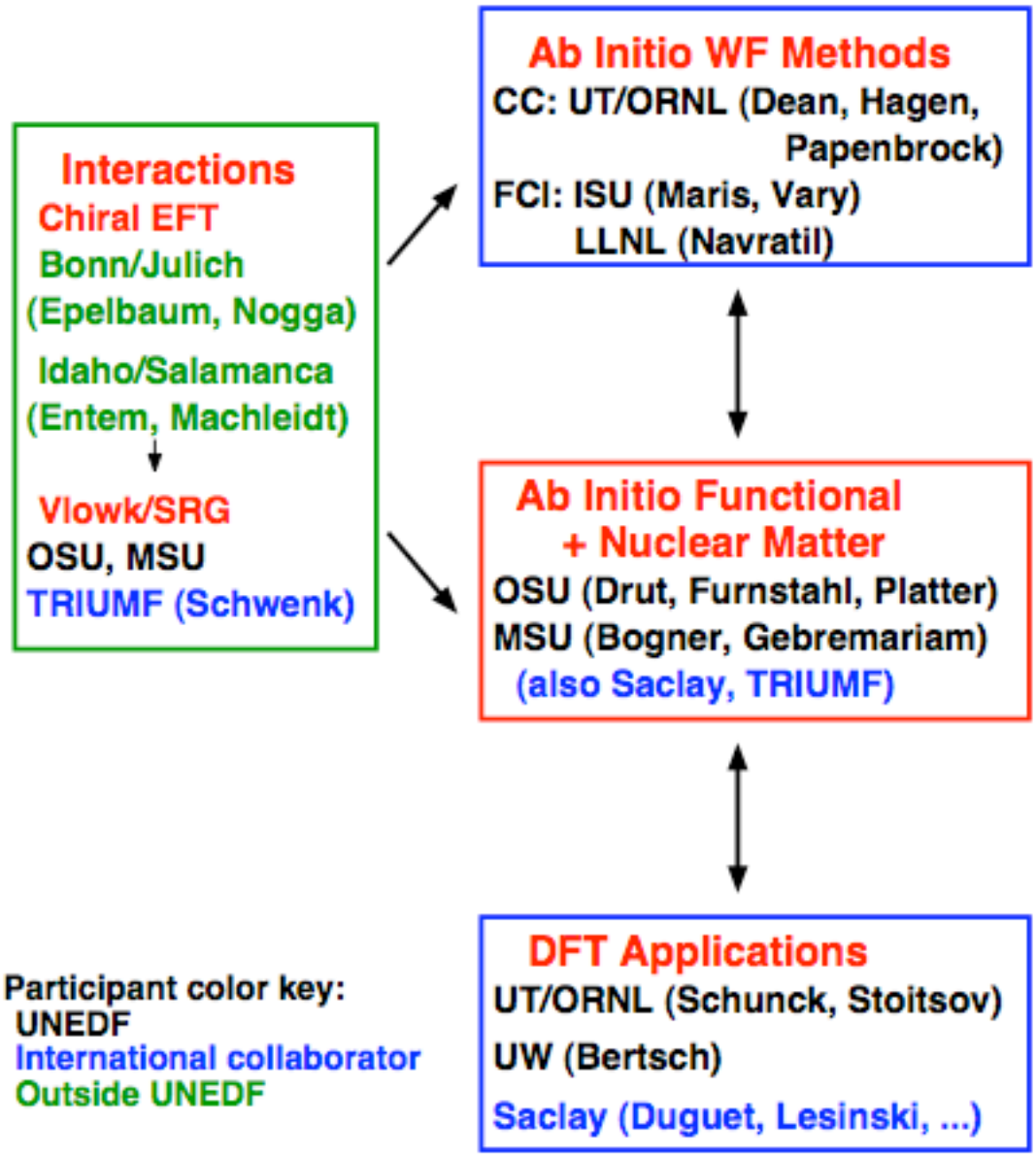
Years 2 & 3: Personnel, Tasks, and Interconnections



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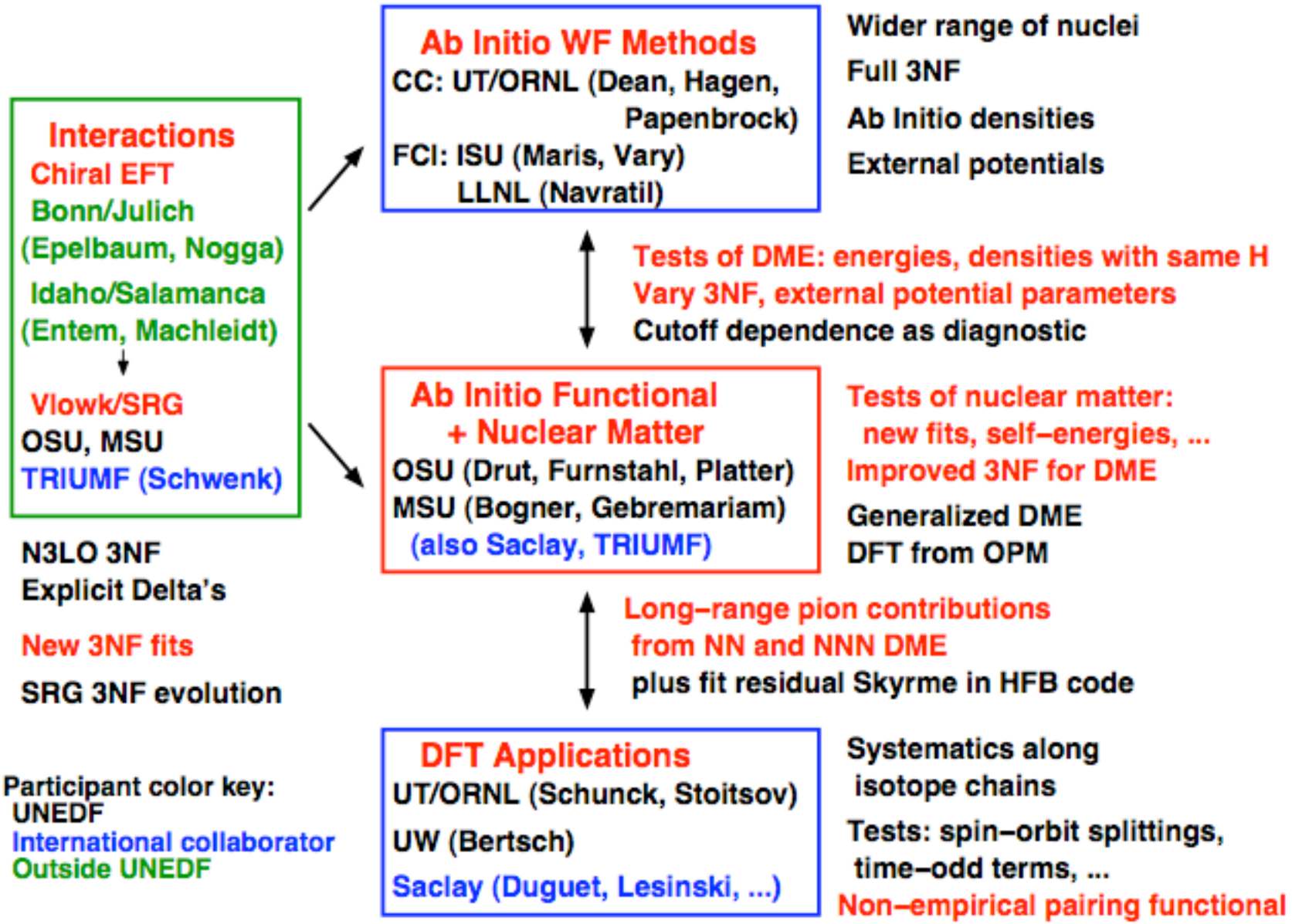


Microscopic EDF's from the DME

- Dominant MBPT contributions to bulk properties take the form

$$\langle V \rangle \sim \mathrm{Tr}_1 \mathrm{Tr}_2 \int d\mathbf{R}\, d\mathbf{r}_{12}\, d\mathbf{r}_{34}\, \rho(\mathbf{r_1}, \mathbf{r_3})\, K(\mathbf{r}_{12}, \mathbf{r}_{34})\, \rho(\mathbf{r_2}, \mathbf{r_4}) \;+\; \mathrm{NNN}\cdots$$

  - density matrices and s.p. propagators
  - finite range and non-local resummed vertices K

  } non-local functionals of ρ

- DME => expand DM in local operators w/factorized non-locality

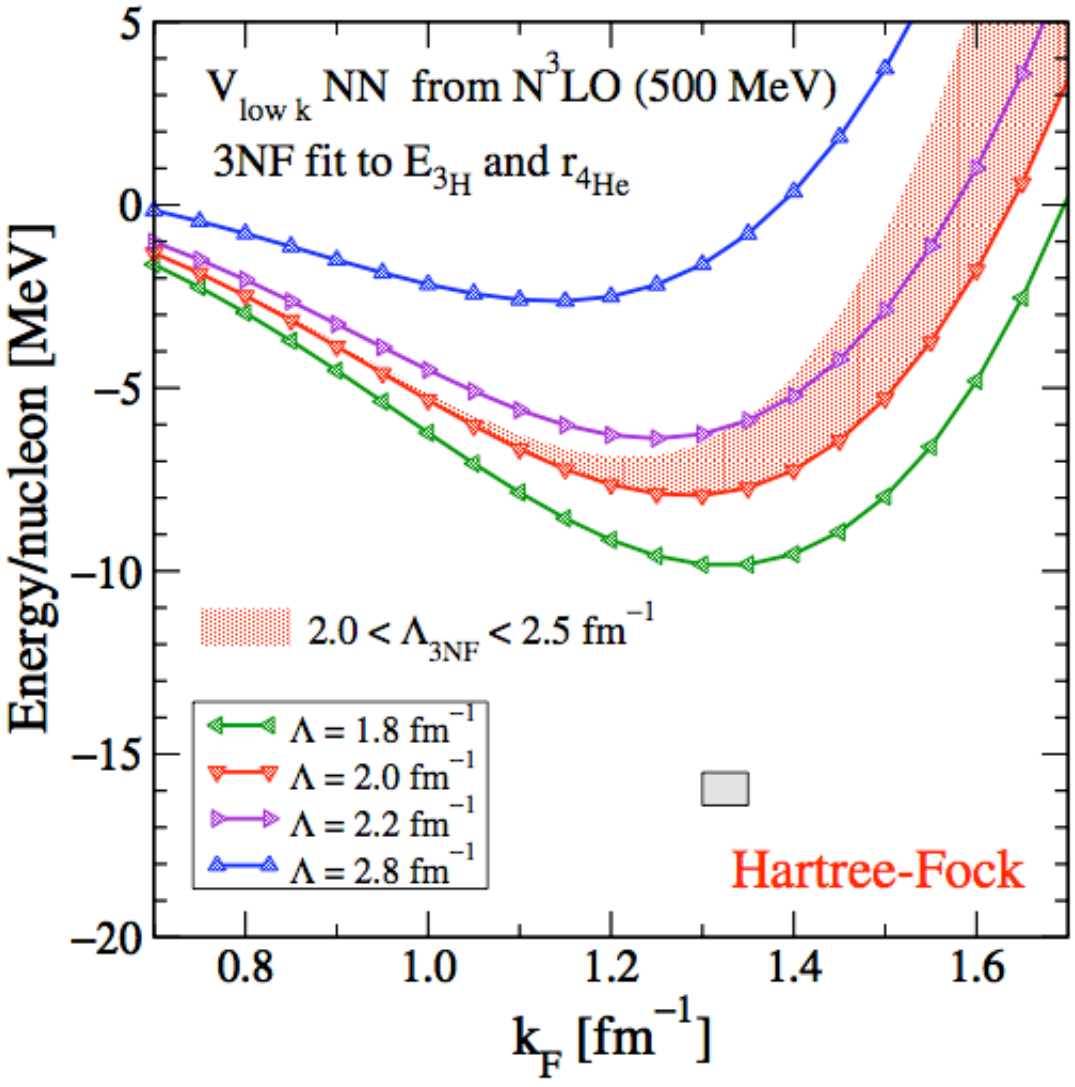
$$\langle \Phi | \psi^\dagger \big(\mathbf{R} - \frac{1}{2}\mathbf{r}\big) \psi \big(\mathbf{R} + \frac{1}{2}\mathbf{r}\big) | \Phi \rangle = \sum_n \Pi_n(\mathbf{r})\, \langle \mathcal{O}_n(\mathbf{R}) \rangle$$

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

Maps <V> into a extended Skyrme-like EDF!

- Original DME => ***calculate*** Π_n from expanding about infinite NM
- Optimized DME => ***Fit*** Π_n, constrain by symmetries and sum rules
- density dependencies, isovector, time-odd,... missing in Skyrme

New low-momentum NNN fits and Nuclear Matter



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

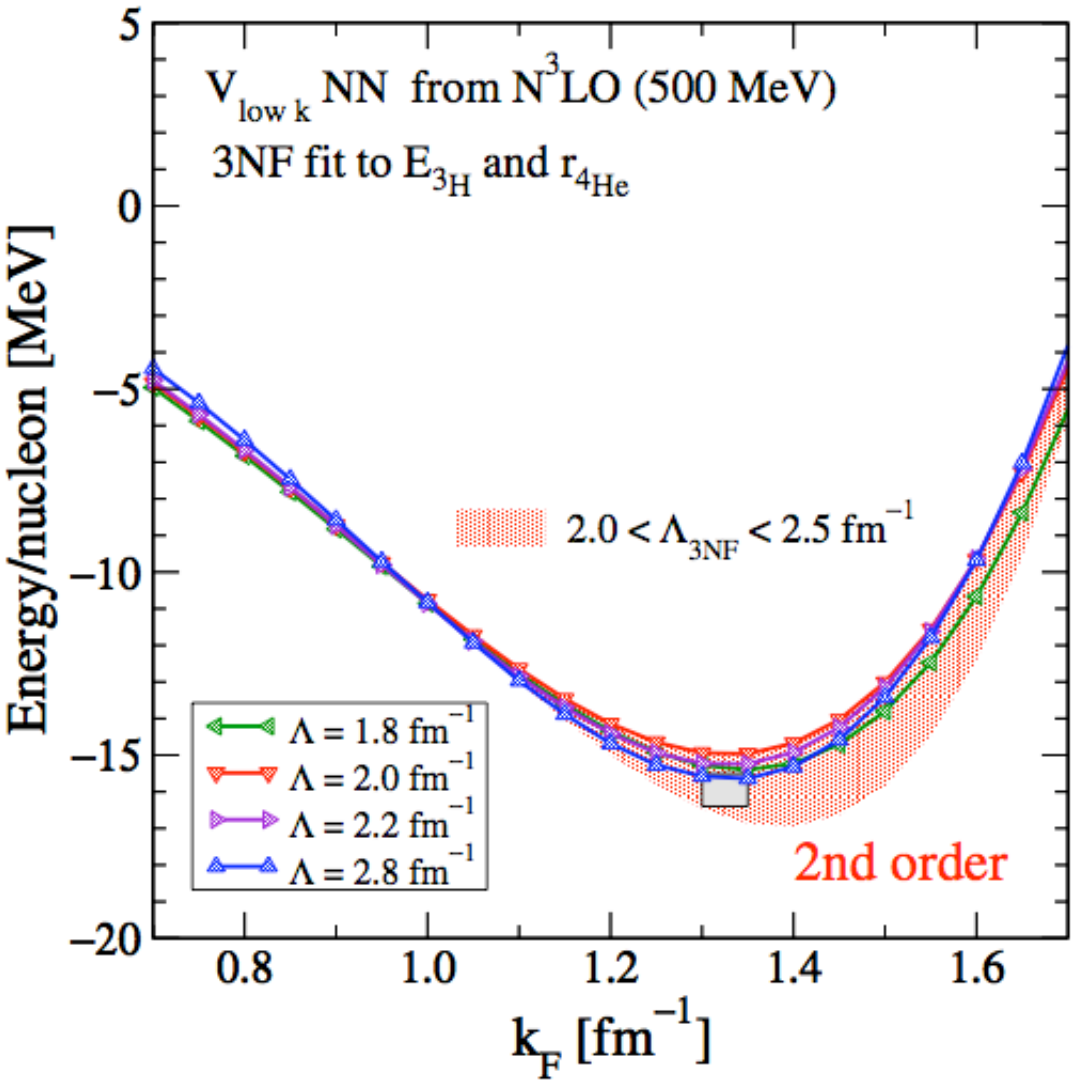
N^{2}LO 3NF fit to A =3,4 B.E. and ^{4}He radii

[A. Nogga]

self-bound w/ saturation

Loop expansion (perturbative) about HF becomes sensible

New low-momentum NNN fits and Nuclear Matter



Knobs to estimate Theoretical error bars:

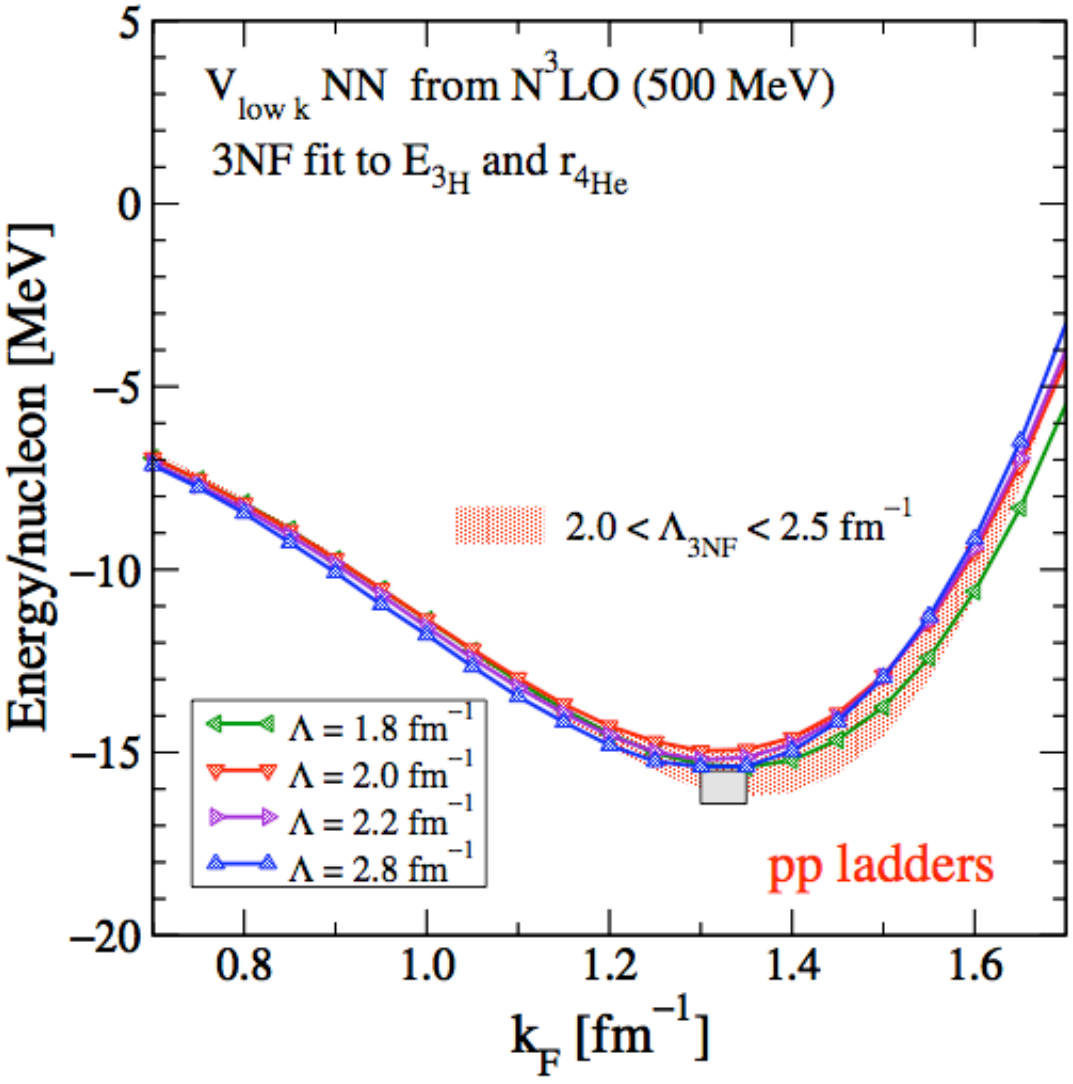
Λ-dependence => theoretical error bands (lower limit)

Assess the impact of large uncertainties in the c_i's appearing in 2- and 3-body TPEP

Vary the order of the underlying EFT

Sensitivity to many-body approximations

New low-momentum NNN fits and Nuclear Matter



To do: asymmetric matter

Ladder sum » 2nd-order

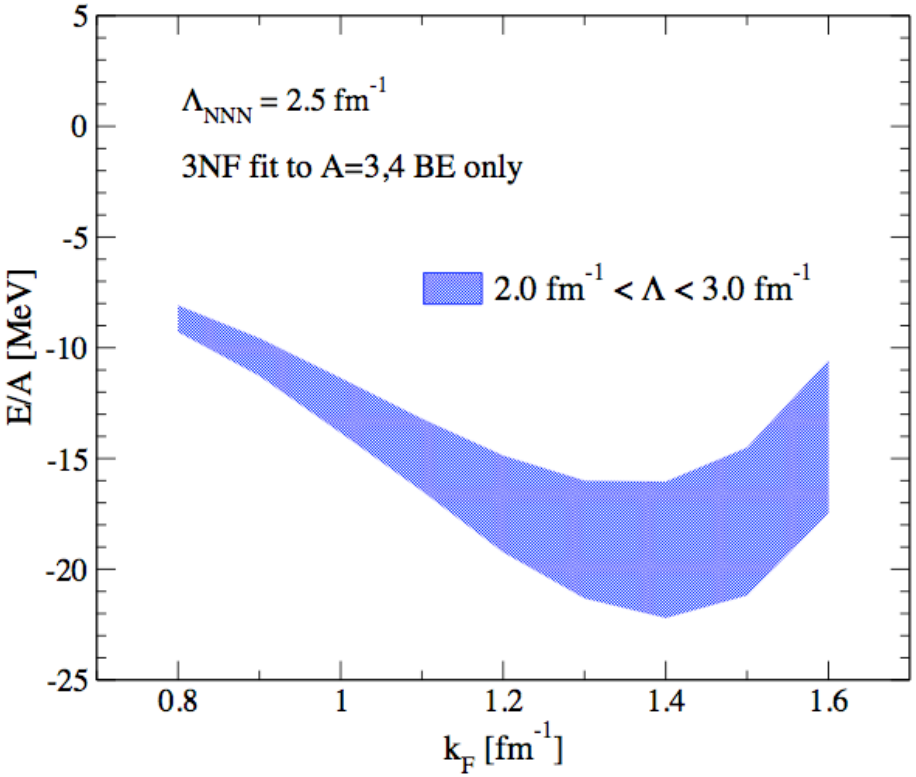
Excellent saturation w/out fine-tuning to nuclear matter

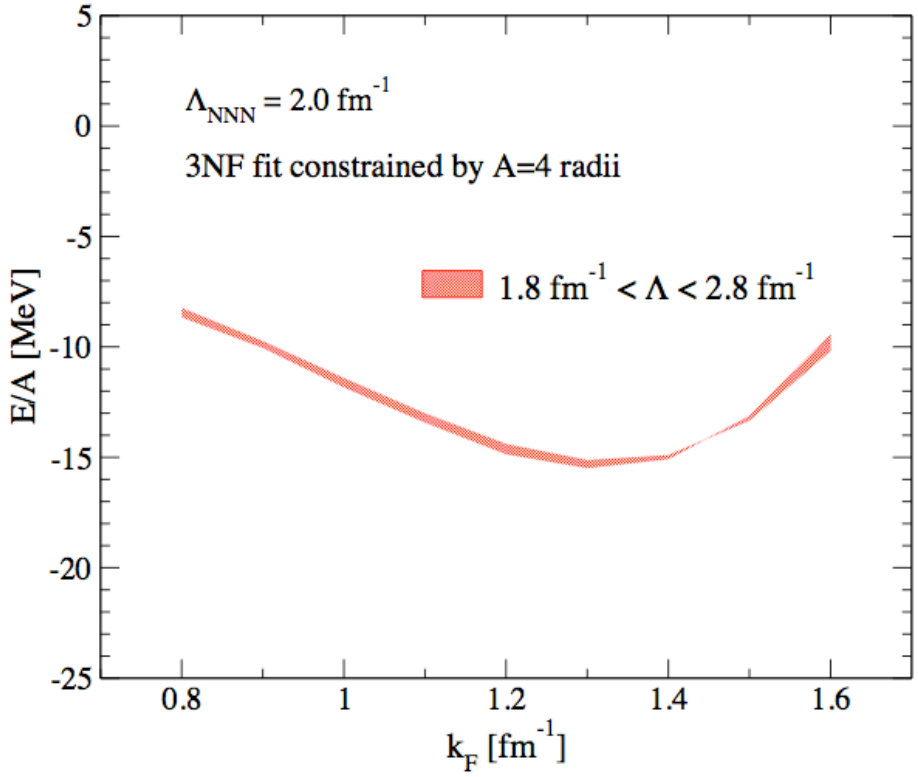
But…

1) V_{NNN} => $V_{2N}(r)$
2) HF propagators
3) Beyond 2-hole lines?
4) Angle-averaging
5) Particle-hole channel
6) …

Coupled-cluster calculations of nuclear matter, ^{16}O and ^{40}Ca would be a huge help!

Guidance from NM for fixing EFT couplings





Different Λ-dependence for the 2 ways of fitting the 3NF lec's

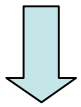
Supports suggestion of Navratil et al. to use ^{4}He radii to constrain fits of 3NF couplings (c_E and c_D)

Large uncertainties in extracting c_3, c_4 from πN and NN => use NM to constrain (sensitivity at the 2-3 MeV level)

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 [energies, densities, density matrices,...]



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

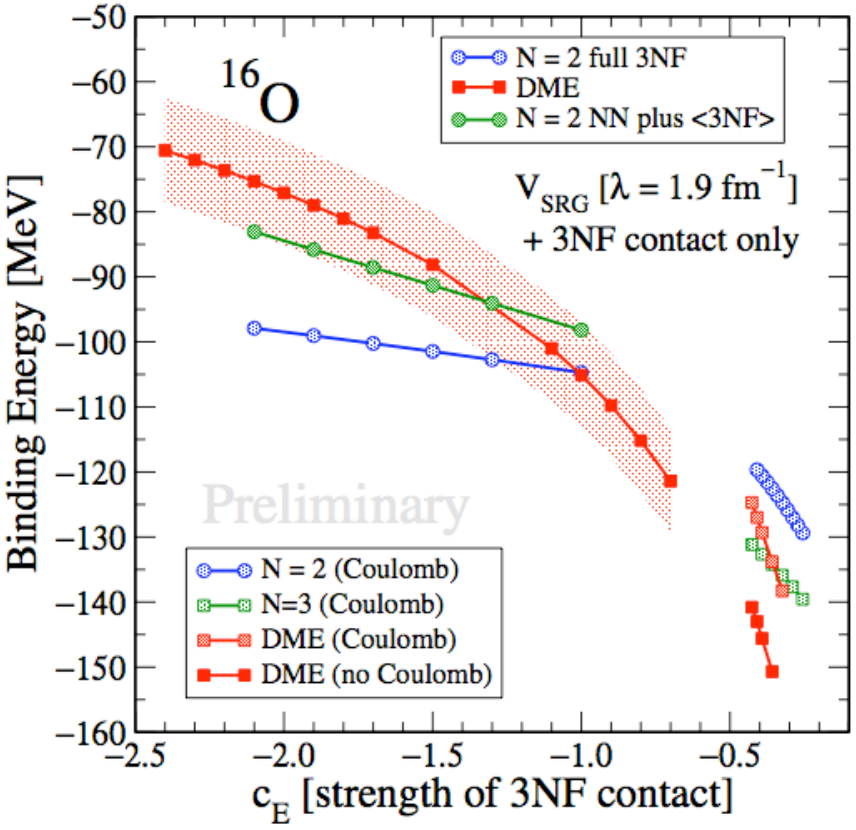
Are systematics reproduced by DME as we vary parameters (e.g., 3NF couplings, RG cutoff Λ, order of input EFT, ...) in H?

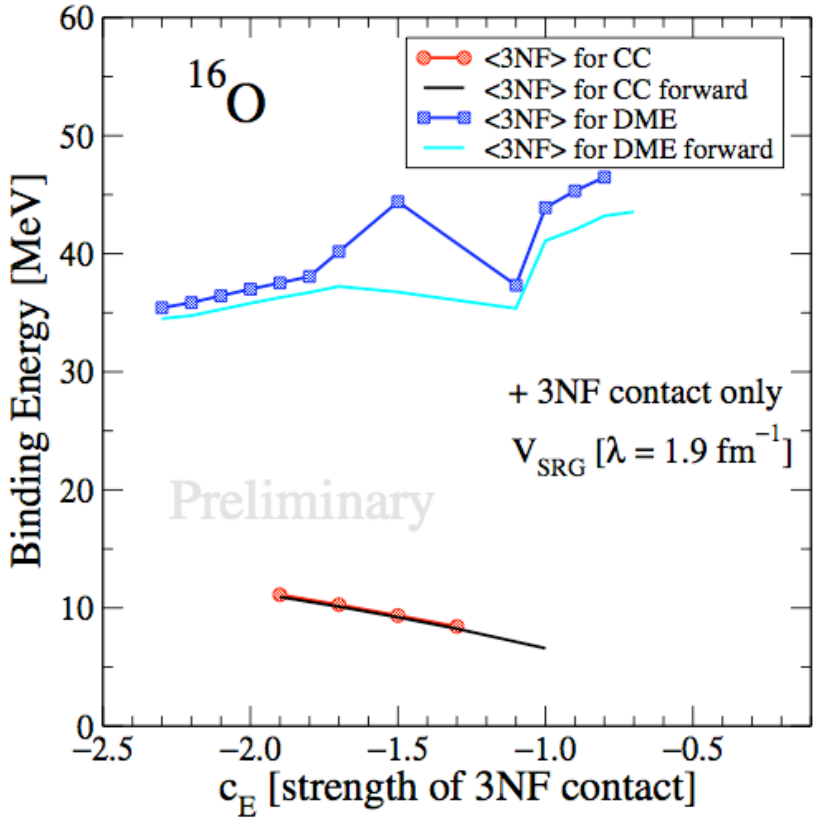
Is the many-body treatment of nuclear matter sufficient?

Early indications are that non-trivial extensions of the DME are needed [see B. Gebremariam and J. Drut later]

Comparison to ab-initio calculations

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



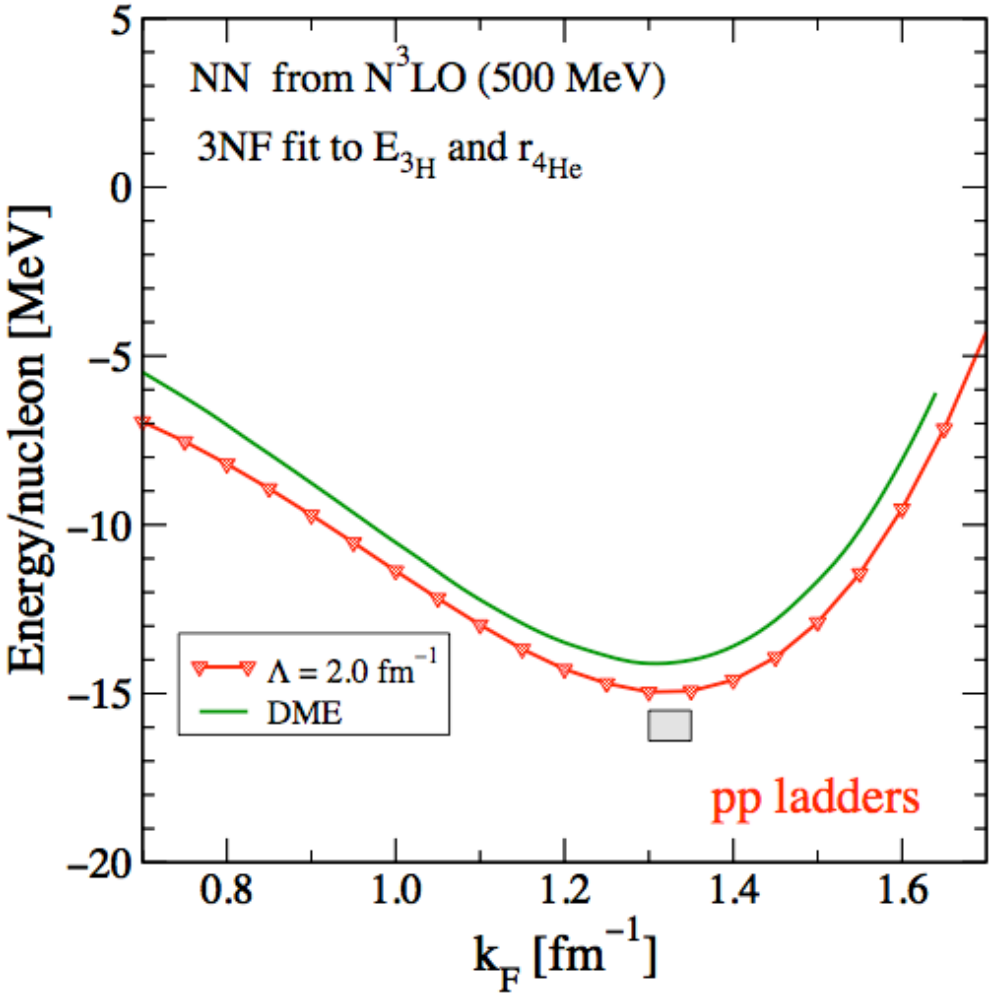


Quantitative and qualitative disagreement btw. coupled-cluster and DFT calculation. What is going on?

Possible Reasons for the Poor Agreement

1) DME averages out too much information

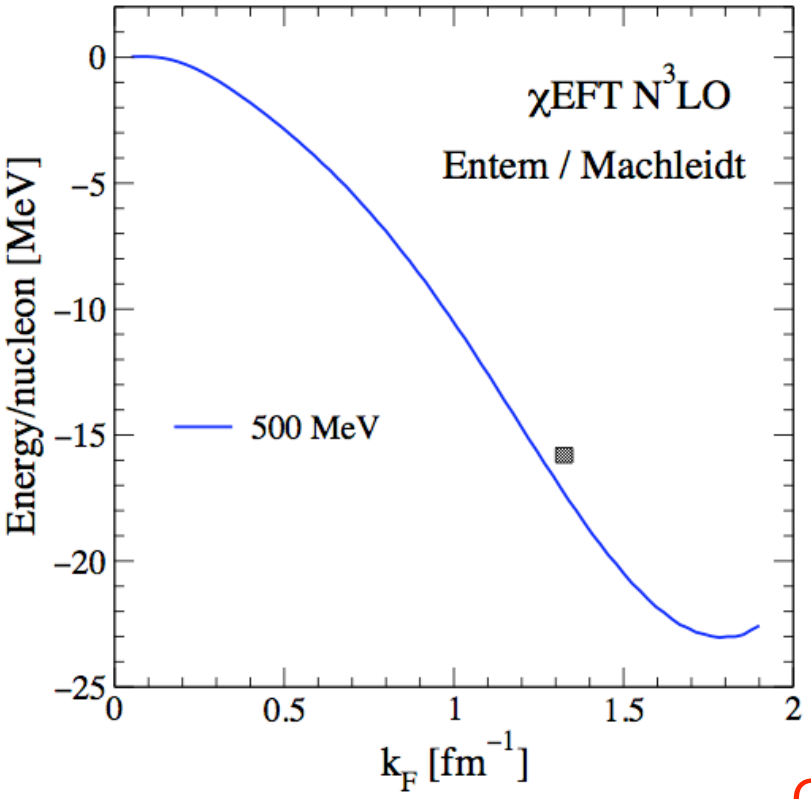
- COM P-dependence (spatial non-locality)
- energy-dependence



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

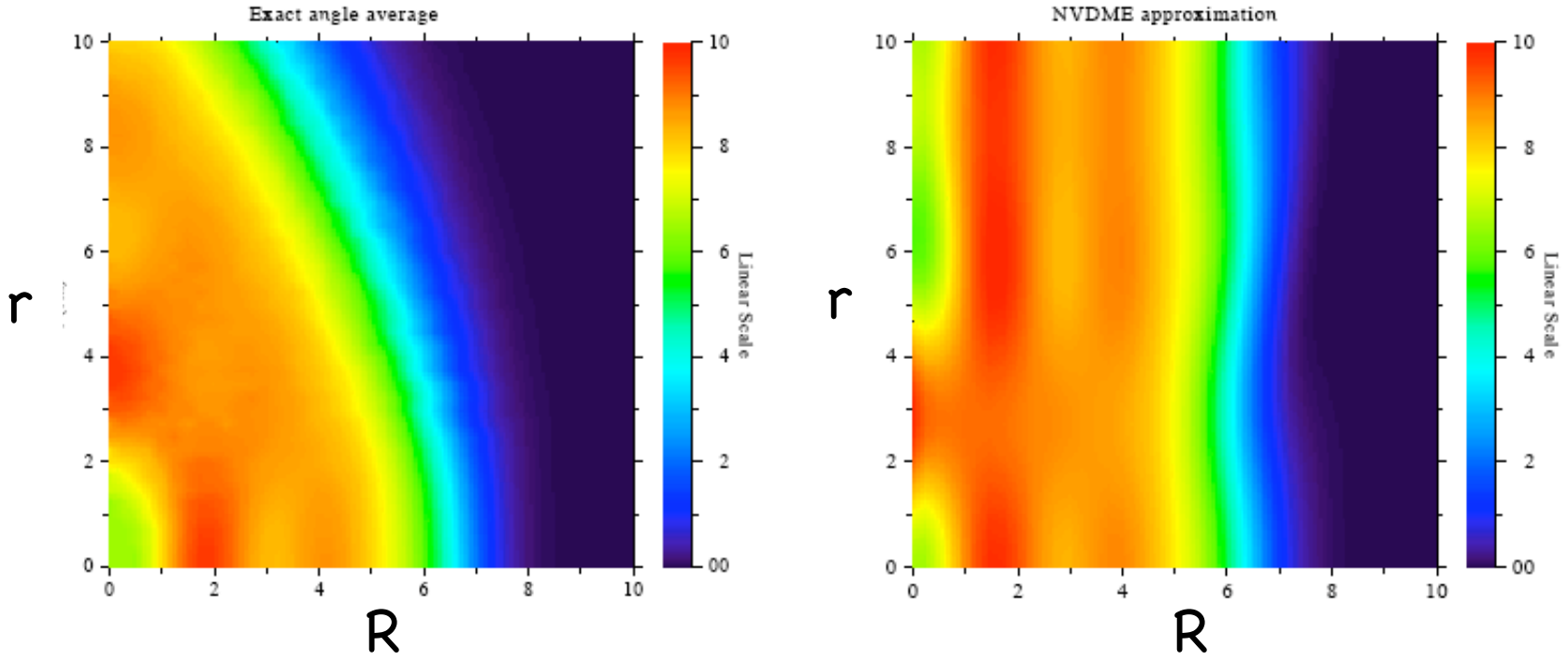
Gradients no longer "small" since DME = expansion about NM?

	O16		Ca40		Ca48	
	Coupled Cluster	DME	Coupled Cluster	DME	Coupled Cluster	DME
E/A	-6.72	-7.89	-7.72	-9.66	-7.40	-10.1
r_{ch}	2.73	2.47	3.35	2.95	3.24	2.84

Possible Reasons for the Poor Agreement

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

Exact $\rho(\mathbf{R}+\mathbf{r}/2)\rho(\mathbf{R}-\mathbf{r}/2)$ DME

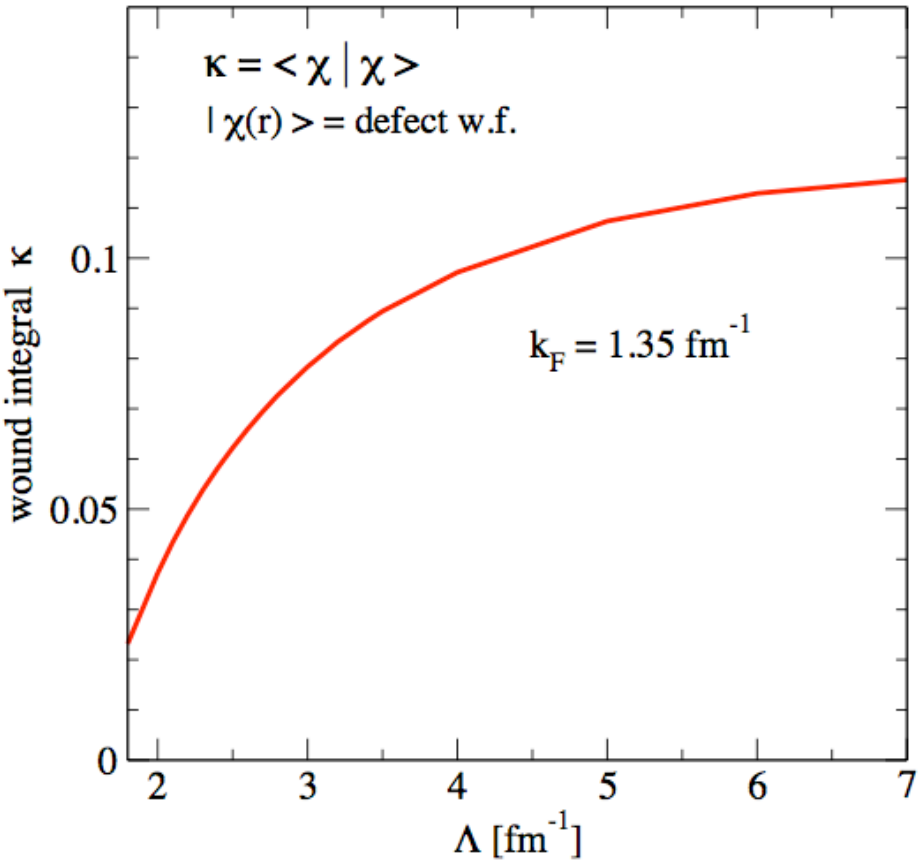


Treat Hartree exactly a-la Coulomb? [Negele and Vautherin, Sprung et al.]

* See B. Gebremariam's talk for the failings of the standard DME and possible solutions.

Possible Reasons for the Poor Agreement

4) Inadequacy of many-body approximations (I.e., LO Brueckner)



$$\frac{\delta E(3\text{hole}-\text{lines})}{E(2\text{hole}-\text{lines})} \sim \kappa$$

3-hole-line correction could contribute at the few MeV level, even at low Λ

Coupled-cluster NM calculation to assess H.O.T. would help!

5) Approximate treatment of 3NF $V_{3N} \rightarrow \mathrm{Tr}_3\left[V_{3N}\mathcal{A}_{123}\right] \approx \mathrm{Tr}_3\left[V_{3N}\right]$

6) Implementation errors in HFBRAD (rearrangement terms, etc.)

Long-range pion NN and NNN contributions to the EDF

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

$$\begin{aligned}\mathcal{E}^{\rho\rho} \equiv \sum_q \int d\mathbf{r} \Big[& A^{\rho\rho}\,\rho_q\rho_q + A^{\rho\Delta\rho}\,\rho_q\Delta\rho_q + A^{\nabla\rho\cdot\nabla\rho}\,\nabla\rho_q\cdot\nabla\rho_q + A^{\rho\tau}\left(\rho_q\tau_q - \mathbf{j}_q\cdot\mathbf{j}_q\right) \\ & + A^{ss}\,\mathbf{s}_q\cdot\mathbf{s}_q + A^{s\Delta s}\,\mathbf{s}_q\cdot\Delta\mathbf{s}_q + A^{\nabla s\circ\nabla s}\,\nabla\mathbf{s}_q\circ\nabla\mathbf{s}_q \\ & + A^{\rho\nabla J}\left(\rho_q\nabla\cdot\mathbf{J}_q + \mathbf{j}_q\cdot\nabla\times\mathbf{s}_q\right) + A^{\nabla\cdot s\nabla\cdot s}\left(\nabla\cdot\mathbf{s}_q\right)\left(\nabla\cdot\mathbf{s}_q\right) \\ & + A^{JJ}\Big(\sum_{\mu\nu} J_{q,\mu\nu}J_{q,\mu\nu} - \mathbf{s}_q\cdot\mathbf{T}_q\Big) + A^{JJ}\Big[\Big(\sum_{\mu} J_{q,\mu\mu}\Big)\Big(\sum_{\mu} J_{q,\mu\mu}\Big) + \sum_{\mu\nu} J_{q,\mu\nu}J_{q,\nu\mu} - 2\,\mathbf{s}_q\cdot\mathbf{F}_q\Big]\Big]\end{aligned}$$

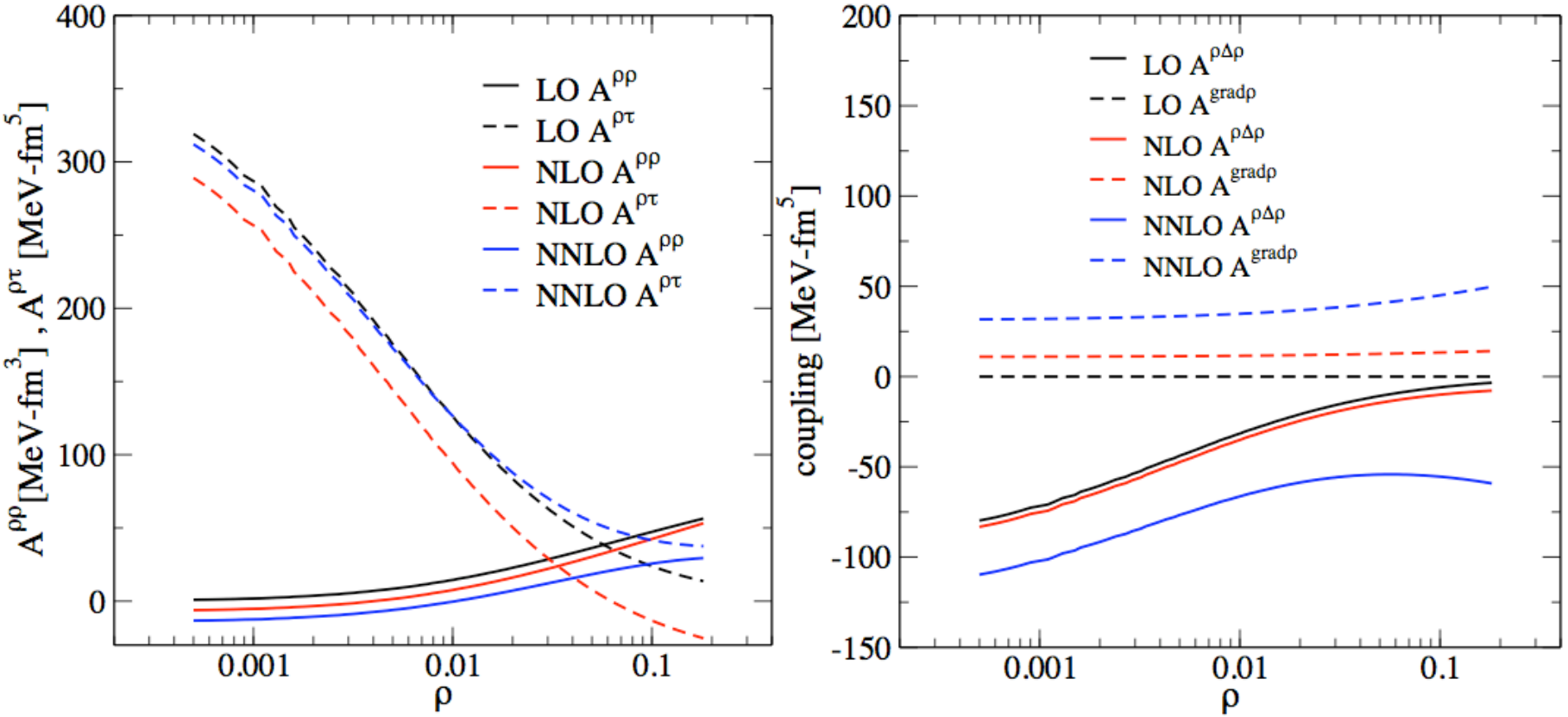
Each coupling function splits into 2 terms

1) Λ-**dependent** Skyrme-like coupling **constants**
2) Λ-**independent** coupling **functions** from pion physics with non-trivial density dependence

Suggests refitting extended Skyrme functionals with non-trivial density-dependence/isovector properties from pion physics

Sensitivity studies? Can we “see” the pion? Trends along isotopic chains?…

Long-range pion NN and NNN contributions to the EDF



Novel density-dependencies driven by 1π and leading 2π exchange

Longest range V <==> Strongest density dependence in EDF

⇨ 3NF 2π contributions will dominate novel density dependencies for spin-orbit terms (coming soon...)

Summary of Y2 Progress

1) New NNN fits for smooth V_{lowk} and V_{SRG}

- nuclear matter (good prelim. results, error bands, code available soon)
- coupled cluster checks of O16/Ca40 (and eventually NM) critical

2) First microscopic DFT comparisons to ab initio made

- CC/FCI calculations starting from same Hamiltonian for O-16, Ca-40, and Ca-48
- many-body approximations made and the DME (in original form) used to derive the EDF may be too crude
- see talks by B. Gebremariam and J. Drut for extensions/alternatives

3) Contributions of long-range pion physics to EDF derived

- NN terms through NNLO of chiral EFT derived and coded
- 3NF contributions to be finished soon
- generalized Skyrme functional in the near term (Stoitsov, Schunk)

See Furnstahl's talk for complete list of Y2/Y3 plans