

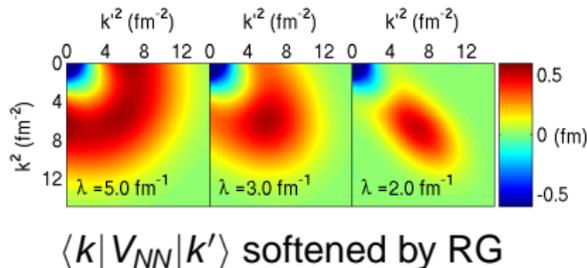
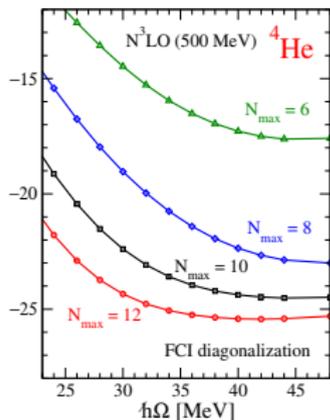
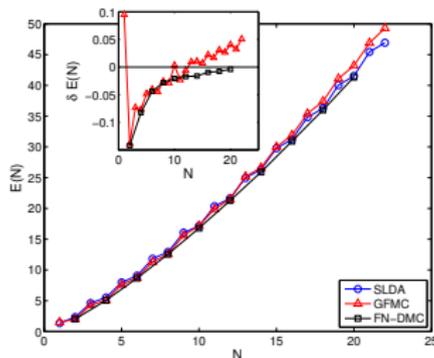
# Microscopic Input to Energy Functionals

R.J. Furnstahl [The OSU]

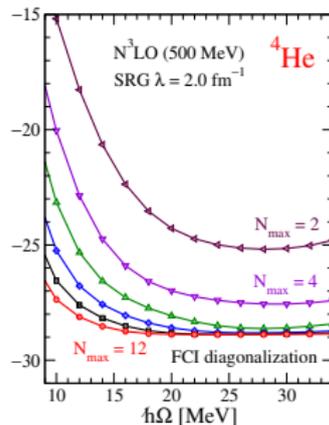
Paths to a Nuclear EDF

- Superfluid LDA as prototype for nuclear DFT
- Insight from neutron drops in external potentials (GFMC)

- **Here:** Constructive DFT from MBPT using chiral EFT and RG



$\langle k | V_{NN} | k' \rangle$  softened by RG



# Ab Initio DFT: Parallel Development

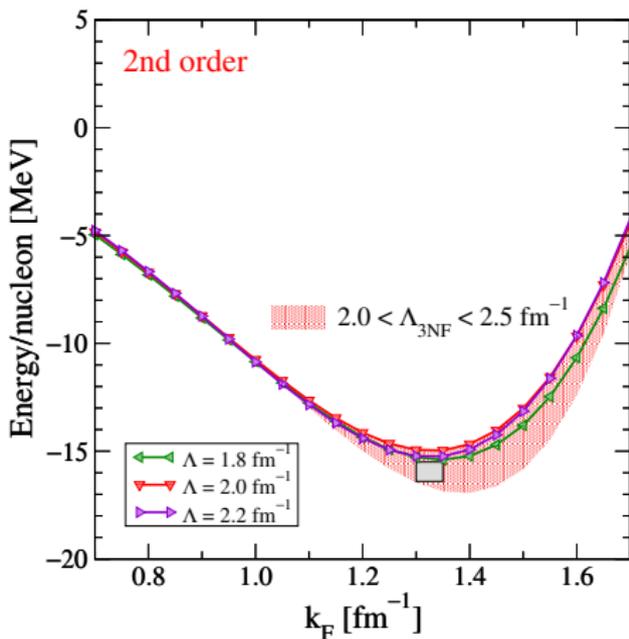
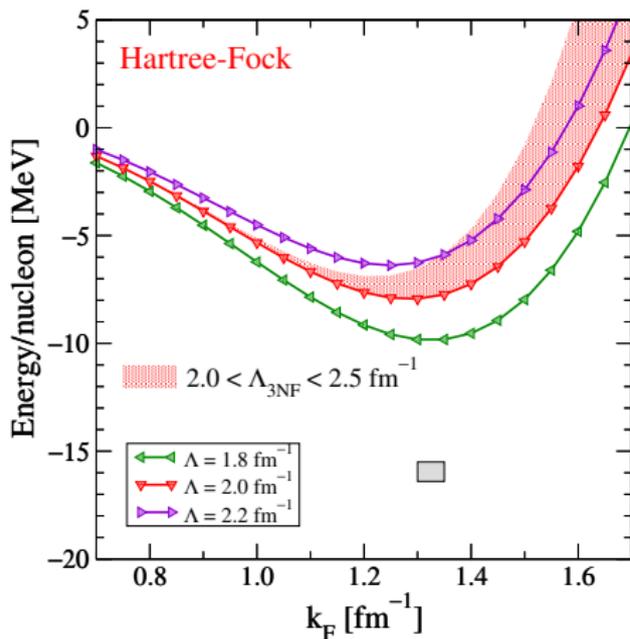
- 1 Momentum-space Renormalization Group (RG) methods to evolve chiral NN and NNN potentials to more perturbative forms as inputs to nuclear matter and ab initio wave function methods (Coupled Cluster; Full Configuration Interaction).
- 2 Controlled nuclear matter calculations based on the RG-softened interactions, as ab initio input to Skyrme EDF benchmarking and microscopic functional.
- 3 Approximate DFT functional, initially by adapting density matrix expansion (DME) including 3NF. Validate against CC, FCI.
- 4 Adaptation to HFB codes; allow for fine tuning. Test vs. data.

## Points of emphasis:

- Systematic upgrade path consistent with existing and developing technology for applying and extending DFT.
- Theoretical error bars on interaction (vary EFT  $\Lambda$  and order of calculation) and on implementation (vary SRG  $\lambda$  or  $V_{\text{low } k}$   $\Lambda$ ).

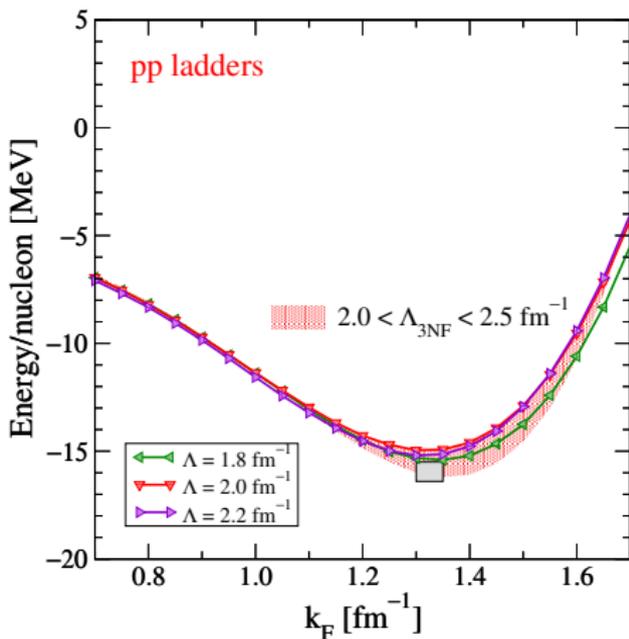
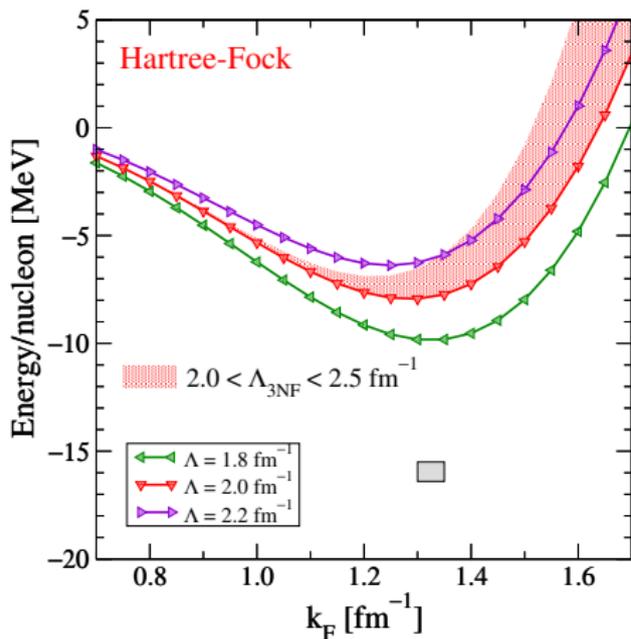
# Short-Term Roadmap for Microscopic Nuclear DFT

- Use a chiral EFT to a given order (e.g.,  $N^3\text{LO}$  below)
- Soften with RG (evolve to  $\Lambda \approx 2 \text{ fm}^{-1}$  for ordinary nuclei)
  - NN interactions fully, NNN interactions (3NF) approximately
- Generate density functional using DME in  $k$ -space



# Short-Term Roadmap for Microscopic Nuclear DFT

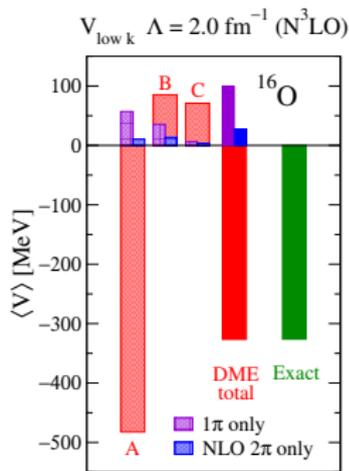
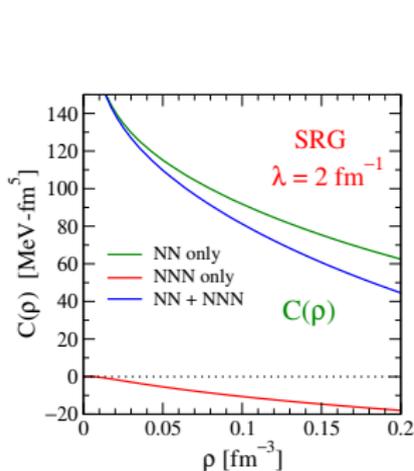
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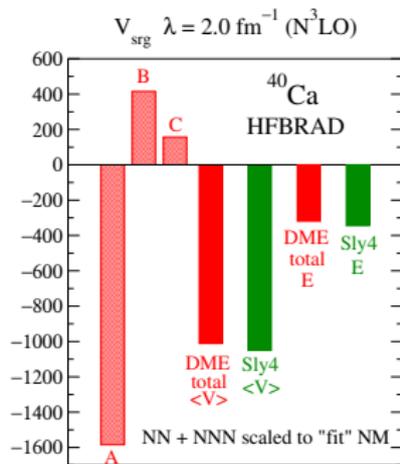
# Adaptation to Skyrme HFB Implementations

$$\mathcal{E}_{\text{Skyrme}} = \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \dots$$

$$\Rightarrow \mathcal{E}_{\text{DME}} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \dots$$



↔  
Tests

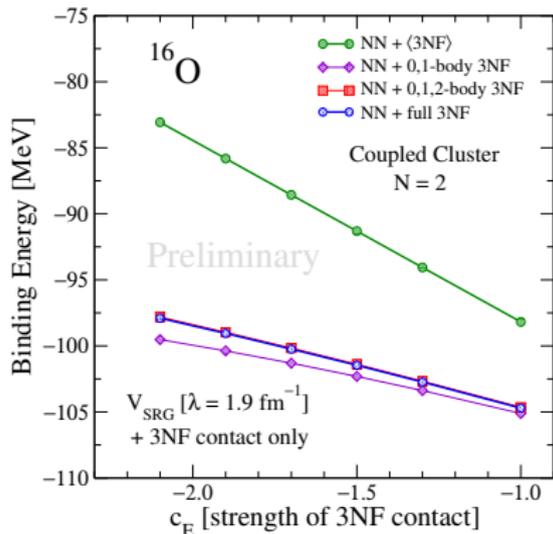


Density dependence: Finite-range pion terms vs. Skyrme-like  $C_n(\Lambda)k^{2n}$

# DFT Validation Against *Ab Initio* Calculations

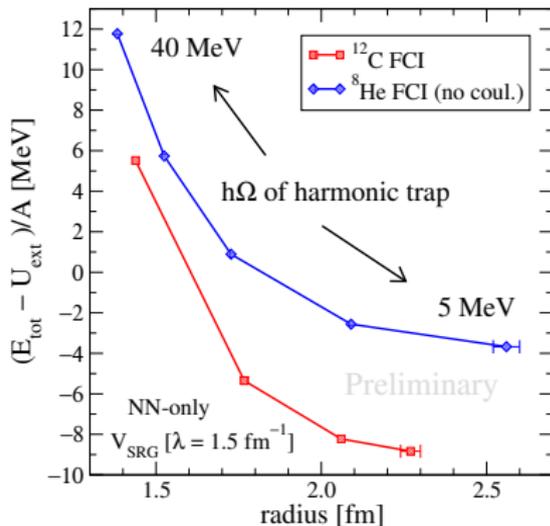
## “Coester Lines”

- Compare systematics, e.g., by varying 3NF coupling in Hamiltonian



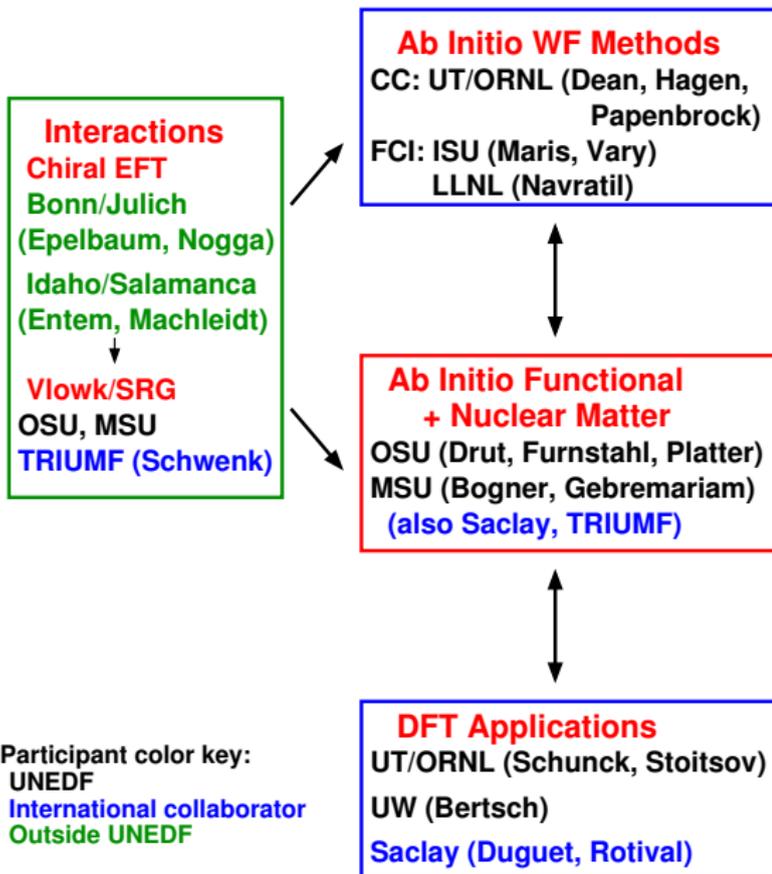
## External Potentials

- DFT from response of energy to perturbation of densities  $\implies$  Apply external fields



- Near future: Full 3NF, more external fields, other nuclei ...

# UNEDF Interconnections for Ab Initio Functionals



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