

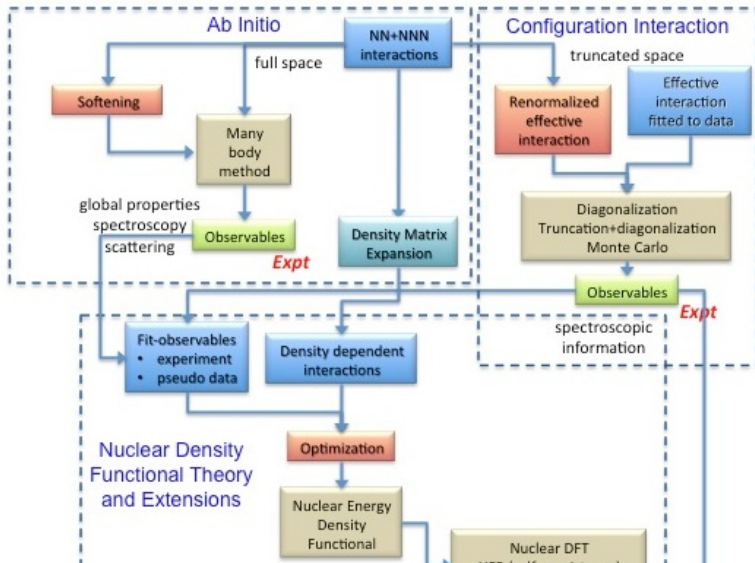
Ab Initio Functionals

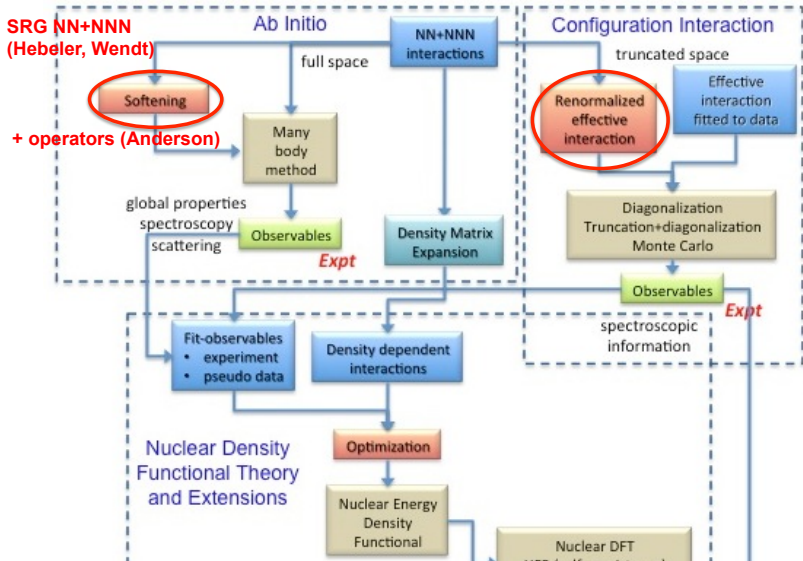
- overview
- status and plans

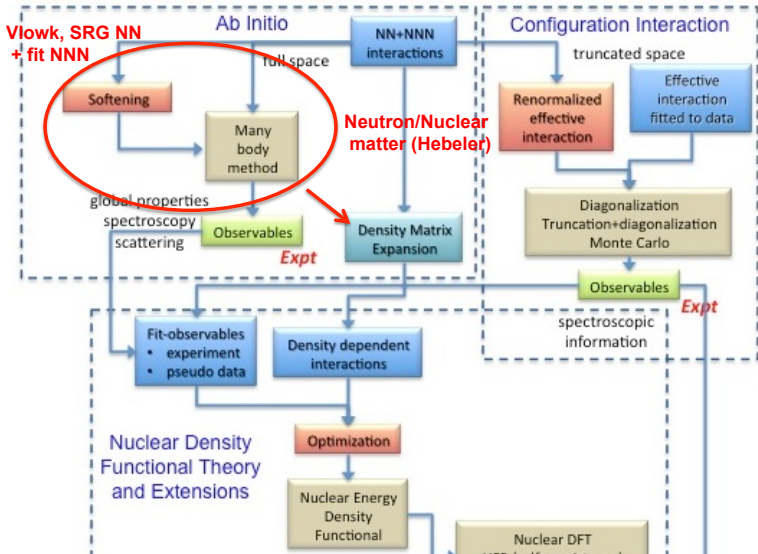
Role and Goals of the Ab Initio Functionals Group

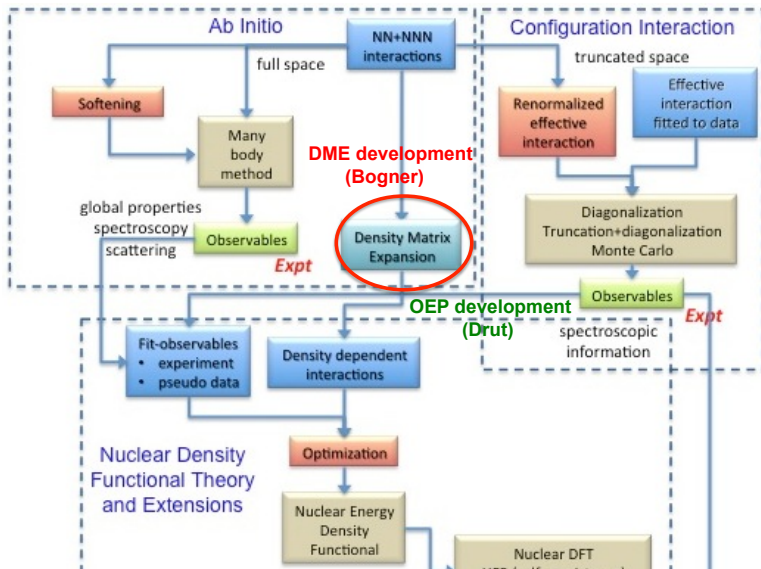
From last year's CPR: (previous talks) (today's talks)

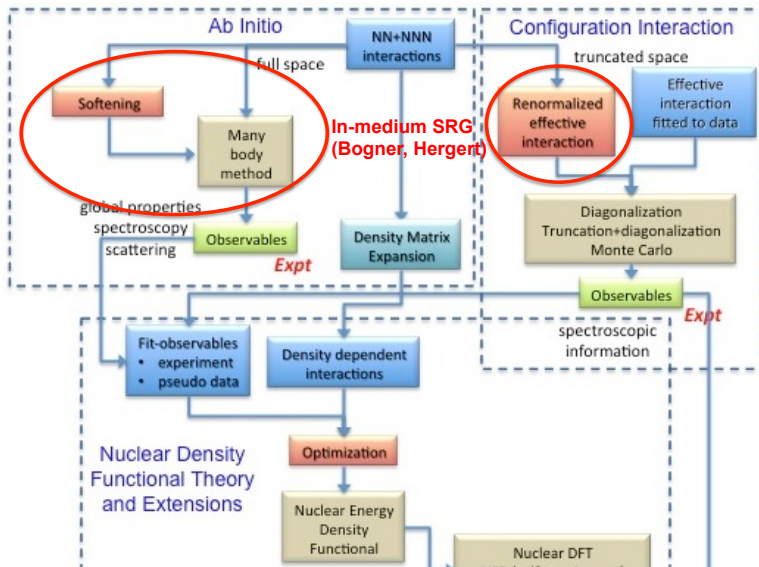
- Develop low-momentum NN and NNN interactions and operators as input to ab initio wave function methods and nuclear matter (Hebeler, Wendt, Anderson)
- Develop nuclear matter calculations with controlled theoretical errors as input to microscopic functionals (Hebeler)
- Construct ab initio functionals in the form of a generalized Skyrme interaction, with theoretical error bars, and understand conceptual issues (Drut, Bogner, Hergert)
- Validate the functionals against ab initio wave function methods (Maris, Kortelainen, Holt)
- Provide guidance to DFT Applications on novel density dependencies for EDF's based on microscopic input (Stoitsov, Hergert, Holt)

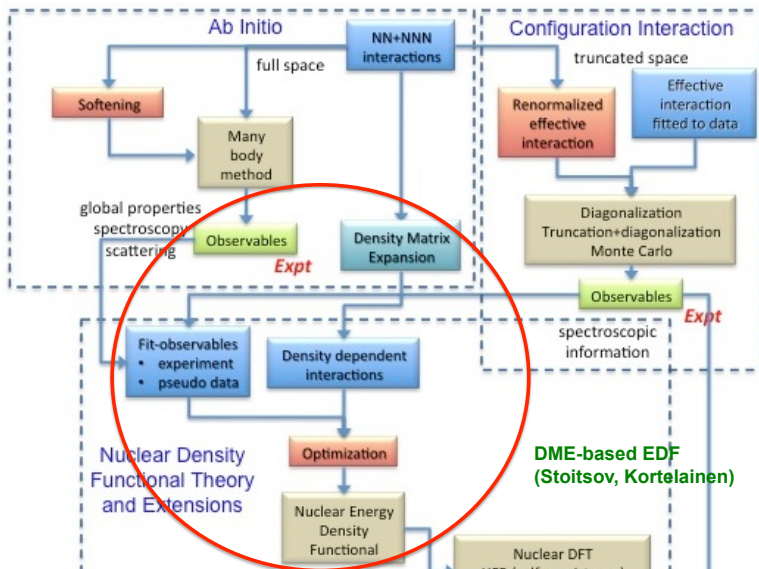


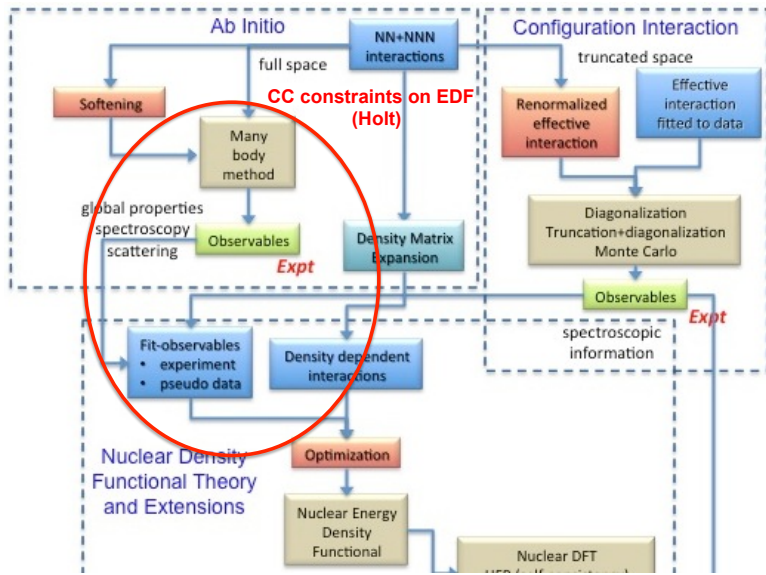












Progress reports in this session

- Kai Hebel, Neutron/nuclear matter with 3NF [Furnstahl]
- Kyle Wendt, SRG developments
- Eric Anderson, SRG-evolved operators
- Scott Bogner, In-medium SRG

Coffee break

- Heiko Hergert, HFB/DME and QRPA calculations
- Jason Holt, Constraints on explicit nuclear density functionals from coupled-cluster theory

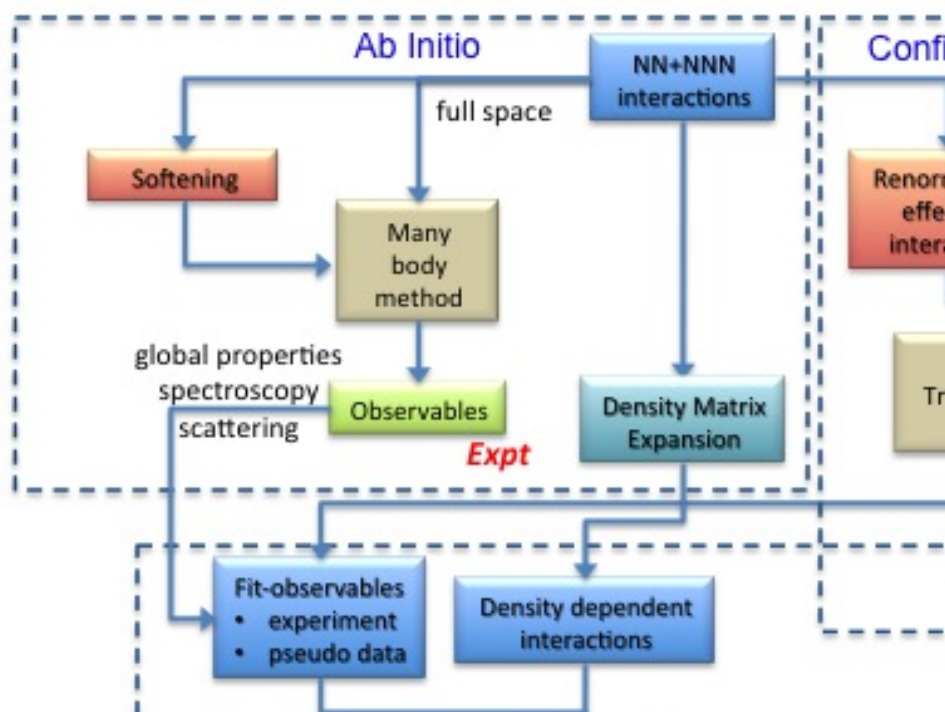
Ab Initio Nuclear DFT Deliverables

Plan for Year-5 from Continuation Progress Report

- Perform neutron drop benchmarks starting from NN and NNN interactions and validate against ab-initio calculations.
- Develop and test improved DME functionals that go beyond HF (microscopic pairing; constrain volume terms from BHF).
- Develop the Optimized Effective Potential (OEP) method for 3D-HFB; compare with HF, HF-DME, and ab initio.
- Use in-medium SRG to develop valence shell model Hamiltonians and effective operators for open-shell nuclei.

Other deliverables from CPR

- Apply $NN + NNN$ low- k SRG interactions in p-shell with NCFC
- SRG: develop few-body operators, test factorization, explore alternative generators to control many-body operators
- Improve and test infinite matter on which DME relies; initial steps toward Monte Carlo and CC calculations
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.



Ab Initio

full space

Many
body
method

Observables

Expt

NN+NNN
interactions

Density Matrix
Expansion

Density dependent
interactions

Configuration Interaction

truncated space

Renormalized
effective
interaction

Effective
interaction
fitted to data

Diagonalization
Truncation+diagonalization
Monte Carlo

Observables

spectroscopic
information

Expt

