

Role and Goals of the Ab Initio Functionals Group

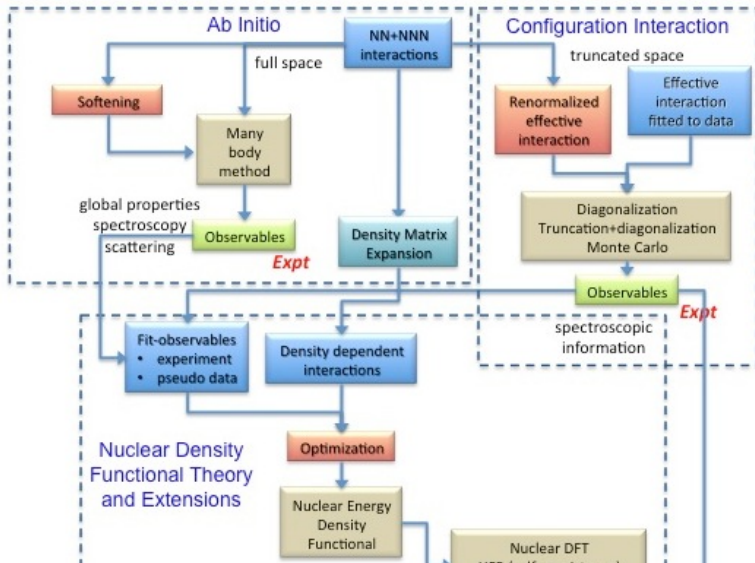
From last year's CPR: (previous talks) (today's talks)

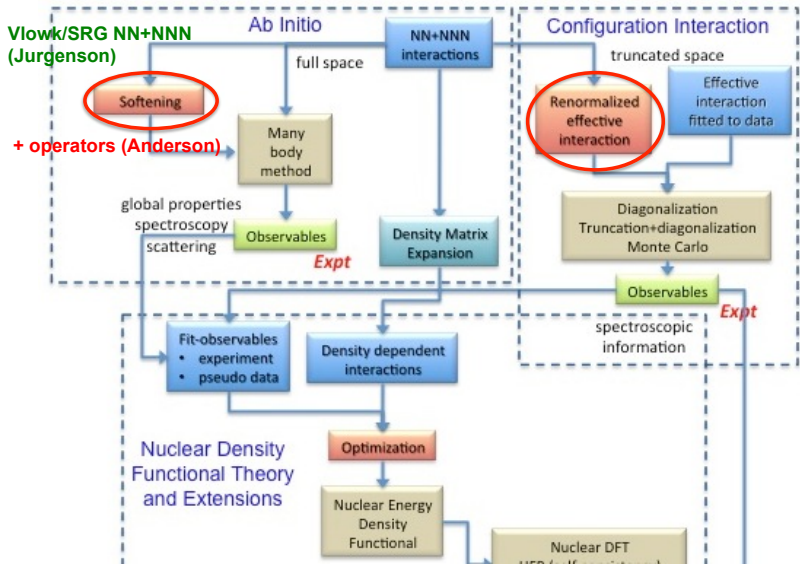
- Develop low-momentum NN and NNN interactions and operators as input to ab initio wave function methods and nuclear matter (Jurgenson, Anderson)
- Develop nuclear matter calculations with controlled theoretical errors as input to microscopic functionals (Hebeler, Hergert)
- Construct ab initio functionals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

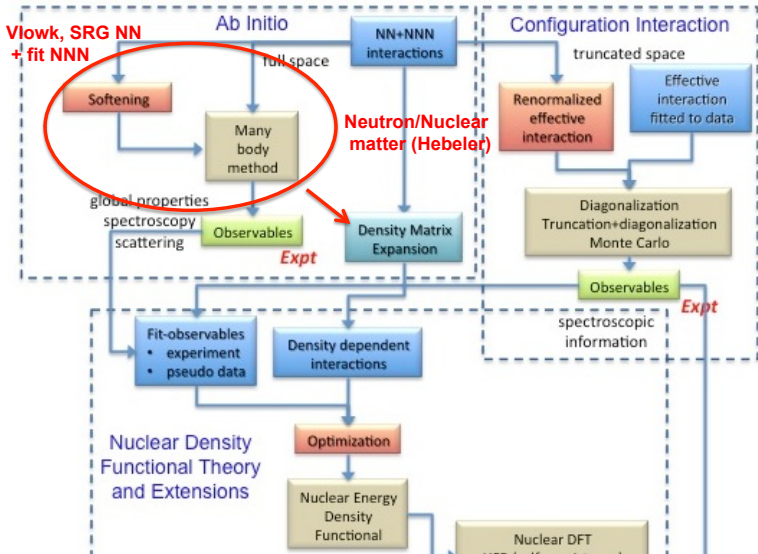
UNEDF junior personnel scorecard

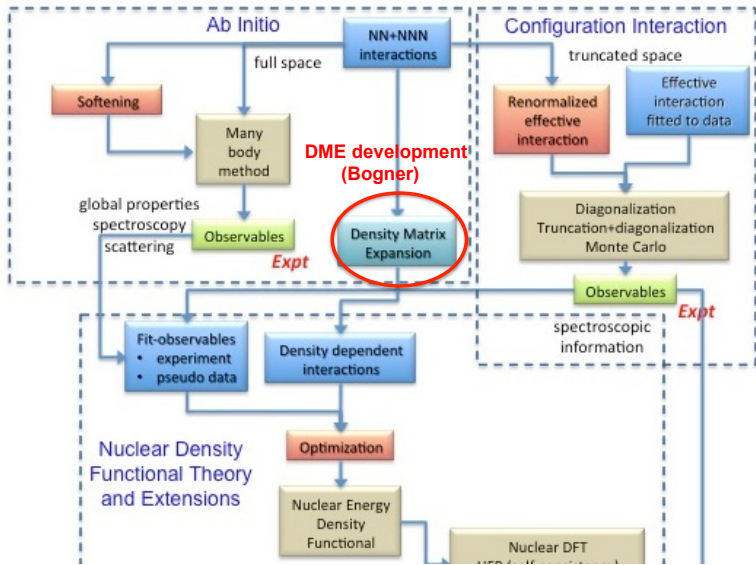
Ab Initio Functional division (and collaborators)

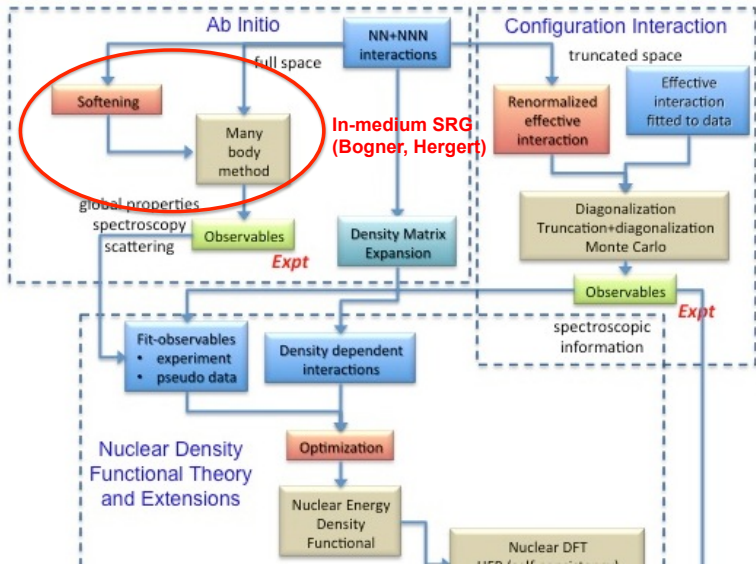
- Recent transitions
 - Biruk Gebremariam: MSU → SAS (5/2010)
 - Eric Jurgenson: OSU → LLNL (10/2009)
 - Lucas Platter: OSU → INT (10/2009)
- Upcoming transitions
 - Joaquín Drut: OSU → LANL (10/2010)
 - Kai Hebler: TRIUMF → OSU (9/2010)
- Metastable
 - Eric Anderson: OSU
 - Heiko Hergert: MSU
 - Markus Kortelainen: ORNL

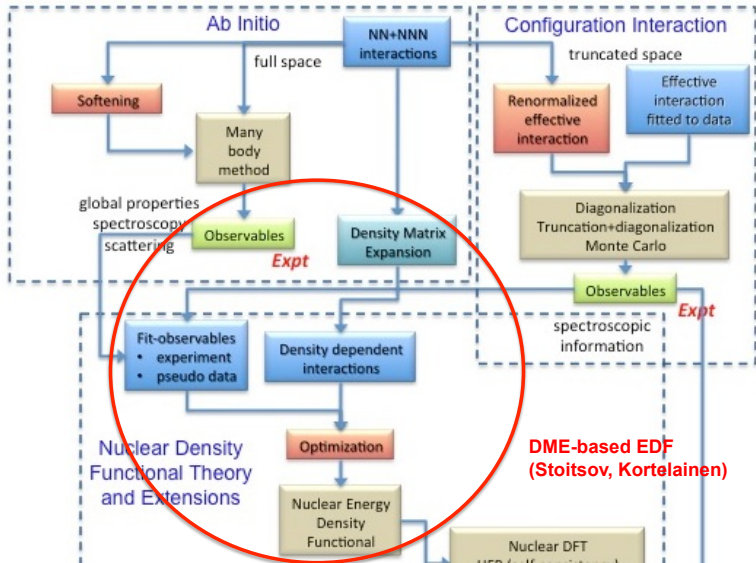












Ab Initio Nuclear DFT Deliverables

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

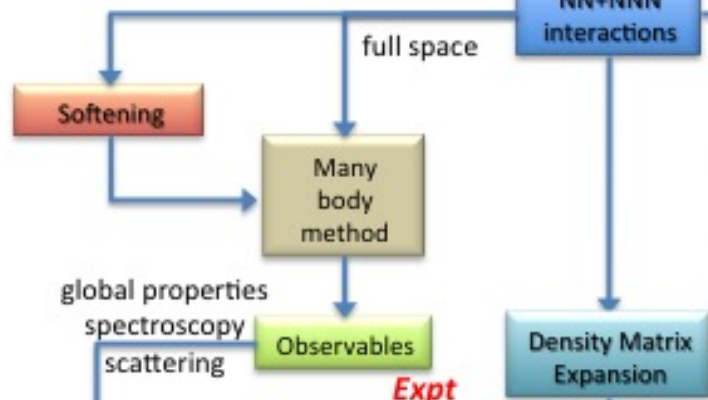
Other deliverables from CPR

- Low- k interactions: evolve, test, export evolved 3D 3NF and evolve operators
- Improve and test nuclear matter on which DME relies
- Upgrade and validate the DME implementation
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
- In-medium SRG: Further closed-shell nuclei and ph channels in nuclear matter
- Develop and test a refit Skyrme functional including universal long-range DME parts

Talks in this session

- Eric Anderson, SRG-evolved operators
- Kai Hebeler, Neutron/nuclear matter with 3NF
- Scott Bogner, DME expansions and in-medium SRG
- Heiko Hergert, In-medium SRG for infinite matter
- Mario Stoitsov, DFT calculations with DME-based EDF
- Markus Kortelainen, Fortran module for density dependent parts of EDF

Ab Initio



Fit-observables
• experiment
• pseudo data

Density dependent interactions

Con

Renormalization
effective interactions

