

# Role and Goals of the Ab Initio Functionals Group

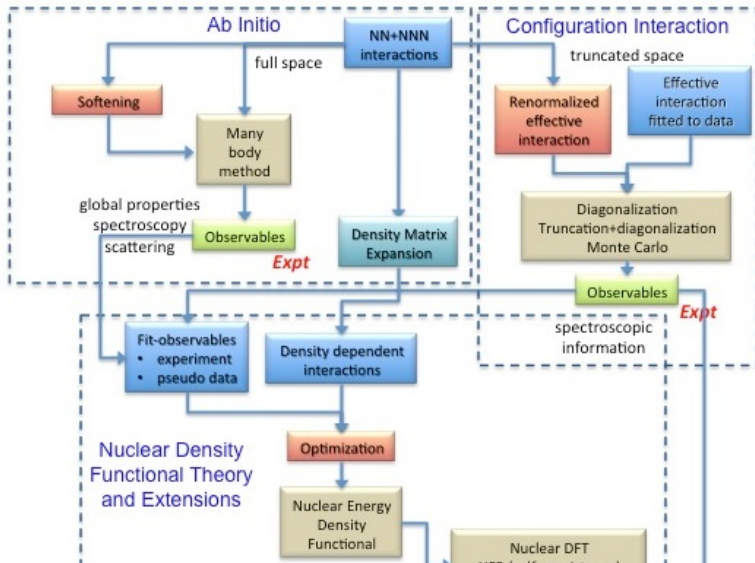
From last year's CPR: (previous talks) (today's talks)

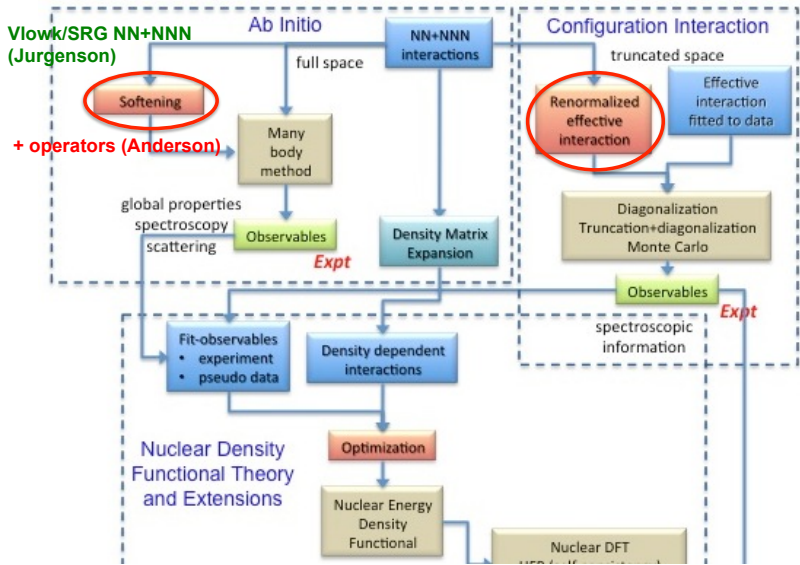
- Develop low-momentum NN and NNN interactions and operators as input to ab initio wave function methods and nuclear matter (Jurgenson, Anderson)
- Develop nuclear matter calculations with controlled theoretical errors as input to microscopic functionals (Hebeler, Hergert)
- Construct ab initio functionals 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)

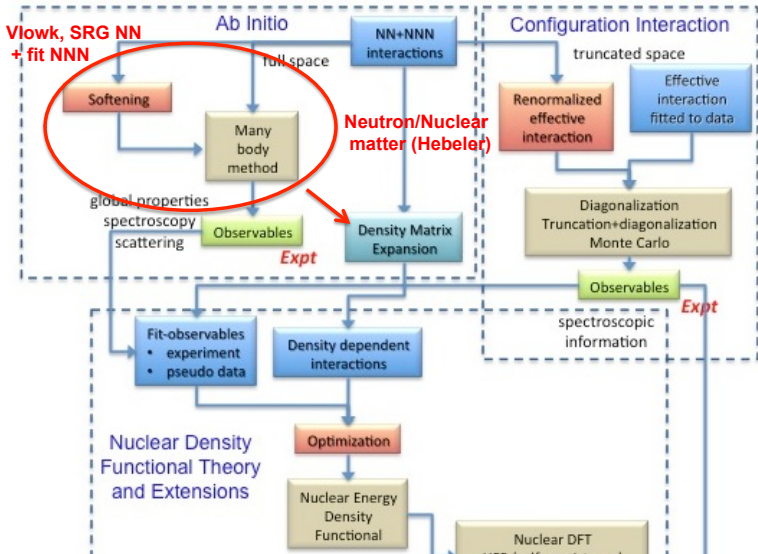
# UNEDF junior personnel scorecard

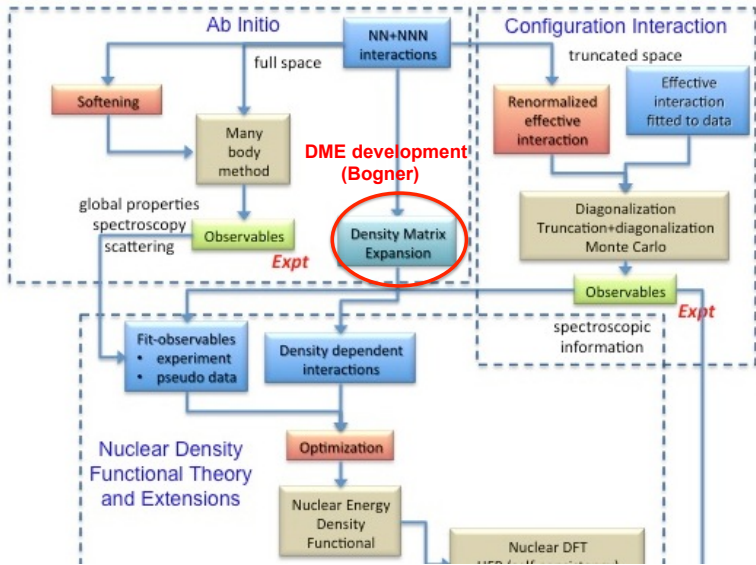
## Ab Initio Functional division (and collaborators)

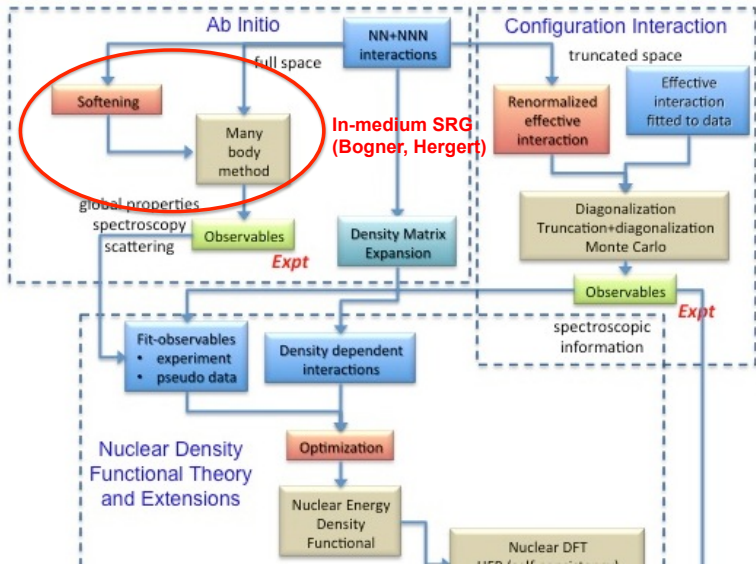
- Recent transitions
  - Biruk Gebremariam: MSU → SAS (5/2010)
  - Eric Jurgenson: OSU → LLNL (10/2009)
  - Lucas Platter: OSU → INT (10/2009)
- Upcoming transitions
  - Joaquín Drut: OSU → LANL (10/2010)
  - Kai Hebler: TRIUMF → OSU (9/2010)
- Metastable
  - Eric Anderson: OSU
  - Heiko Hergert: MSU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



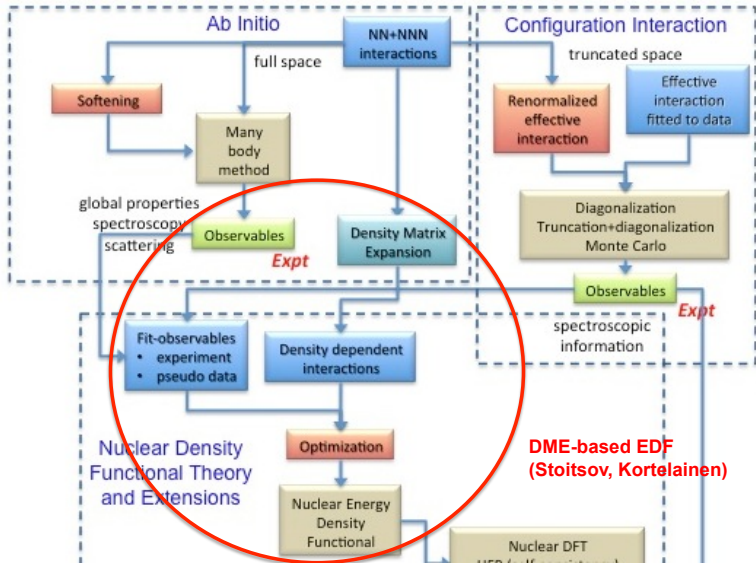












# Ab Initio Nuclear DFT Deliverables

## Plan for Year-4 from Continuation Progress Report

- Extend DME and validate against ab initio calculations. Initial work toward  $^{40}\text{Ca}$  DME comparisons
- Further development of  $\pi$ -DME functionals; include pairing
- Continue development and testing of orbital-based DFT

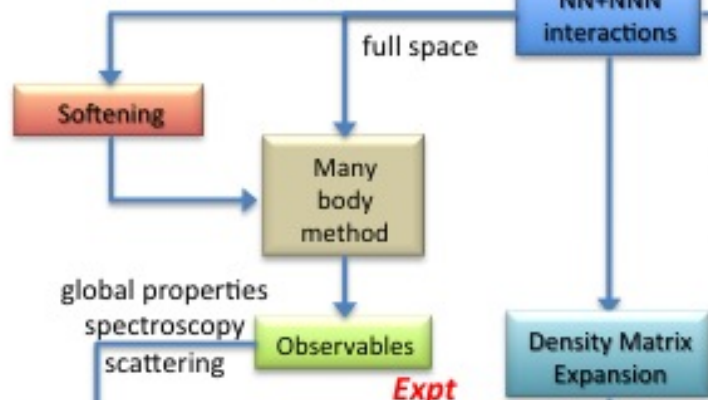
## Other deliverables from CPR

- 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

