SciDAC Collaboration: UNEDF

The NuShellX Configuration Interaction Codes

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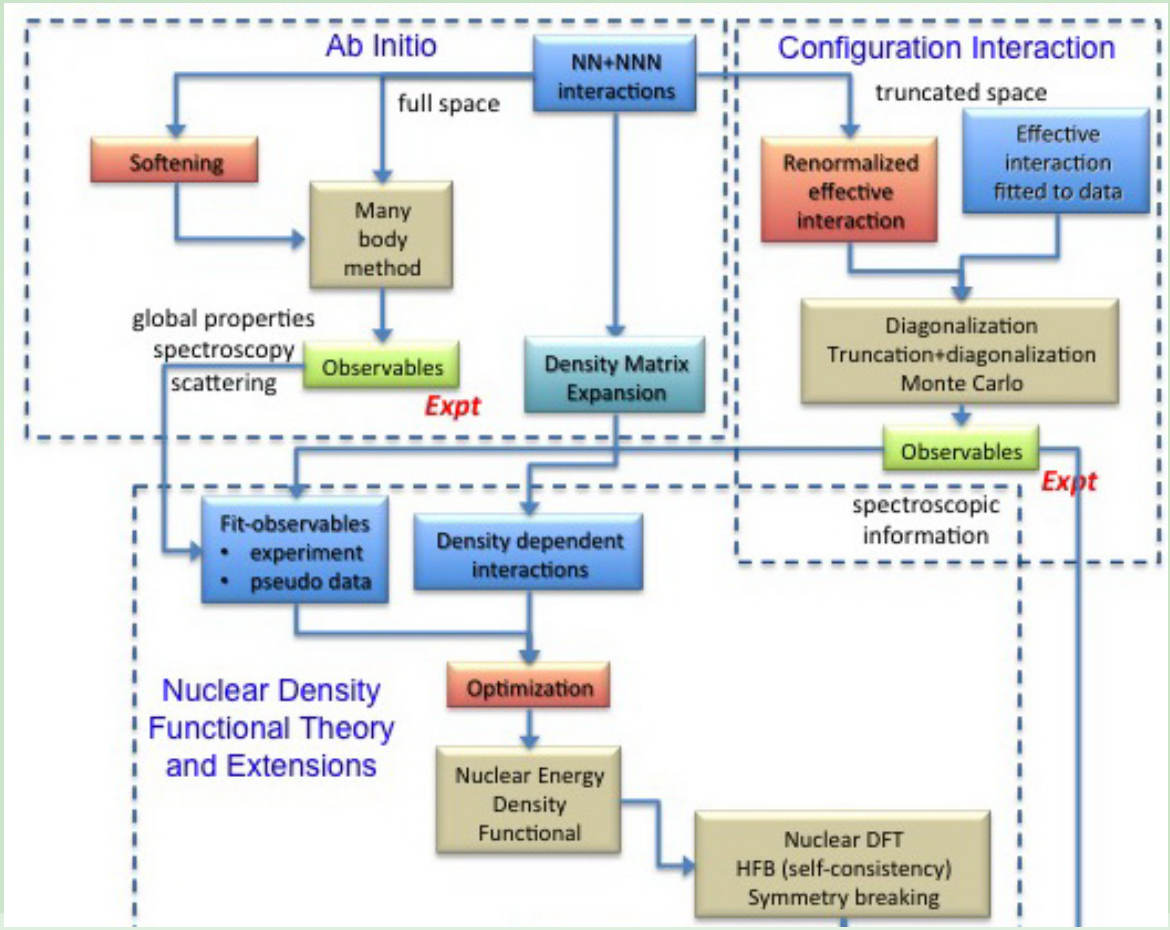
What is UNEDF?

- UNEDF: Universal Nuclear Energy Density Functional
- Density functional theory for the nucleus.
- Looking for predictive power that can scale to heavy nuclei.
- A universal density functional is still being sought.

Schematic: UNEDF Program



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What is NuShellX?

- A set of shell model configuration interaction (CI) codes.
  - Matrix elements calculated on-the-fly.
  - OpenMP-parallelization of Lanczos solvers.
- CI codes, DFT codes, and ab initio codes complement one another in various ways. Hence the desire to further develop this CI code.

Challenges

- The size of the configuration space for CI codes becomes very large at the fp shells and beyond.
- Some mitigation can be achieved algorithmically. Thick Restart Lanczos, for example.
- Codes also need to scale well to take advantage of massive parallelization.

Questions?

Shameless Plug

- The Institute for Cyber Enabled Research at Michigan State is looking for a few good research specialists.
- Must have a Ph.D. and experience in computational science.
- Not my position, but feel free to talk to me for more information during the workshop....

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