SciDAC Collaboration: UNEDF
The NuShellX Configuration Interaction Codes
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.
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?
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....