UNEDF-TOPS eigensolver collaboration:
Breakthrough nuclear science

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About the graphics:

- The plot in the upper left hand corner shows a 2D slice of a 3D harmonic oscillator basis function used in defining the basis space.
- The plot in the center shows the reductions in execution time for different versions of MFDn on NERSC's Franklin using 4,950 cores. The vertical axis gives the Wallclock Times.
- The plot in the lower right corner shows the latest strong scaling tests on NERSC's Franklin. The vertical axis gives the Aggregated Times of All Cores.

This is a collaboration between TOPS and UNEDF ("Universal Nuclear Energy Density Functions").

UNEDF is a SciDAC project. Its vision is to arrive at a comprehensive and unified description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons. In particular, an ab initio approach is used to understand the dynamics of nucleons. The calculations are performed using MFDn (Many-Fermion Dynamics), a parallel code for configuration interaction modeling in a harmonic oscillator basis (see figure in upper left corner). Collaboration among Physics, Applied Mathematics, and Computer Science has resulted in critical improvements in MFDn by a factor of 3-6 on the Cray XT-4 at NERSC and XT-5 at ORNL.

Improvements in MFDn include the development of new discrete and combinatorial algorithms for manipulating the sparsity of the Hamilton; the incorporating of new data structures for the Lanczos iterations; and enhanced inner loop and I/O performance.

The figure in the center shows the reductions in execution times of a number of versions of MFDn, running on a standard test case using 13C with 2-body and 3-body potentials. Here, V10-B05 (April 2007) is the pre-SciDAC version and V12-B09 is the latest production version. The times reported are Wallclock Times on NERSC's Franklin using 4,950 cores.

The figure in the lower right corner shows the excellent behavior of MFDn in a strong scaling test on 3,000 to 8,000 cores using the NERSC Franklin system. The times reported are the Aggregated Times of All Cores. The curve labeled V13 is the latest code that uses hybrid OpenMP/MPI, which gives slightly better performance.

On-going simulations show that MFDn runs efficiently on 30,000 cores and above on ORNL's Cray XT-5.

The latest production version of MFDn was used in advanced simulations to predict the properties of ^{14}F, an exotic nucleus with an extreme proton to neutron ratio, not previously discovered. The properties of this "beyond proton drip line" nucleus present significant constraints on theories of strong interactions and is an example of exotic nuclei that will be measured at the planned DOE facility for rare isotope beams. Texas A&M is attempting to measure this nucleus using their newly upgraded cyclotron. Computing the 15 lowest eigenstates using the improved MFDn for ^{14}F requires about 3 hours using 30,504 cores on the Cray XT-5 at ORNL. This would have taken at least 18 hours using previous versions of MFDn.

This collaboration involves Lawrence Berkeley National Laboratory (Esmond G. Ng, Philip Sternberg, Chao Yang), Iowa State University (Pieter Maris, James Vary), and Ames Laboratory (Masha Sosonkina).