Computing Masses of Atomic Nuclei

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References:
[1] "Axially deformed solution of the Skyrme–Hartree–Fock–Bogolyubov equations using the transformed harmonic oscillator basis. The program HFBTHO (v1.66p)" M.V. Stoitsov, J. Dobaczewski ,W. Nazarewicz, P. Ring, Comput. Phys. Commun. **167** (2005) 43–63
[2] http://orph02.phy.ornl.gov/workshops/lacm08/UNEDF/database.html
[3] http://massexplorer.org/
[4] J. Dobaczewski, *et al*., Comput. Phys. Commun. **180** (2009) 2361

About the graphics:
Top-Left: Deviations between theoretical and experimental nuclear masses for the SLy4 parameterization of the Skyrme energy functional. Calculations are performed with the HFBTHO solver [1] at the Hartree-Fock-Bogoliubov level with a contact pairing interaction in a harmonic oscillator basis of 20 full shells.
Bottom-Left: Same as Top-Left figure for the UNEDFpre parameterization of the Skyrme energy functional.
Bottom-Middle: Convergence of the POUNDERs model-based optimization algorithm as function of compounded CPU-time, compared to a Nelder-Mead approach, on the 12-parameter fit of the Skyrme energy functional.
Bottom-Right: Illustration of the interpolation of the multi-dimensional surface (in parameter space) in model-based algorithms

What was accomplished:
We have developed and applied a new model-based method to the problem of functional optimization in the nuclear Density Functional Theory (DFT). In DFT, energy functionals depend on a number of free parameters that must be adjusted to experimental data. The computational cost of this adjustment (optimization) can be very high, since the time of calculation of one nucleus only can reach a few hours in specific configurations: this is why until now all optimization strategies were restricted to data in spherical nuclei only. Model-based optimization methods rely on the minimization of a trial, or surrogate, model which is a local approximation to the exact function. We have found that such approaches provide significant reductions in the required number of function evaluations and yield better solutions: previous methods were unable to find an acceptable solution in 2160 CPU-hours while our new method found one in $\sim$ 200 CPU-hours. This development therefore makes possible the calibration of expensive simulations, such as DFT optimization problems using non-spherical nuclei. The parameterization UNEDFpre of the Skyrme energy functional that we have obtained correctly reproduces many

features of ground-state properties of atomic nuclei and closely approaches the predicted quality limit of Skyrme DFT.

The impact this accomplishment will have on science, computing, energy, or the environment:
Improving the accuracy and precision of DFT is the core of the UNEDF effort and will impact many areas of nuclear science. In nuclear astrophysics, the understanding of nucleo-synthesis relies heavily on nuclear masses in very neutron-rich nuclei, where no experimental data exists and only theoretical models can be used. The search for superheavy elements is driven by theoretical predictions of nuclear stability which are all obtained in the framework of DFT. Also, nuclear fission is another example of a fundamental scientific and societal problem, the understanding of which ultimately depends on the quality of the energy functionals used in the calculation (see slide "Microscopic description of nuclear fission").

Resources and approaches (facilities, computing resources, software, innovative approaches, etc.) used:
DFT calculations have been performed with the HFBTHO solver [1] on NERSC Cray XT4 Franklin supercomputer. The experimental database was determined by the Oak Ridge group and is publicly available at the address given [2]. Various properties of the UNEDFpre parameterization of the Skyrme functional can be consulted online on the MassExplorer website [3]. The POUNDERs algorithm is written in Matlab and a Fortran interface is currently under development.

What future efforts associated with and/or motivated by this accomplishment are proposed and why?
The performance of the POUNDERs algorithm, combined with supercomputing resources, paves the way to comprehensive optimization of the nuclear DFT probing all the channels of the energy functional. In particular:
§ Including experimental data related to very deformed configurations is crucial for a precise description of nuclear fission (see slide "Microscopic description of nuclear fission").
§ Spectroscopic properties of DFT can be improved if data on odd nuclei are included
Such datasets require either many more DFT calculations for a given function evaluation (case of blocking calculations in odd nuclei) or more sophisticated and CPU-intensive 3D solvers like HFODD [4] that can describe non-axial shapes (fission barriers). Work in this direction is currently in progress and part of Year 4 of the UNEDF effort.

The Team:
This collaboration involves Argonne National Laboratory (Jorge Moré, Jason Sarich, Stefan Wild) and Oak Ridge National University/University of Tennessee (Markus Kortelainen, Thomas Lesinski, Witek Nazarewicz, Nicolas Schunck, Mario Stoitsov.)
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