Discovering the Secrets Buried in Theories

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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

About the graphics:
Left: Pair-wise correlations at the solution of a (restricted) 8 parameter fit of the Skyrme energy functional
Top-Right: Specific sensitivity of each of the 12 parameters of the Skyrme functional to global changes in experimental data . For example, parameter #6 is mostly sensitive to changes in the values of nuclear masses and odd-even mass differences, but almost insensitive to r.m.s. radii of spherical nuclei.
Bottom-Right: Global sensitivity (% of change) of the parameterization of the Skyrme functional to specific changes in experimental data by 0.1σ, where σ is the typical error associated with each type of data (mass, radii, odd-even mass difference)

What was accomplished:
We have applied powerful methods of Statistics (correlation matrix, confidence intervals, etc.) to study the properties of the UNEDFpre parameterization of the Skyrme nuclear energy functional (see slide "Computing Masses of Atomic Nuclei"). This information is extremely important, as it allows to study the stability of the solution of the optimization problem, extract correlations between the various parameters of the nuclear energy functional, extract possibly redundant parameters and study the dependence of the parameterization under small changes in the experimental data. The major achievement was the development of a surrogate (model-based) approach to carry out the statistical analysis, which allows to extend this type of studies to costly function evaluations. This new method is highly scalable: we have computed correlations on 5616 cores at NERSC Cray XT4 Franklin supercomputer.

The impact this accomplishment will have on science, computing, energy, or the environment:
One key measure of the reliability of a theory is its capacity to provide theoretical error bars. Since nuclear DFT depends on a set of free parameters adjusted to data, it is crucial to assess the dependence of a given parameterization on the

experimental data that was used to obtain it. If this dependence is too high, the parameterization may be instable and its predictive power can be questioned. Our accomplishment is therefore the first step towards delivering theoretical predictions of nuclear observables such as masses with built-in error bars. This could help constrain better calculations in other fields where nuclear data is used as input (r-process calculations, fission, etc.)

Resources and approaches (facilities, computing resources, software, innovative approaches, etc.) used:
DFT calculations have been performed with the HFBTHO solver [1]. The experimental database was determined by the Oak Ridge group and is publicly available at the address given [2]. Sensitivity analysis using the surrogate method developed here was carried out on NERSC Cray XT4 Franklin supercomputer. For *n* parameters, *m* nuclei, *p* cores per nucleus simulation, this technique can exploit up to 5(n+1)(n+2)m×p/2 cores.

What future efforts associated with and/or motivated by this accomplishment are proposed and why?
The significant amount of correlations between the parameters of the Skyrme functional suggest that the standard parameterization of the latter, which was used in this work, may not be the most appropriate. It may also suggest that the experimental dataset was not complete enough to constrain effectively each parameter. Ideally, one would like to find a representation of a functional in terms of N *independent* parameters that would be unambiguously constrained by the data. Current work in this direction, building on the results reported here, includes using additional data such as one-particle separation energies or energies at large deformations in the optimization procedure.

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.) It is supported by UNEDF grant DE-FC02-09ER41583.