Microscopic Description of Nuclear Fission

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References:

"Microscopic description of complex nuclear decay: multimodal fission," A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. C 80, 014309 (2009).
"Broyden's method in nuclear structure calculations", A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck, and M.V. Stoitsov, Phys. Rev. C 78, 014318 (2008).

About the graphics:

Top-Left: Potential energies of ^{252}Fm and ^{258}Fm, along optimum fission paths plotted against the quadrupole moment (defining the elongation of the nuclear shape), drawn in the common scale relative to the ground-state minima. The ground state of a fissionable system corresponds to energy minimum confined inside the first (inner) fission barrier. During the fission process, the system penetrates the barrier by the process of quantum mechanical tunnelling through the classically forbidden region. In this region, marked by yellow, the total energy is less than the potential energy, and in classical physics there would be no probability of finding a particle. In some nuclei, such as ^{252}Fm, a metastable superdeformed state, a fission isomer, appears that is protected by a second (outer) fission barrier. At very large elongations outside the outer barrier, the nucleus splits into two fission fragments. The difference between potential energies of ^{252}Fm and ^{258}Fm can be attributed to shell effects, which vary from nucleus to nucleus.
Top-Right: A comparison between linear mixing and modified Broyden's mixing applied in the self-consistent convergence scheme in the DFT solver HFODD for the constrained configuration in ^{252}Fm at the quadrupole moment of Q_{20}=20 eb. The number of unknown variables (i.e., the size of the Broyden vector) is about 7,000,000. Much faster convergence has been achieved in comparison with the linear-mixing procedure, which is often used in such types of calculations.
Center: Two-dimensional total energy surface for ^{258}Fm in the plane of two collective coordinates: elongation, Q_{20}, and reflection-asymmetry, Q_{30}. Dashed lines show the fission pathways: symmetric compact fragments (sCFs) and asymmetric elongated fragments (aEFs). Nuclear shapes are shown as three-dimensional images that correspond to calculated nucleon densities.
Bottom-Left: The calculated fission half lives of even-even fermium isotopes, with $242 \le A \le 260$, compared with experimental data.
Bottom-Right: The summary of fission pathway results obtained in this study. Nuclei around ^{252}Cf are predicted to fission along the asymmetric path aEF; those around ^{262}No along the symmetric pathway sCF. These two regions are separated by the bimodal symmetric fission (sCF + sEF) around ^{258}Fm. In a number of the Rf, Sg,

and Hs nuclei, all three fission modes are likely (aEF + sCF + sEF; trimodal fission). In some cases, labeled by two-tone shading with one tone dominant, calculations predict coexistence of two decay scenarios with a preference for one. Typical nuclear shapes corresponding to the calculated nucleon densities are marked.

What was accomplished:
We study the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory (DFT). Our results show that the observed bimodal fission can be explained in terms of pathways in multidimensional collective space corresponding to different geometries of fission products. From the calculated collective potential and collective mass, we estimated spontaneous fission half-lives, and good agreement with experimental data was found. We also predict a new phenomenon of trimodal spontaneous fission for some rutherfordium, seaborgium, and hassium isotopes.

The impact this accomplishment will have on science, computing, energy, or the environment:
Understanding of the fission process is crucial for many areas of science and technology. Fission governs existence of many transuranium elements, including the predicted long-lived superheavy species. In nuclear astrophysics, fission influences the formation of heavy elements on the final stages of the r-process in a very high neutron density environment. Fission applications are numerous. Improved understanding of the fission process will enable scientists to enhance the safety and reliability of the nation's nuclear stockpile and nuclear reactors. The deployment of a fleet of safe and efficient advanced reactors, which will also minimize radiotoxic waste and be proliferation-resistant, is a goal for the advanced nuclear fuel cycles program. While in the past the design, construction, and operation of reactors were supported through empirical trials, this new phase in nuclear energy production is expected to heavily rely on advanced modeling and simulation capabilities.

Resources and approaches (facilities, computing resources, software, innovative approaches, etc.) used:
This work was carried out under the INCITE award "Computational Nuclear Structure". The calculations were performed at ORNL on a Cray XT3/XT4 Jaguar supercomputer systems. The algorithmic developments for this project have been funded through SciDAC-2 UNEDF project. We used a symmetry-unrestricted DFT framework based on the solver HFODD capable of treating simultaneously all the possible collective degrees of freedom that might appear on the way to fission. The novel features include the implementation of the modified Broyden's method to solve self-consistent equations involving over 7,000,000 variables and the use of the Augmented Lagrangian Method to solve the optimization problem with many constraints. Because a single HFODD run with all self-consistent symmetries broken takes between 1 and 10 hours of CPU time, depending on how sophisticated calculations are, it takes 3-30 CPU-years to carry out the full fission pathway analysis for 20 isotopes; hence, massively parallel computer platforms are required. The DFT solver has been highly optimized under a joint collaborative effort

involving scientists from Tennessee, Argonne, Poland, and Finland, all involved in UNEDF project.

What future efforts associated with and/or motivated by this accomplishment are proposed and why?

This work represents an important step towards the long-term goal of dynamic, microscopic description of nuclear fission. In the near term, we intend to improve the theory of fission by considering multidimensional inertia tensors and by performing the direct minimization of the collective action in a multidimensional collective space. In the long term, the theory will be extended to account for nonadiabatic effects by means of the imaginary-time propagation. In addition, quality microscopic input for fission calculations is needed. Of particular importance is the development of an optimized nuclear energy density functional with improved prediction of bulk nuclear properties and spectroscopy. Work along these lines is in progress under the UNEDF SciDAC project. Extreme scale computing affords us the opportunity to relax assumptions so that we can calculate fission properties with increasing fidelity, and therefore enables validation with experiments. We see this trend continuing during the next 5-10 years as supercomputing reaches toward the exascale. Indeed, during the recent workshops on extreme computing, the microscopic description of nuclear fission has been identified as the priority direction for high performance computing in nuclear structure.

The Team:

This collaboration involves Andrzej Staszczak, Andrzej Baran, Jacek Dobaczewski, and Witold Nazarewicz (University of Tennessee-ORNL-Lublin-Warsaw fission collaboration); David Dean, Mario Stoitsov, Nicolas Schunck (ORNL/University of Tennessee); Jorge Moré and Jason Sarich (ANL). It is supported by UNEDF and NNSA SSAA grants DE-FC02-09ER41583 and DE-FG03-03NA00083.