Figure 1: Fission pathway for ^{240}Pu along the mass quadrupole moment calculated with the SkM*, UNEDF0, and UNEDF1 energy density functionals. E_{II}, E_A, and E_B denote the experimental energy of the fission isomer and the inner and outer barrier heights, respectively.
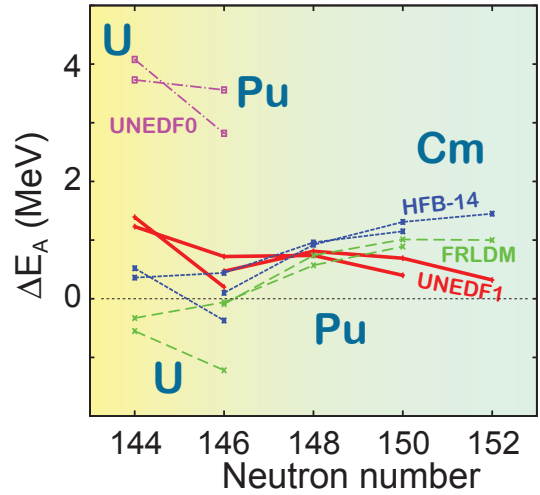

Figure 2: Difference between theoretical and experimental inner fission barriers in U, Pu, and Cm nuclei for the UNEDF0 and UNEDF1 functionals, and FRLDM and HFB-14 models; see Ref. [4] for further details.

Quality Input for Microscopic Fission Theory

Soon after its discovery in 1938, Bohr and Wheeler [1] developed the first theory of *nuclear fission*, a fundamental nuclear decay of great relevance to science and society at large. Bohr and Wheeler predicted that significant further theoretical progress would not occur as rapidly because "an accurate estimate for the stability of a heavy nucleus against fission in its ground state will ... involve a very complicated mathematical problem" [1]. Their prognostication has proved true: almost 75 years later our understanding of this complex phenomenon, involving hundreds of strongly interacting protons and neutrons moving inside a splitting nucleus, remains largely incomplete. There are great expectations, however, that with the help of today's high-performance computers the secrets of fission may finally be unlocked.

Under the SciDAC UNEDF program [2] and a Stewardship Science Academic Alliance grant [3], nuclear physicists at the University of Tennessee, Lawrence Livermore National Laboratory, and Oak Ridge National Laboratory, in collaboration with computational mathematicians at Argonne National Laboratory, have recently delivered a validated input for the microscopic description of the fission process in nuclei [4]. The principal goal of this study, which is based on the nuclear density functional theory (DFT) and focuses on the actinide and transactinide regions of the nuclear mass table, is to deliver fission models capable of providing nuclear data not only of a higher quality, but also with quantified uncertainties. For many applications of interest to the NNSA, the required data on fission cross-sections and fission products cannot be obtained experimentally because neutron-rich nuclei with short half-lives are required. Understanding fission— and, in particular, properties of fission fragments—is essential to successfully analyzing fission yields under a variety of conditions and is the starting point for the complex modeling of the prompt fission neutron spectrum.

One of the focus areas of the UNEDF fission effort is the development of high-quality input for microscopic fission calculations. Without such input, even the most sophisticated fission approaches based on many-body theory would not be able to produce reliable results. Verified and validated theoretical input is crucial for interpreting experimental data, assessing the importance and feasibility of planned measurements, predicting nuclear properties in the regions that are impossible to access experimentally, and defining future research directions.

The quality of a DFT calculation relies on the form and parameterization of an underlying energy density functional. Since the functional's parameters cannot be derived or computed, they must be optimized based on experimental data. A previous study [5] employed advanced optimization algorithms and high-performance computing to carry out a state-of-the-art optimization of the functional; the resulting parameterization UNEDF0 yields good agreement with experimental masses, radii, deformations, and other global nuclear properties. Recently, in order to develop a high-quality functional for fission, this study was extended by adding excitation energies of fission isomers (superdeformed states on the path to fission) in four actinide nuclei.

A striking feature of the new functional UNEDF1 [4] is its ability to reproduce the empirical fission barriers in the actinide region listed in the Reference Input Parameter Library at IAEA [6]. As seen in Figures 1 and 2, the quality of UNEDF1 predictions for inner and outer fission barriers is comparable to that obtained in more phenomenological models [6]. Furthermore, UNEDF1's new status as the input of choice when it comes to the microscopic study of the nuclear fission process sacrifices little. Indeed, UNEDF1 provides a description of global nuclear properties that is almost as good as that of UNEDF0. Researchers are encouraged by the finding that deformation properties of the functional can be well-constrained by including only a handful of data relevant to fission. Although the quest for the microscopic fission theory is far from over, a crucial milestone towards this lofty goal has been reached.

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[3] *Theoretical Description of the Fission Process*, a project supported by the National Nuclear Security Administration under the Stewardship Science Academic Alliance program through DOE grant DOE-DE-FG52-09NA29461. http://www.phys.utk.edu/witek/fission/fission.html

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