Exploring the nuclear chart using density functional theory

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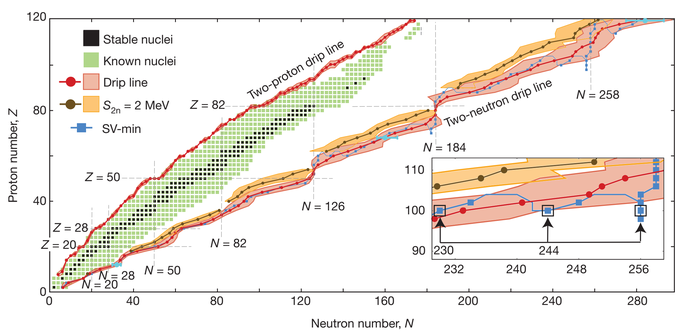
Introduction

More than a century after their discovery, atomic nuclei remain one of the oldest and most exciting challenges of contemporary physics. Nowadays, Density Functional Theory (DFT) represents the best compromise between accuracy and simplicity, allowing for the microscopic description of a wide variety of nuclear properties and phenomena across the nuclear chart.



Method

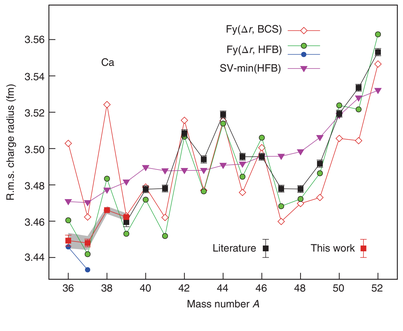
DFT describes the nuclear quantum many-fermion system in terms of the one-body normal ρ and transition κ densities. These are calculated by solving the Hartree-Fock-Bogoliubov (HFB) equation, where the many-body wavefunction is obtained via minimization of the total energy:

$$\delta E[|\psi\rangle] = 0 \quad \text{with} \quad E = \langle\psi|\hat{\mathcal{H}}|\psi\rangle = E[\rho,\kappa]\,.$$

The HFB equation form a self-consistent set of non-linear integro-differential equations involving dense linear algebra with matrices of the order of 2,000×2,000 or more, which must be solved either iteratively or by direct minimization of the energy via gradient method. The development of an efficient computational infrastructure is thus crucial to properly tackle problems such as large-scale surveys or the theoretical description of fission.

Sizes of extreme calcium isotopes

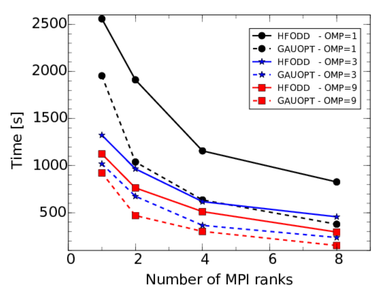
Current DFT calculations require a fitting of a dozen model parameters to selected experimental data: A proper optimization procedure is thus a crucial step to fully exploit the capabilities of this theoretical framework. The usage of Bayesian analysis in the calibration process, together with a proper selection of experimental data and the development of more advanced models could thus boost the capabilities of DFT calculations.

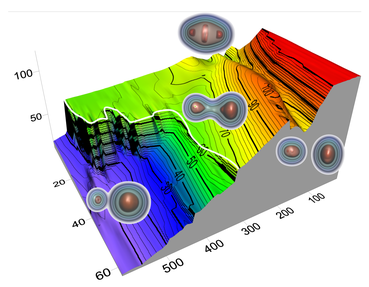


In [1], DFT calculations showed that novel interactions and state-of-the art mean-field methods can properly describe the interplay of of both weak binding and superfluidity, reproducing the intricate behaviour of charge radii along the chain of calcium isotopes.

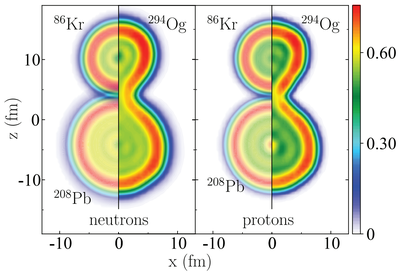
Fission of exotic nuclei

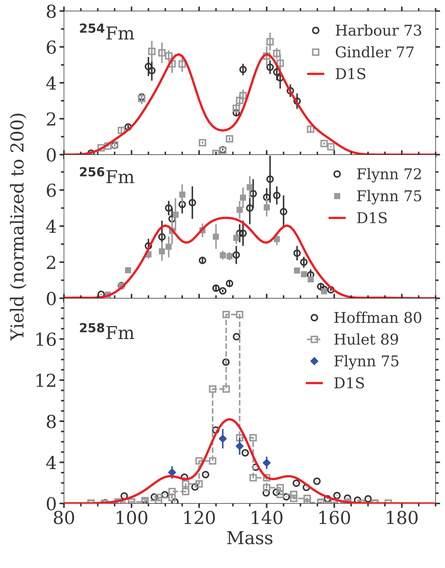
The theoretical description of fission demands the computation of the nuclear energy and collective inertias in a multidimensional space comprising all the relevant collective degrees of freedom. This requires solving the HFB equations over millions of configurations describing the different shapes of the nucleus. In the NUCLEI project we develop highly optimized DFT solvers capable of performing such very large-scale ensemble runs on leadership computing facilities.





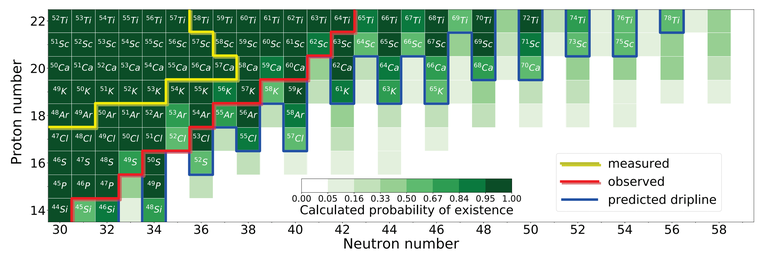
Below are two examples of the predictive power of our approach. In [2], we calculated the spontaneous fission yields of $^{294}_{118}$Og, the heaviest known isotope, using for the first time a 4D deformation mesh. We predicted that cluster emission, a very asymmetric fission mode, is the dominant decay channel of this nucleus, and proved that this prediction is model-independent. In [3], we reproduced the features of fission fragment distributions in neutron-rich Fermium isotopes by simulating directly the time-evolution of the fissioning system in the collective space. We could reproduce how adding just a few neutrons can completely alter the characteristics of the yields, from asymmetric to symmetric fission.



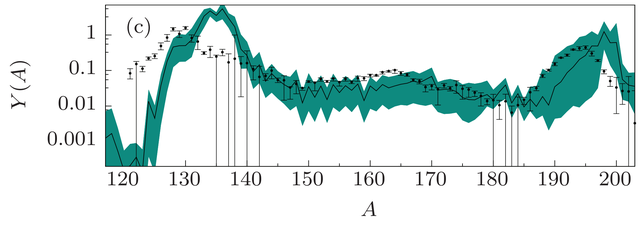


Uncertainty Quantification in DFT

In order to asses the predictive power of any nuclear model, a proper quantification of its intrinsic uncertainties is in order. In recent years, the usage of Bayesian methods became a powerful tool for estimating the statistical uncertainties in EDF calculations.



In [4], the probability of nuclei to be bound to neutron emission is estimated using Bayesian model averaging analysis and DFT calculations. In [5], the DFT statistical uncertainties on binding energies are propagate in r-process calculations, quantifying the impact of new experimental data.



These studies show that supervised machine learning techniques can provide reliable estimations of predictions' uncertainties and guide the optimization process of the functionals, increasing the DFT predictive power in regions far from stability.

Acknowledgments

This work was supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Nuclear Physics under Award No. DE-SC0018083 (NUCLEI SciDAC-4 collaboration).

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project

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