# UNEDF2: the Endpoint of Skyrme DFT

Objectives

- Develop predictive nuclear density functional theory to compute properties of light to heavy nuclei to understand global properties of nuclei, nuclear fission, and the formation of elements in the universe.

- Use the advanced optimization framework POUNDERS and carefully selected nuclear data to produce the well-calibrated Skyrme-type nuclear energy density functional UNEDF2 that represents an effective nuclear interaction.

Impact

- Enable rigorous, data-driven, predictive modeling of nuclear structure, which will reduce uncertainties stemming from nuclear science inputs in:
  - basic science research such as tests of fundamental symmetries and nuclear astrophysics
  - stockpile science and reactor physics

- Provide benchmark and template for future developments of nuclear structure models
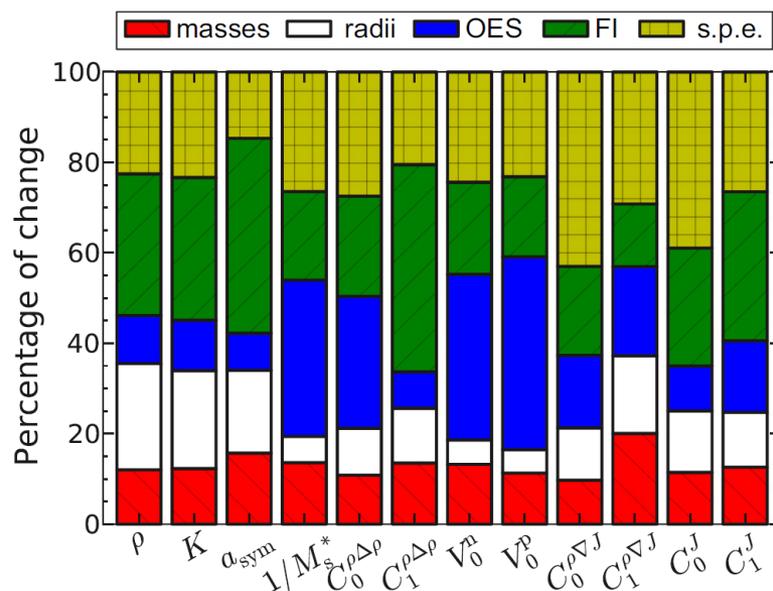
Sensitivity of the UNEDF2 parameters of the Skyrme energy density to different data types: atomic masses (red), charge radii (white), odd-even mass differences (blue), fission isomer excitation energies (green), and single-particle energies (yellow). The 4 fission isomer excitation energies and 9 single-particle energies represent only about 10% of the experimental data used but have a major impact on the final parameters.

Accomplishments

1. We have developed a general framework to solve the self-consistent equations of nuclear density functional theory.

2. We have shown that:
   - to constrain nuclear density functional, and provide uncertainty quantification, different types of data are required;
   - traditional Skyrme functionals are intrinsically limited.

3. We have used the POUNDERS optimization framework and fast solver HFBTHO, developed and published under UNEDF/ NUCLEI SciDAC projects.

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI
Nuclear Computational Low-Energy Initiative