Uncertainty Quantification in Nuclear Density Functional Theory

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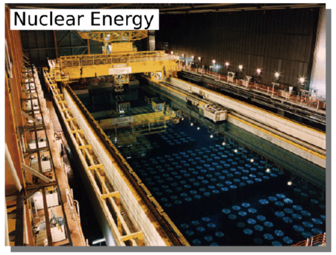
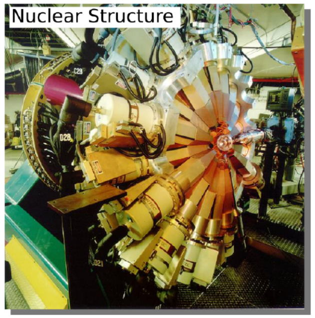
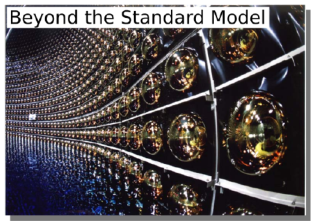
Abstract

- Nuclear density functional theory (DFT) is needed to compute properties of atomic nuclei for basic science and applications.
- Energy density functionals (EDF) depend on a handful of model parameters that must be fitted on experimental data.
- We built the first optimization and uncertainty quantification (UQ) framework to determine EDF model parameters, and quantify and propagate the resulting statistical uncertainties.

Nuclear Structure and Reactions







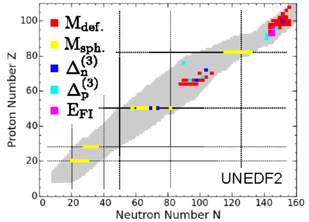
- Detailed knowledge of nuclear properties is needed both for basic science and applications:
  - Elements in the universe are formed in complex nuclear reactions networks in stellar environments;
  - Current experiments on the nature of the neutrino depends very sensitively on a handful of nuclear matrix elements that must be computed very precisely;
  - Nuclear fission powers nuclear reactors and determines the limit of nuclear stability.
- The Facility for Radioactive Ion Beam (FRIB) is DOE's largest investement and will provide experimental data in very exotic, neutron-rich nuclei;
- Many atomic nuclei of critical importance to superheavy physics, nuclear astrophysics, or fission will nevertheless remain out of reach: a predictive theory is essential.

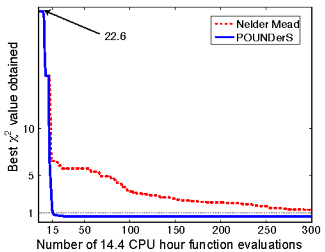
Nuclear Density Functional Theory

- Density functional theory is a general approach for solving quantum many-body problems such as nuclei, atoms, or molecules.
- In nuclear physics, its main input is the nuclear energy density functional:
  - The nuclear EDF effectively maps out nuclear forces into a functional of the density of particles (neutrons and protons);
  - The EDF depends on a handful of coupling constants (= model parameters) that must be fitted on experimental data (= calibration).
- Given the EDF, nuclear DFT solvers determine the actual density of particles by solving a non-linear system of coupled integro-differential integrations.
- Solving the DFT equations take between a few minutes up to a few days on a node; large-scale applications such as surveys of nuclear properties or fission require hundredof thousands to millions of such calculations.

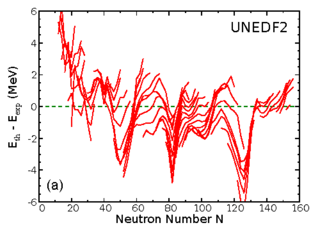
Optimization

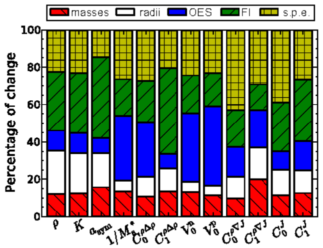
- Our calibration of the nuclear EDF uses different types of data across the nuclear chart [1-3].
- Calculations are performed with the derivative-free POUNDERS algorithm using the fast DFT solver HFBTHO on leadership computing facilities [1].





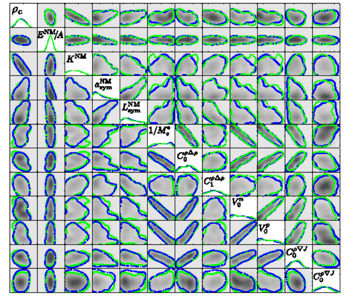
- We perform a full sensitivity analysis of the solution to highlight correlations among parameters and the importance of data types in determining parameters [1-3].
- We show that current forms of nuclear energy functionals are not predictive enough [3].



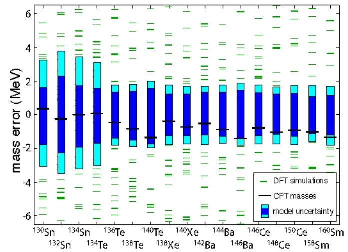


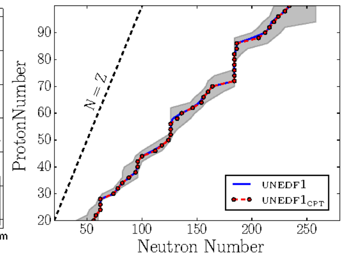
Uncertainty Quantification

- We compute the full Bayesian posterior distribution of the UNEDF1 nuclear EDF by Markov Chain Monte Carlo sampling [4].
- To mitigate the prohibitive cost of MCMC simulations, we build a response function of our χ_2 function using Gaussian processes [4,5].
- 200 full DFT calculations are used to train the GP model.



- Uncertainties extracted from the posterior distribution are compatible with those from the covariance analysis [6].





- We draw random samples from the posterior distribution to propagate stastistical uncertainties to predictions of masses of neutron-rich nuclei and the limits of stability (neutron drip line).
- We find that recent mass measurements of neutron-rich nuclei at the Caribu facility (ANL) do not provide enough information to reduce current (large) uncertainties [7].

Conclusions

- Our new optimization and UQ framework will provide reliable theory guidance for DOE and NSF experimental programs and helps identify limitations in predictive power of models.
- POUNDERS (optimization) and GPMSA (UQ) codes were developed during successive SciDAC collaborations and have transformed how nuclear DFT is implemented.

References

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