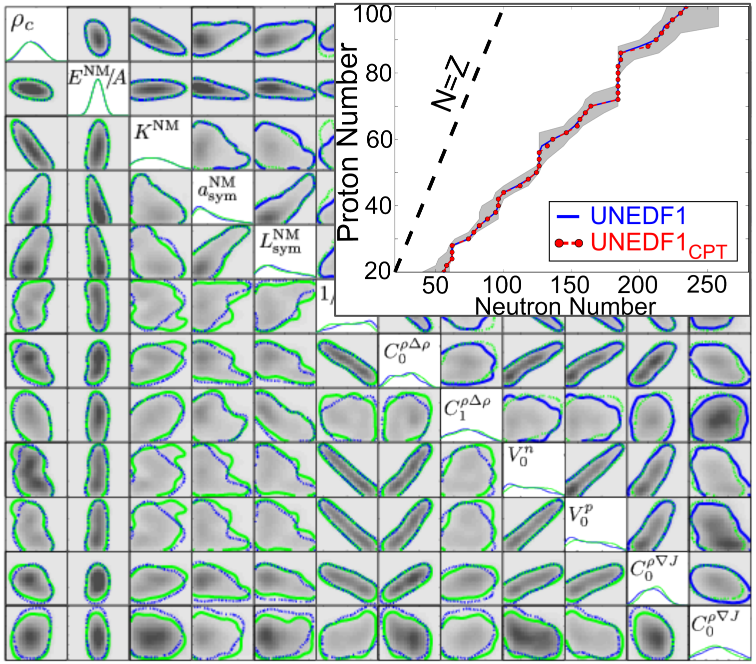
Quantifying the Nuclear Unknown with Bayesian Inference

Objectives

- Quantify theoretical uncertainties in nuclear density functional theory (DFT) for applications in basic science and national security.
- Assess the information content of experimental observables with respect to current theoretical models.
- Enhance the feedback in the "observation-theory-prediction-experiment"- cycle of the scientific method.

Impact

- Provide reliable theory guidance with controlled uncertainties for experimental programs.
- Identify limitations in predictive power of theoretical models.
- Provide template for the deployment of uncertainty quantification methodology (UQ) to nuclear structure and reactions.



Bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT $UNEDF_1$ parameterization. ***Inset****: Position of the two-neutron dripline predicted by the $UNEDF_1$ functional (blue) and by its refit $UNEDF_{CPT}$, which incorporates new mass measurements from the CPT facility at ANL (red). Statistical uncertainties at the 90% confidence level computed in the Bayesian analysis are represented by the grey band.*

Accomplishments

1. Developed a Bayesian framework to quantify and propagate statistical uncertainties of nuclear energy functionals.
2. Showed that new precise mass measurements do not impose sufficient constraints to lead to significant changes in the current DFT models.
3. Coupled the fast DFT solver HFBTHO, POUNDERS optimization framework, and the GPMSA UQ code, developed under the UNEDF/NUCLEI , SUPER, and QUEST SciDAC projects.

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI Nuclear Computational Low-Energy Initiative

Reference: J. McDonnell *et al.*, Phys. Rev. Lett., in press (2015); arXiv:1501.03572

Contact: N. Schunck, schunck1@llnl.gov