Uncertainty Quantification in Nuclear Density Functional Theory

Information and Statistics in Nuclear Experiment and Theory (ISNET-3)

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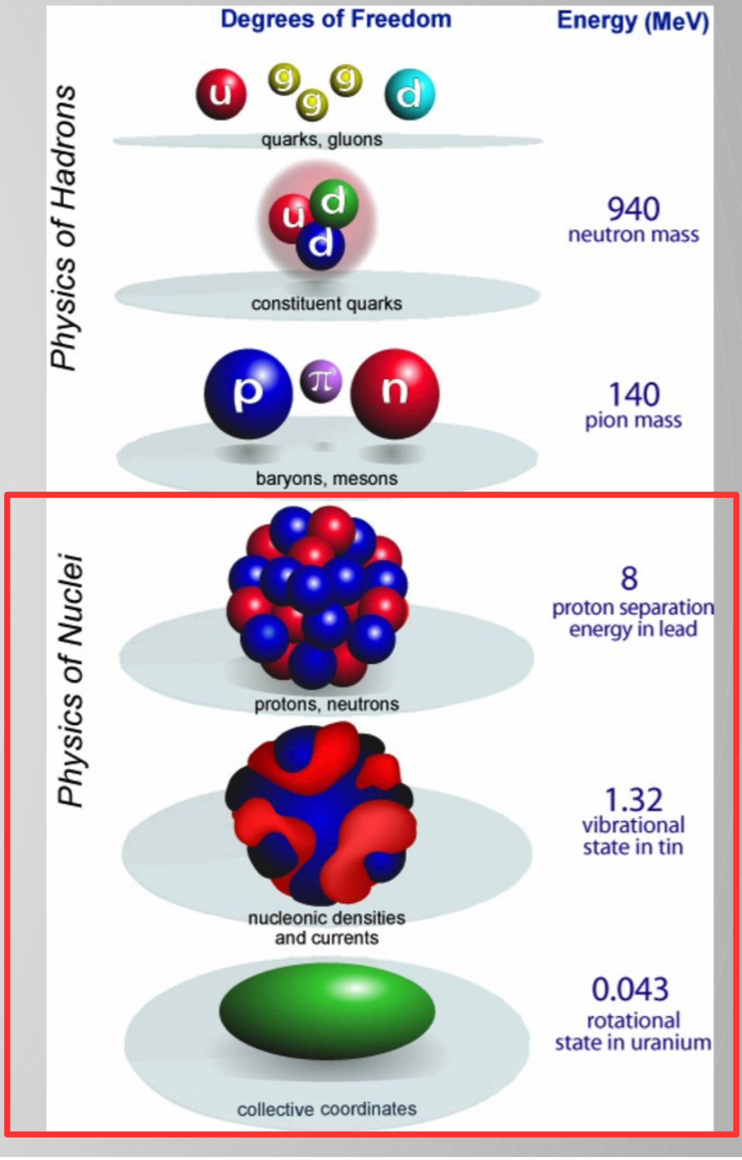
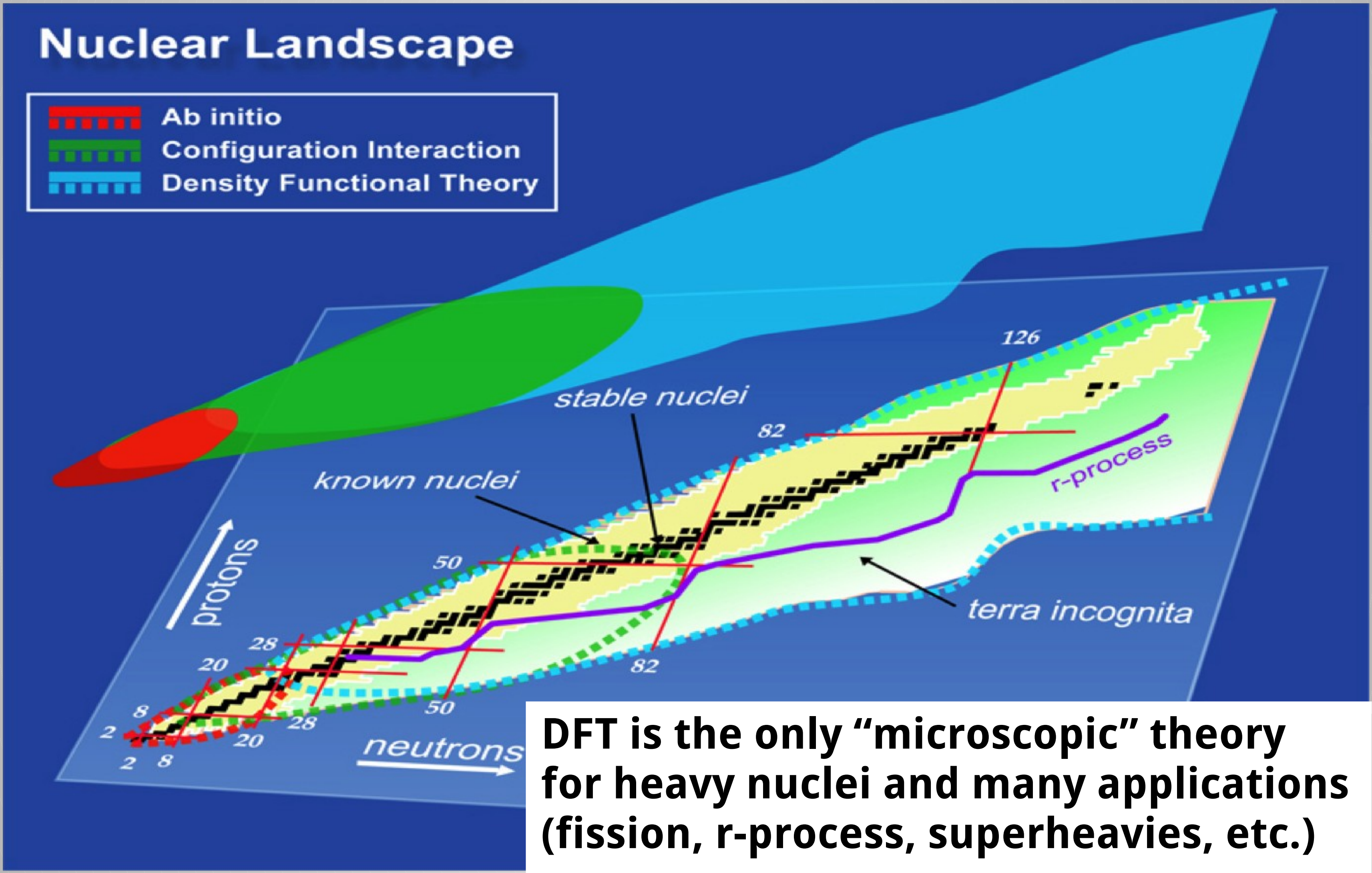
The Nuclear Hierarchy

- Hierarchy of degrees of freedom
  - Quarks and gluons
  - Point-like protons and neutrons
  - Densities of nucleons
  - Collective coordinates
- The physics of nuclei is based on nucleons and densities of nucleons

  ⇒ All approaches to nuclear structure are phenomenological models!
- Nuclear density functional theory (DFT)
  - Built on effective nuclear energy density functional (or interactions)
  - Densities of nucleons are basic degrees of freedom



The Realm of Nuclear DFT



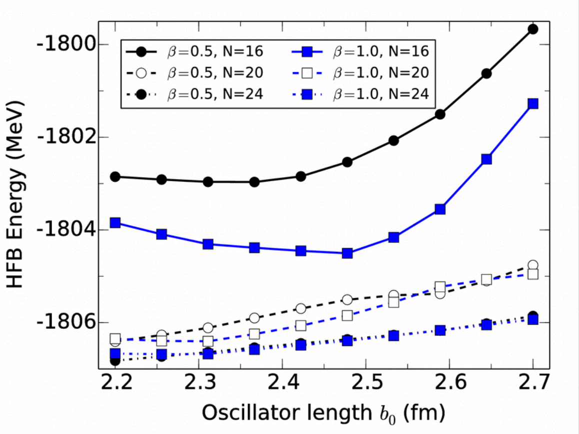
DFT is the only "microscopic" theory for heavy nuclei and many applications (fission, r-process, superheavies, etc.)

Nuclear DFT for Dummies

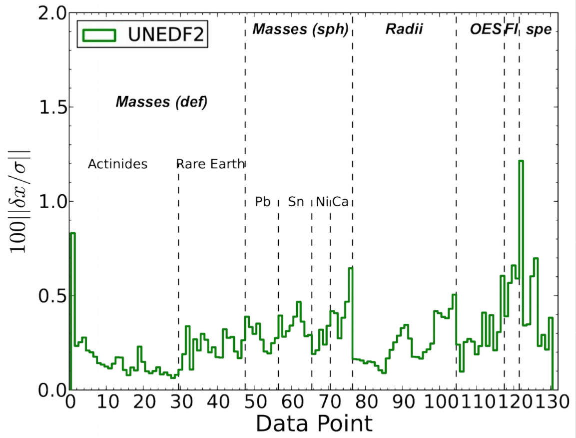
- System of independent particles ⇒ uncorrelated wave-function
- Total energy is a functional of the density of nucleons: concept of energy density functional (EDF)
- Cannot take the EDF from realistic nuclear forces: many-body physics cut-off by assumption of independent particles
  - Design and optimize effective nuclear forces
  - Use guidance from theory of nuclear forces and ab initio methods
  - Symmetry breaking (=deformation) the key to success
- Compared to ab initio methods with realistic potentials, EDFs are more phenomenological by design
  - Connection with QCD/EFT is loose (at best)
  - No power counting, perturbative expansion, etc.
- Examples: Skyrme (zero-range) and Gogny (finite-range) forces

DFT as a Model

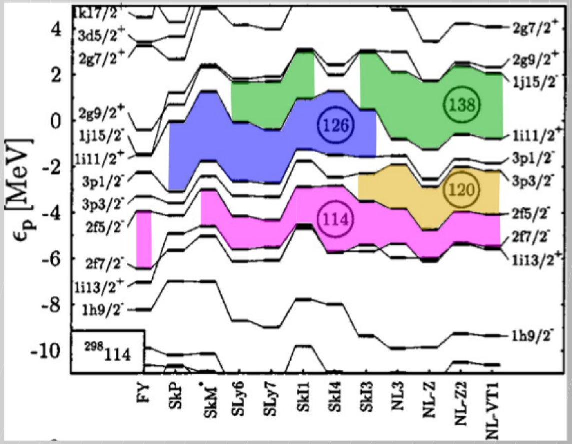
- A mathematician view of DFT: given a set of parameters, we produce a set of outputs by solving the DFT equations (to determine the actual density ρ(r) in the system)
- Sources of uncertainties/errors
  - Numerical <u>errors</u> due to implementation of DFT equations on a CPU
  - Statistical uncertainties induced by the fit of model parameters on data
  - Systematic uncertainties caused by the choice of the functional



Numerical errors
J. Phys. G.: Nucl. Part. Phys. **42**, 034024 (2015)



Statistical uncertainties
PRC **89**, 054314 (2014)



Systematic uncertainties
From PRC **61**, 034313 (2000)

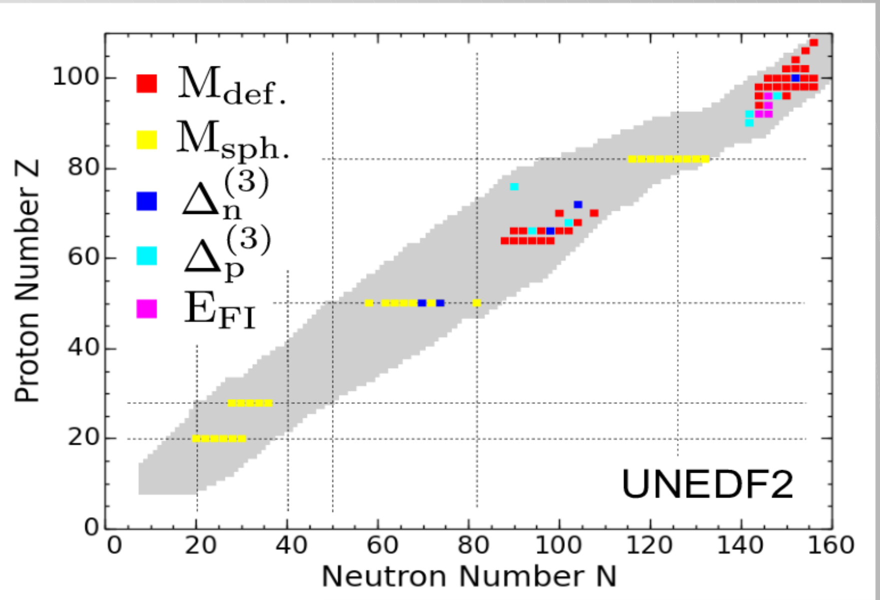
Skyrme Energy Density Functional

- Start from the Skyrme two-body effective potential
  - Write expectation value of Skyrme potential on independent particle state (Slater determinant or HFB vacuum)
  - Recast result as integral over space of functional of local density (EDF)
- Skyrme EDF (particle-hole channel)
  - Characterized by 10 parameters (time-even channel only)
  - 5 of them can be expressed as function of nuclear matter properties ⇒ better constrained
- Practical implementation of DFT in nuclear structure
  - HFB ansatz for the ground-state wave function
  - Degrees of freedom are the one-body density matrix and the pairing tensor
- Pairing channel: surface-volume EDF
  - Contains only 2 adjustable parameters
  - Only Odd-Even Mass (OEM) staggerings taken into account

The UNEDF Protocol

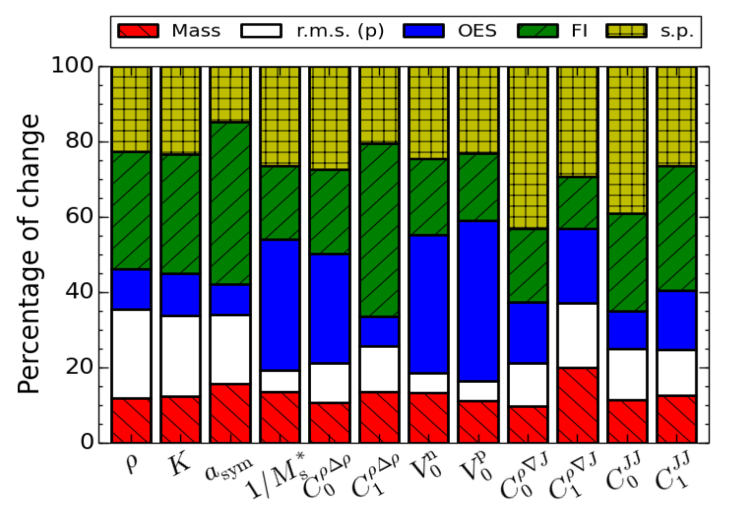
PRC **82**, 024313 (2010),
PRC **85**, 024304 (2012),
PRC **87**, 054314 (2014)

- First fit at deformed HFB level ⇒ should reduce bias of the fit
- Composite χ_2 depends on n_x parameters, T data types, and contains n_d data points
- Supplement "best-fit" with full covariance and sensitivity analysis

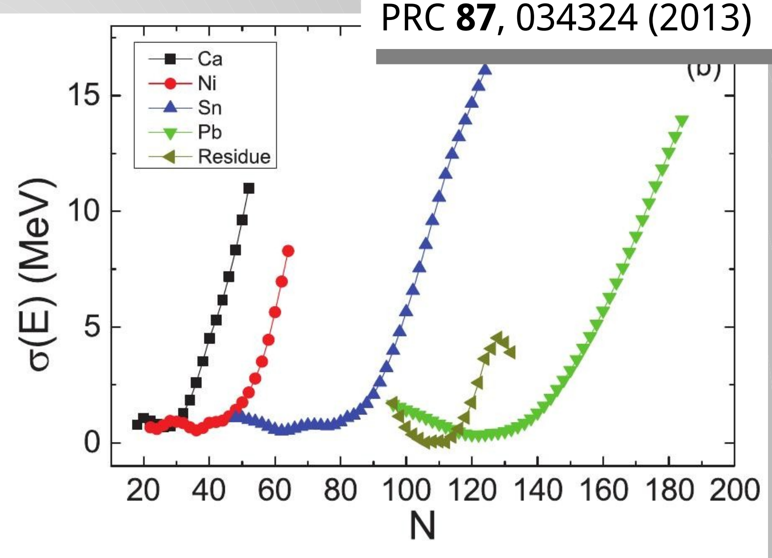


	UNEDF0	UNEDF1	UNEDF2
Number of parameters *n_x*	12	12	14
Type of data *t*	Masses, r.m.s. radii, OES (*T=3*)	Masses, r.m.s. radii, OES, E* fission isomer (*T=4*)	Masses, r.m.s. radii, OES, E* fission isomer, s.p. splittings (*T=5*)
Number of data points *n_d*	108	115	130

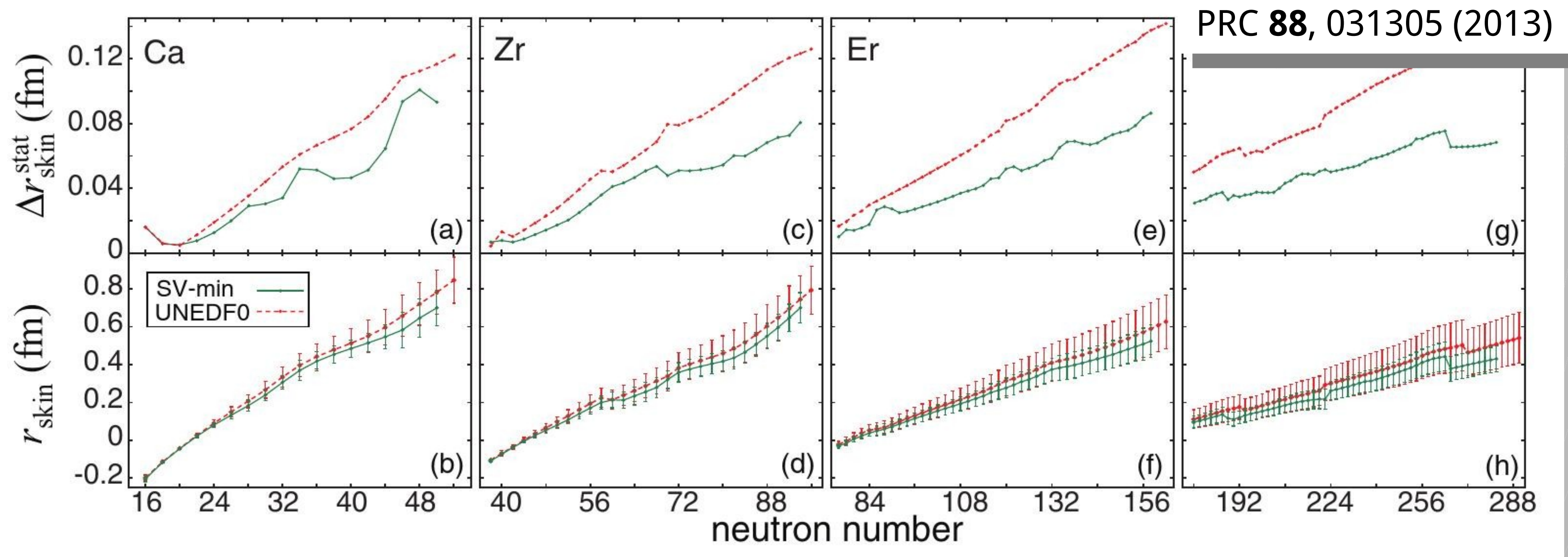
Sensitivity and Covariance Analysis



PRC **87**, 034324 (2013)



PRC **88**, 031305 (2013)



Quantifying the Unknown: Bayesian Inference

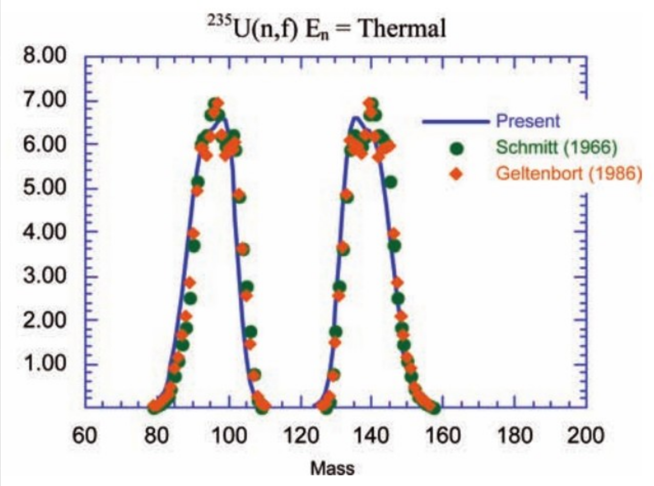
- DFT model parameters are treated as genuine random variables
  - No such thing as 'exact value of the parameter'
  - Interval of confidence ➔ probability distribution
- Bayesian inference techniques allow for rigorous determination of the probability distribution of parameters (=posterior distribution)
- The posterior distribution depends on some metric defined by a χ_2

$$L(\text{model}) \approx e^{-\chi_2}$$

- Consequences
  - Use of statistical techniques always imply some “fitting” to data
  - Potential conflict with desired predictive power of physics model...

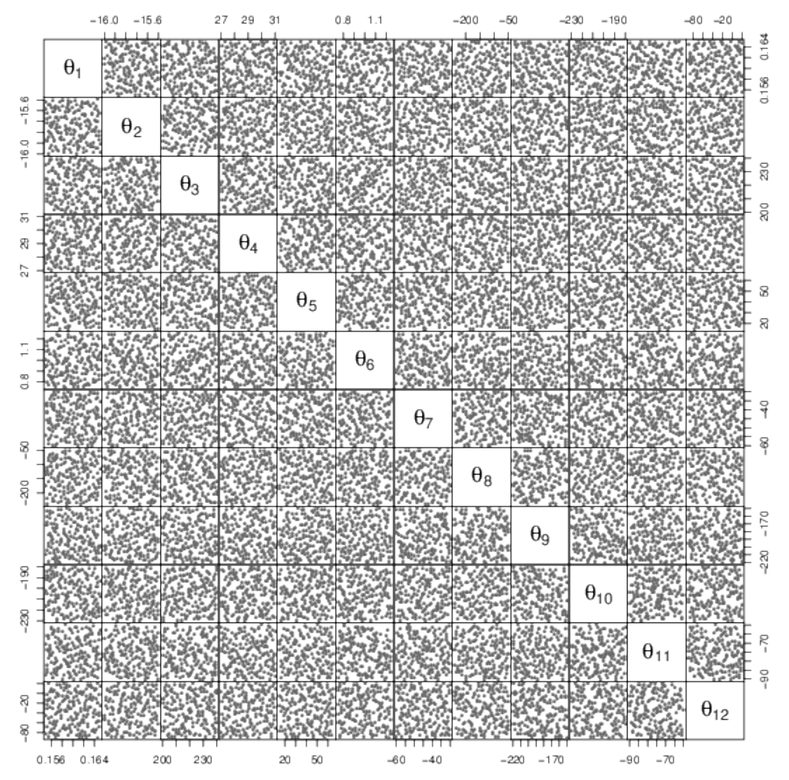
Example: Prediction of fission product yields (FPY), see David Regnier's talk

- DFT: Compute FPY from EDF fitted on g.s. properties (mostly) using only hypothesis of adiabaticity of large amplitude collective motion and quantum mechanics
- IAEA: Five-Gaussian models containing 8 parameters adjusted on data in actinides



Response functions

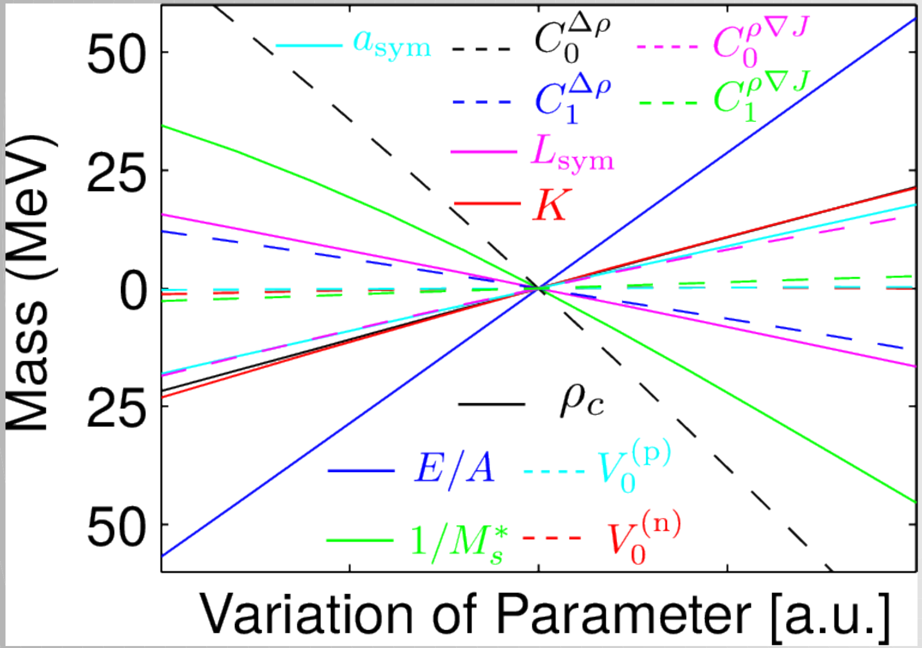
- UNEDF1 objective function involves about 100 deformed HFB calculations
  - 1 HFB = 6 cores for 5 minutes
  - 1 χ_2 evaluation ~ 600 cores for 5 minutes
- Mitigation: use response function to emulate the true χ_2
- Three-step process
  - Train the model with genuine χ_2 calculations (= generate “data”)
  - Determine a response function, and treat parameters as random variables
  - Run MCMC to build the distribution for the parameters of the emulator
- Model emulation becomes parts of the uncertainty quantification and propagation



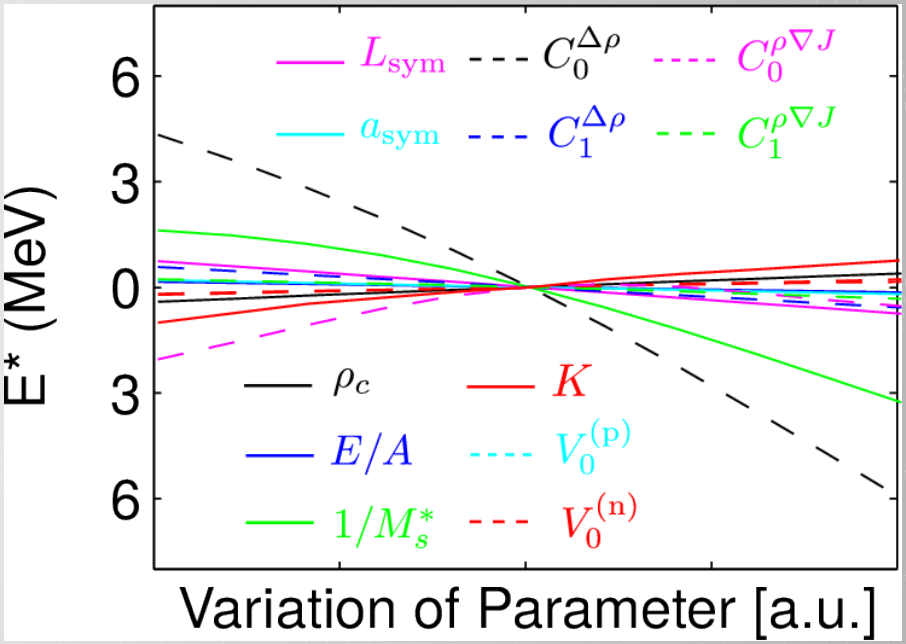
Initial sampling of parameter space in the construction of the emulator for UNEDF1

Linear approximation

- Use emulator to easily quantify dependence of data on parameters
  - Masses vary linearly across a relatively large range
  - Fission isomers show more non-linearities



Dependence of nuclear masses on parameters near UNEDF1 solution

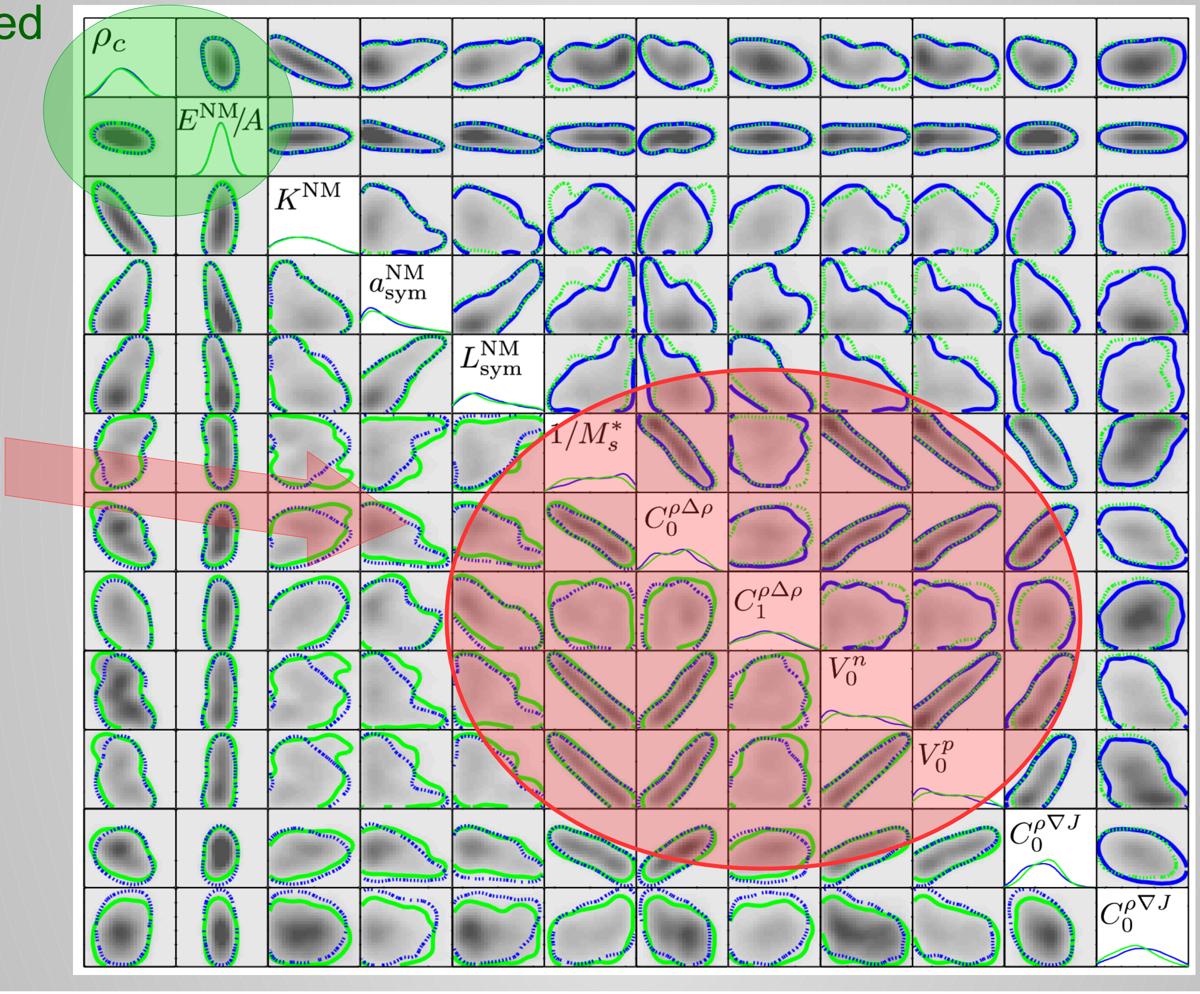


Dependence of fission isomer E* on parameters near UNEDF1 solution

UNEDF1 Posterior Distribution

PRL **114**, 122501 (2015)

Well-constrained parameters



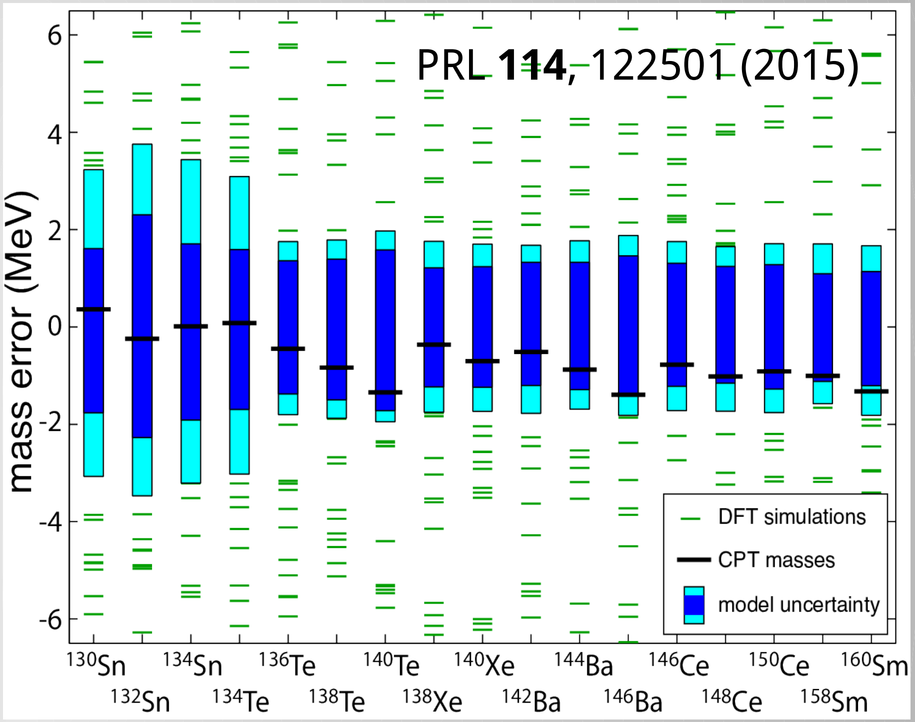
Not so well-constrained parameters

Attention: 2σ intervals

Bivariate posterior distribution for the UNEDF1 Skyrme functional.

Propagating Uncertainties

- Propagation of uncertainties done by
  - sampling the posterior distribution (=generating a EDF parametrizations)
  - calculating observables of interest with sampled EDF
- Results obtained with uniform prior
- Two main sources of statistical uncertainties
  - UNEDF1 parametrization
  - Emulator

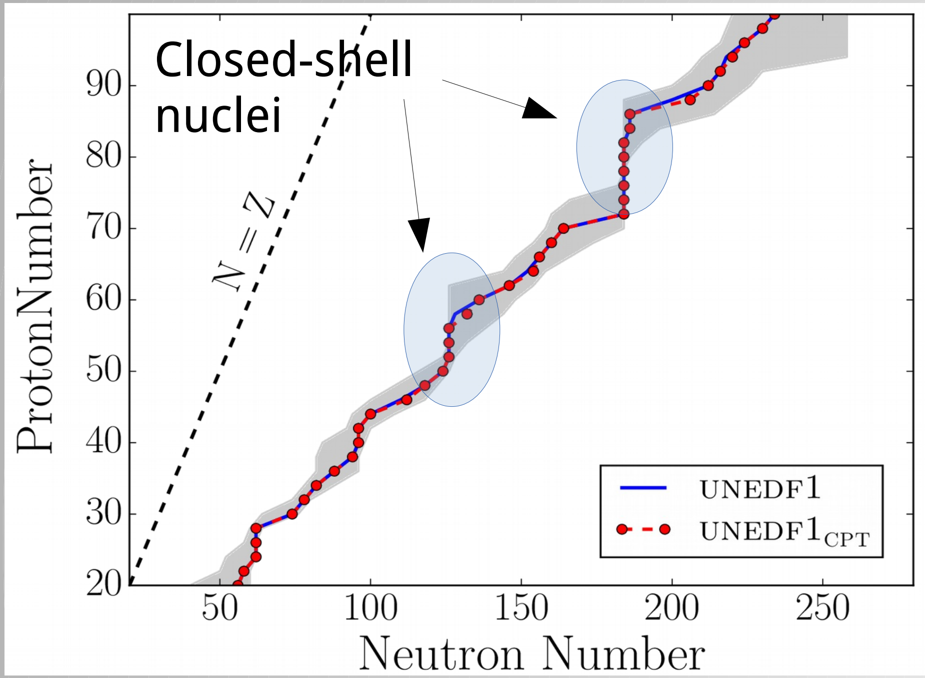


PRL **114**, 122501 (2015)

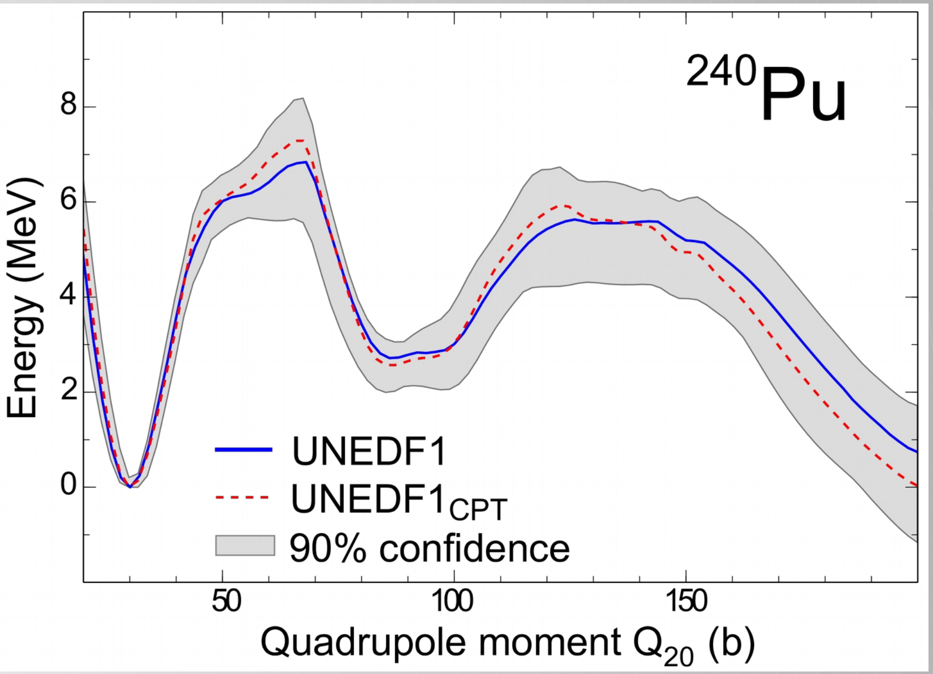
Errors and uncertainty of masses in neutron-rich nuclei measured at ANL. Black lines: deviation between experiment and UNEDF1 values

Predictive Power

PRL **114**, 122501 (2015)



Two-neutron driplines



Fission barrier in ^{240}Pu

- Large statistical uncertainties in extrapolations caused by
  - Lack of relevant data in optimization? (Ill-constrained parameters show up)
  - Intrinsic limitations of the model? (Skyrme HFB is not predictive enough)
  - Misconceptions? (Deformation properties are not well-constrained, 90% CI is too broad)

Outlook for DFT Optimization

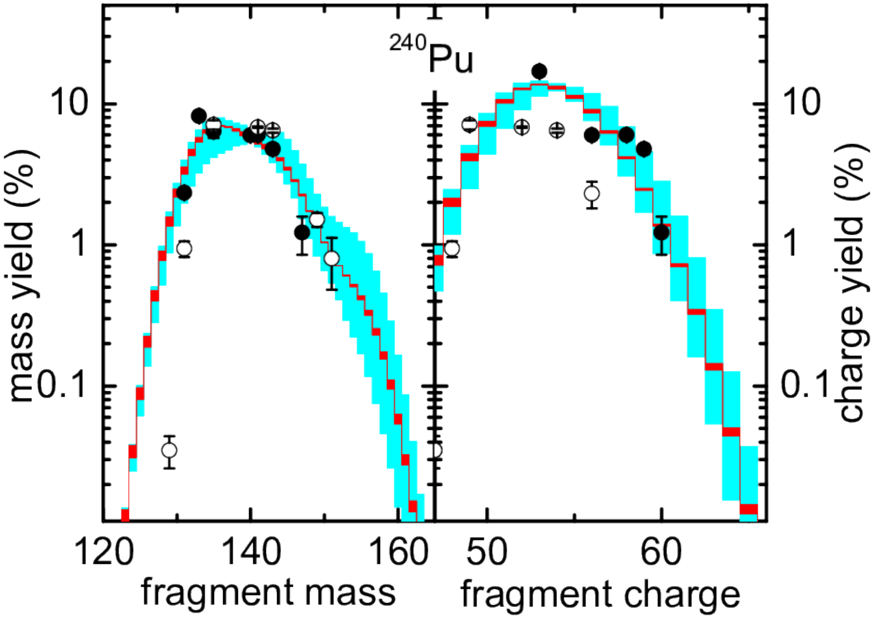
- Include uncertainties from model-dependent data (s.p. splittings) with possibly large experimental error bars into EDF fit
  - Option 1: simply include “some” experimental error
  - Option 2: propagate uncertainty of model used to extract data.

    Example: DBWA analyses for single-particle states, discrepancies in fission isomer data
- Combine numerical, statistical and systematic uncertainties in a unique framework
- Put more emphasis on pairing functional
  - Hard to constrain by data (especially if functional involves several parameters) ⇒ good candidate for uncertainty propagation
  - Good candidate to estimate systematic errors?
- EDF from realistic NN and NNN forces

Challenges of Uncertainty Propagation

- Fission product yields
  - Energy density functional
  - Potential energy surface
  - Collective inertia tensor
  - Scission configurations
  - (SF: Least action principle)
  - Definition of initial state
  - Dissipation
- Example of major challenges
  - Emulators of PES and scission to propagate EDF uncertainties down to FPY
  - Predicting impact on FPY of going from low fidelity (=2D PES) to high fidelity (>2 collective variables)

arXiv:1510.08003



Mass (left) and charge (right) distribution of fission products in spontaneous fission of ^{240}Pu from DFT + Langevin dynamics

For a (short) review: arXiv:1503.05894

Coming soon: INT Program in 2016

Bayesian Methods in Nuclear Physics (ISNET-4)
June 13 to July 8, 2016
R.J. Furnstahl, D. Higdon, N. Schunck, A.W. Steiner

A four-week program to explore how Bayesian inference can enable progress on the frontiers of nuclear physics and open up new directions for the field.
Among our goals are to

Registration is still open (for a short while)!
http://www.int.washington.edu/PROGRAMS/16-2a/

- learn from the experts about innovative and advanced uses of Bayesian statistics, and best practices in applying them;
- learn about advanced computational tools and methods;
- critically examine the application of Bayesian methods to particular physics problems in the various subfields.

Existing efforts using Bayesian statistics will continue to develop over the coming months, but Summer 2016 will be an opportune time to bring the statisticians and nuclear practitioners together.

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