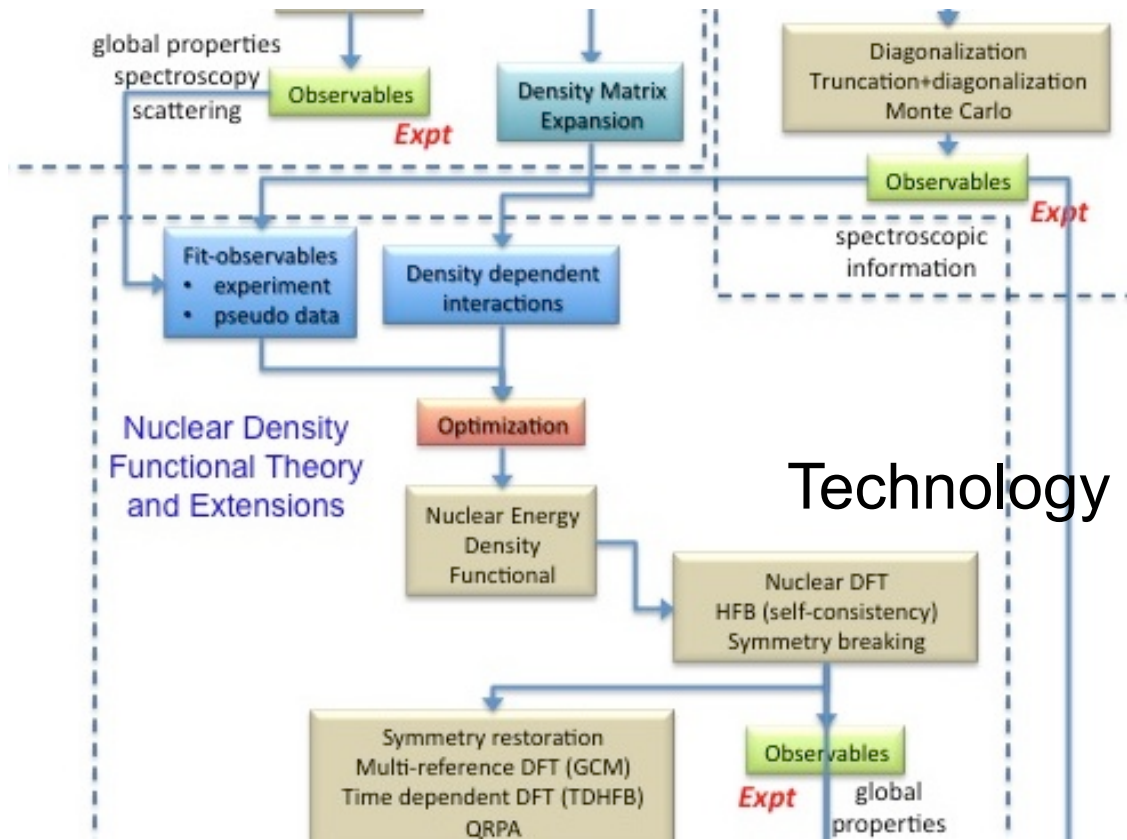# DFT Applications

Technology to calculate observables
*Global properties*
Spectroscopy
DFT Solvers
Functional form
Functional optimization
Estimation of theoretical errors

TABLE VIII: Binding energy and fission first barrier height for ^{240}Pu in units of MeV for SLy4, SkM*, UNEDF0, and UNEDF1. These are compared to the experimental value of [48].

| Functional	Binding Energy	First Barrier Height
SLy4	1801.5	11.9
SkM*	1804.3	9.4
UNEDF0	1811.8	9.6
UNEDF1	1811.8	6.8
Exp	1813.5	6.1
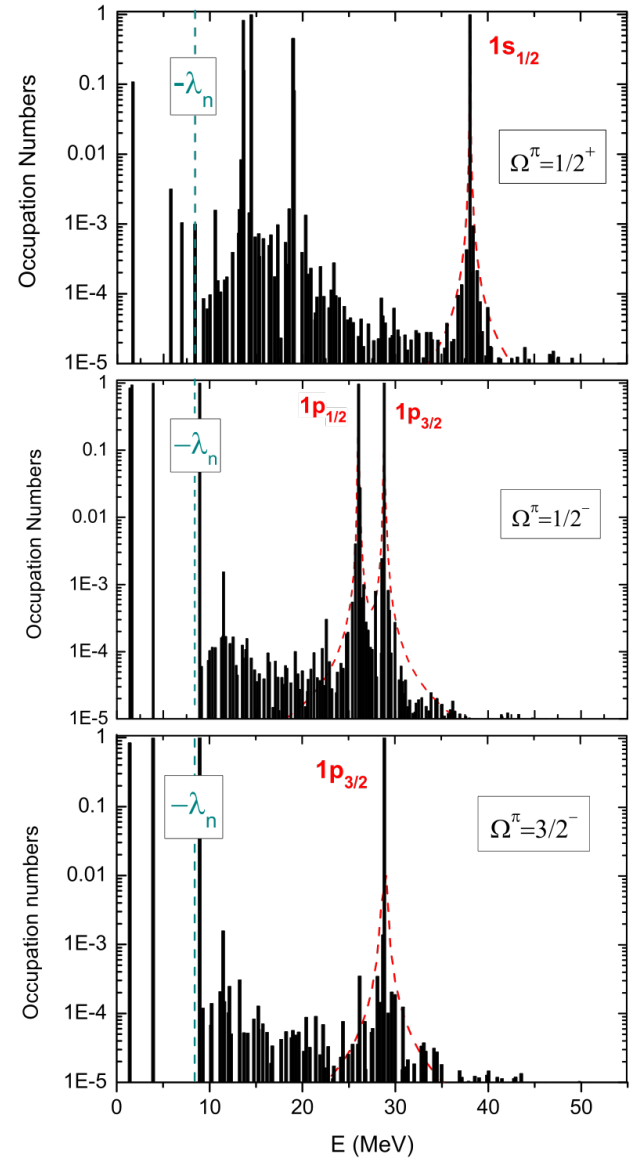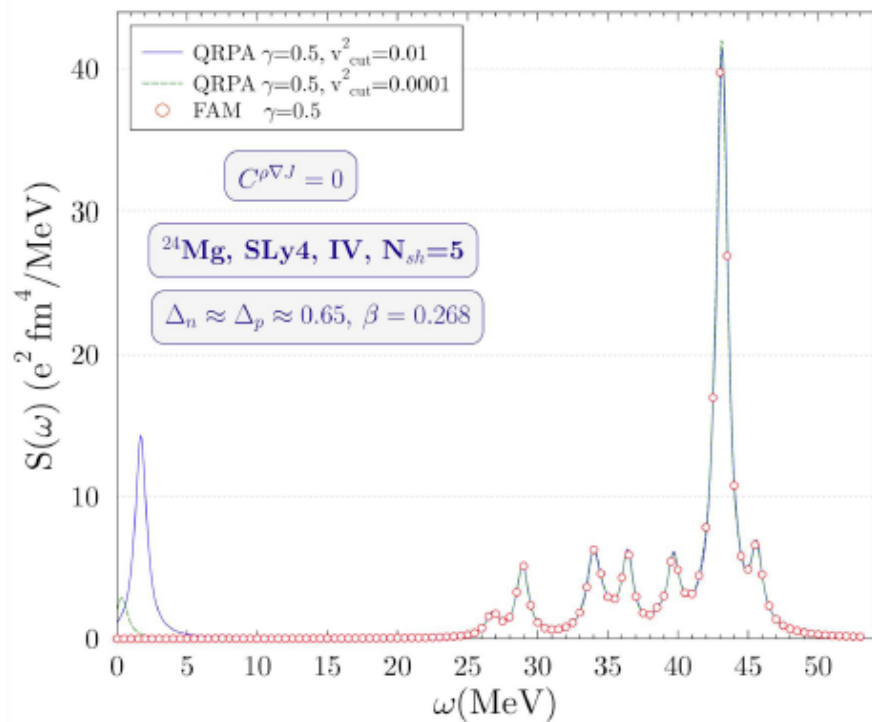
Optimization Algorithms for Calibrating Extreme Scale Simulations

Typical Challenges

- Computational expense of simulation only allows for evaluating a few sets of parameter values
- Derivatives with respect to parameters can be unavailable or intractable to compute/approximate
- Experimental data incomplete or inaccurate
- Sensitivity analysis/confidence regions desired

New Algorithm POUNDERS

- Exploits mathematical structure in calibration problems
- Benefits from expert knowledge
  - data, weights, uncertainties, etc.
- Obtains good fits in minimal number of simulations

POUNDERS obtains better solutions faster
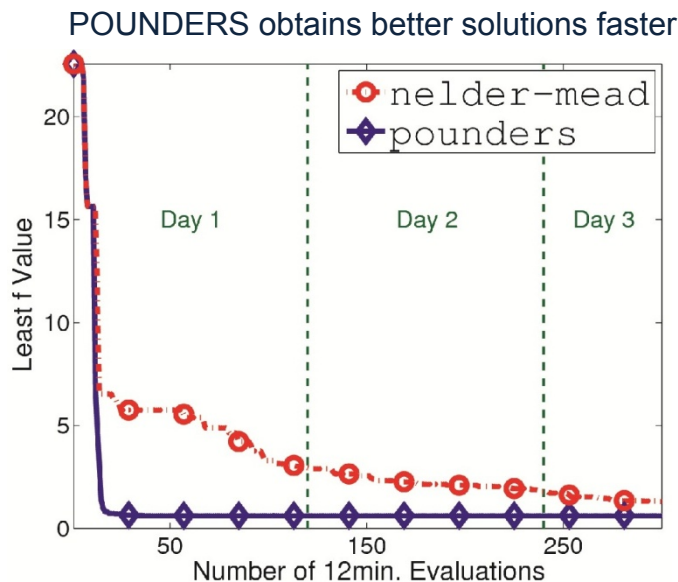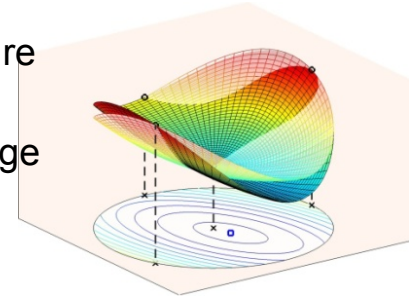
Energy density functionals (EDFs) for UNEDF

- Enables fitting of complex, state-of-the-art EDFs
  - Optimization previously avoided because too many evaluations required to obtain desirable features
- Substantial computational savings over alternatives
- Using resulting EDF parameterizations, the entire nuclear mass table was computed and is now distributed at **www.massexplorer.org**
  - *Nuclear Energy Density Optimization. Kortelainen et al., Physical Review C 82, 024313, 2010*
  - *Three joint physics & optimization publications @ SciDAC11!*

Quality Control

Integral to this project is the verification of methods and codes, the estimation of uncertainties, and assessment.
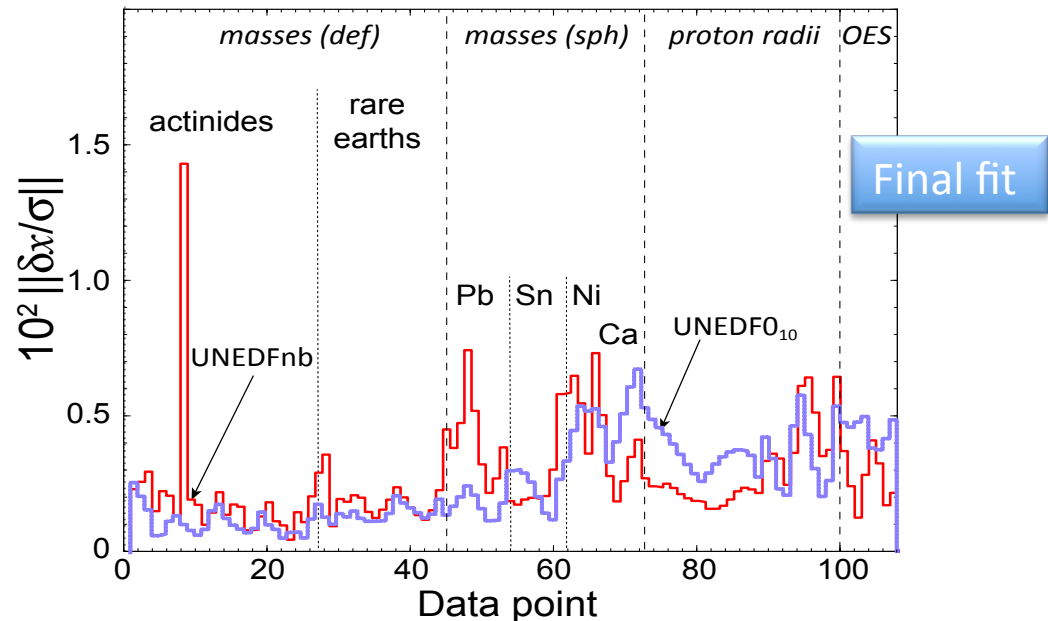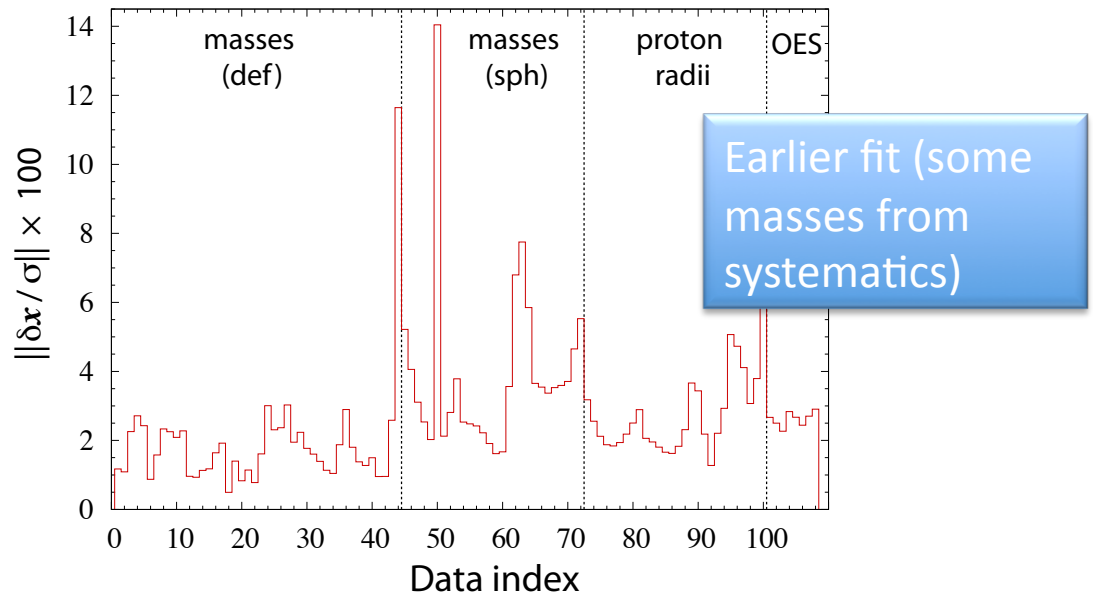
Verification and Validation
- Cross-check of different methods and codes
- Benchmarking

Uncertainty Quantification and Error Analysis
- Tools for correlation analysis to estimate errors and significance
- Uncertainty analysis

Assessment
- Development and application of statistical tools
- Analysis of experimental data significance

- UNEDF1 functional – optimized for large deformations and fission
- UNEDF2 functional – shell effects + neutron droplets added
- UNEDF3 functional – novel density dependence + GRs added
- POUNDERS in action!
- MADNESS-HFB; treatment of HFB continuum
- Orbital-based DFT
- Phenomenological N3LO functionals