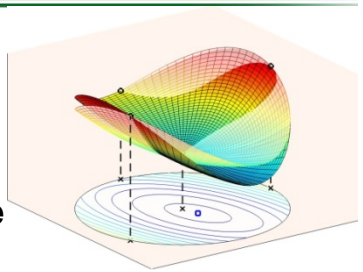
“Derivative-free Optimization for Density Functional Calibration” - Moré & Wild, ANL

ASCR- Applied Mathematics Highlight

Objectives

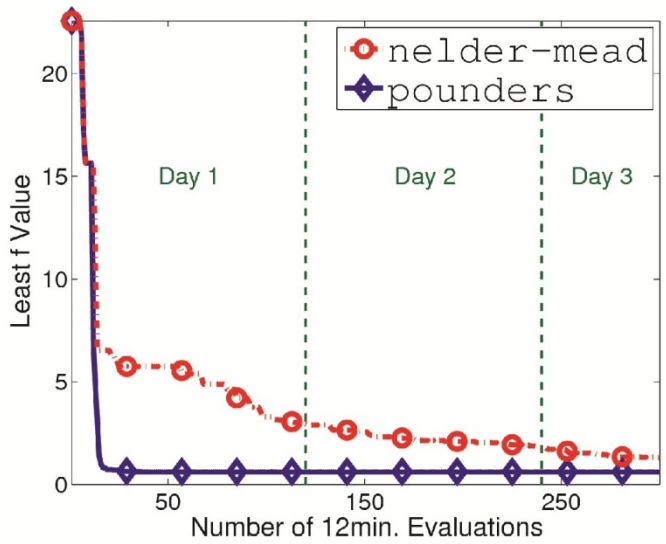
- **Develop optimization algorithms for calibrating UNEDF energy density functionals (EDFs) to selected experimental observables**
- **Exploit the mathematical structure of this calibration problem**
- **Enable sensitivity analysis**



Impact

- **Provide UNEDF with properly optimized functionals for wide classes of nuclei and diverse physical observables**
- **New computational tools for calibrating large scale computer simulations for applications outside of UNEDF project**
- **New statistical tools for providing uncertainty quantification and error analysis, and new experimental data assessment**

POUNDERS obtains better solutions faster



Progress / Accomplishments 2010

- New code, POUNDERS, yields substantial computational savings over alternative algorithms
- Enables fitting of complex EDFs -- previous optimizations required too many evaluations to obtain desirable features
- Using the resulting EDF parameterization, *UNEDF0,* the entire nuclear mass table was computed
- “Nuclear Energy Density Optimization.” M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. Stoitsov, and S. Wild. Physical Review C **82**, 024313 (2010).