Quantifying Uncertainties in Nuclear Density Functional Theory

P(ND)2-2 – Second International Workshop on Perspectives on Nuclear Data for the Next Decade

October 14 – 17, 2014

Nicolas Schunck

Lawrence Livermore National Laboratory

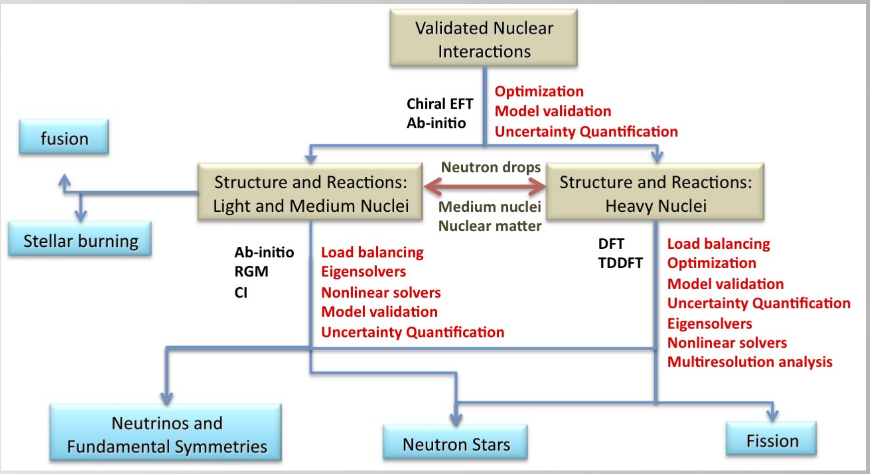
LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

The NUCLEI SciDAC 3 Collaboration

NUCLEI Mission Statement

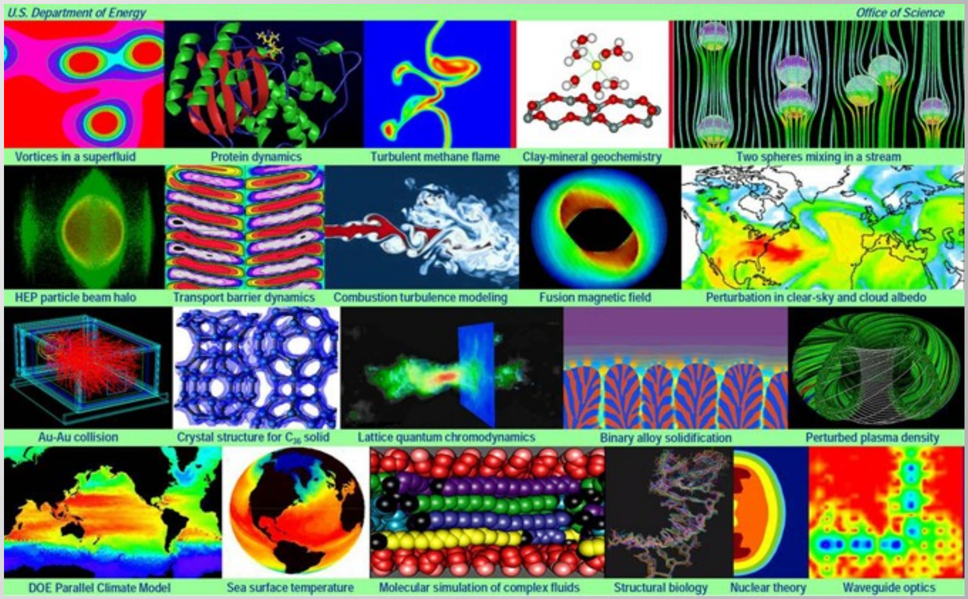
The NUCLEI (Nuclear Computational Low-Energy Initiative) SciDAC project builds upon recent successes in large-scale computations of atomic nuclei to provide results critical to nuclear science and nuclear astrophysics, and to nuclear applications in energy and national security.



NUCLEI
Nuclear Computational Low-Energy Initiative

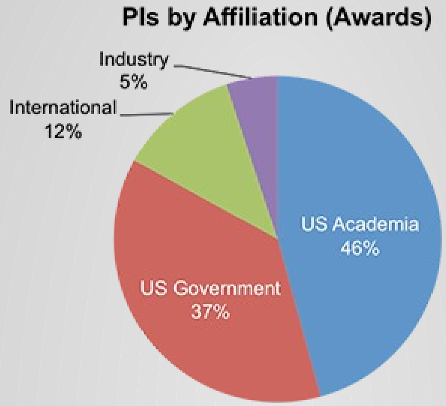
SciDAC Mission Statement

The U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program was created to bring together many of the nation's top researchers to develop new computational methods for tackling some of the most challenging scientific problems



The INCITE Program

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING



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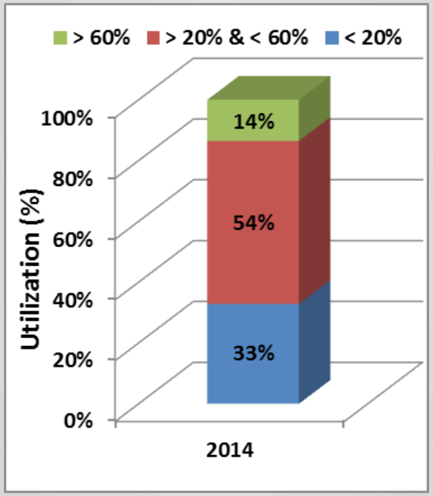
The U.S. Department of Energy (DOE) Office of Science provides a portfolio of national high-performance computing facilities housing some of the world's most advanced supercomputers. These leadership computing facilities enable world-class research for significant advances in science.



Types of jobs

Type: New
Title: "Nuclear Structure and Nuclear Reactions"

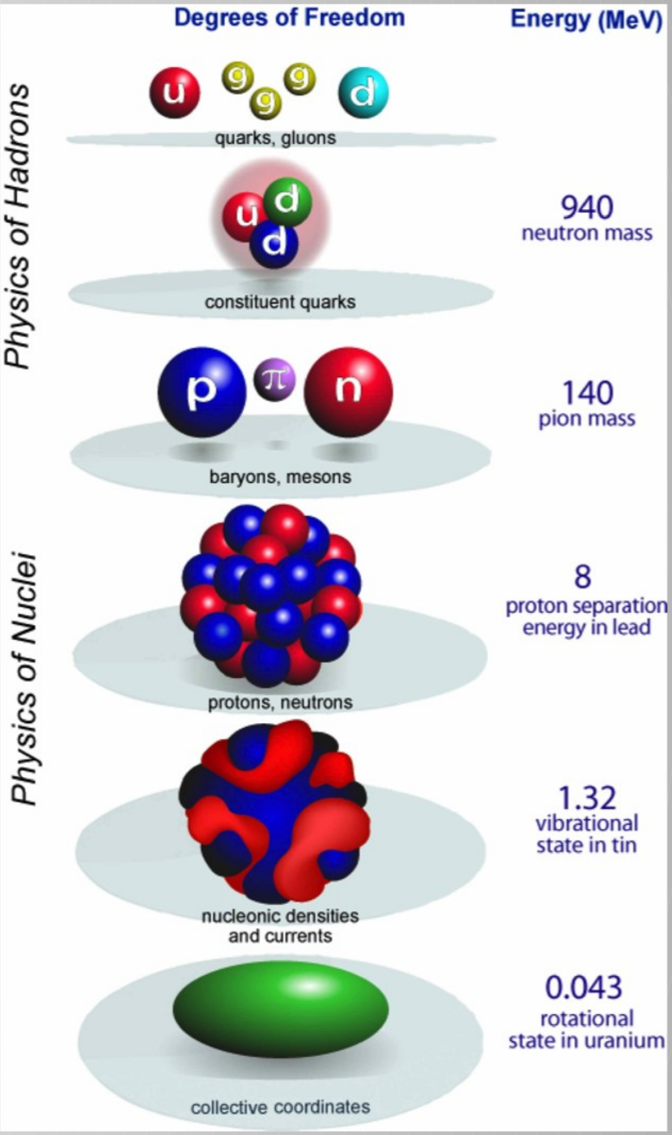
Principal Investigator: James Vary, Iowa State University
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Gaute Hagen, Oak Ridge National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Oak Ridge National Laboratory
Petr Navratil, TRIUMF
Witold Nazarewicz, University of Tennessee-Knoxville
Steven Pieper, Argonne National Laboratory
Nicolas Schunck, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **204,000,000 processor hours**
Site: Oak Ridge National Laboratory **Machine (Allocation):** Cray XK7 (104,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

- 4th largest allocation for 2014-2017
- Supports 6 programs solving the nuclear many-body problem
- Hybrid MPI/OpenMP model, some with GPU, scale up to full machine

The Nuclear Hierarchy



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- Hierarchy of degrees of freedom
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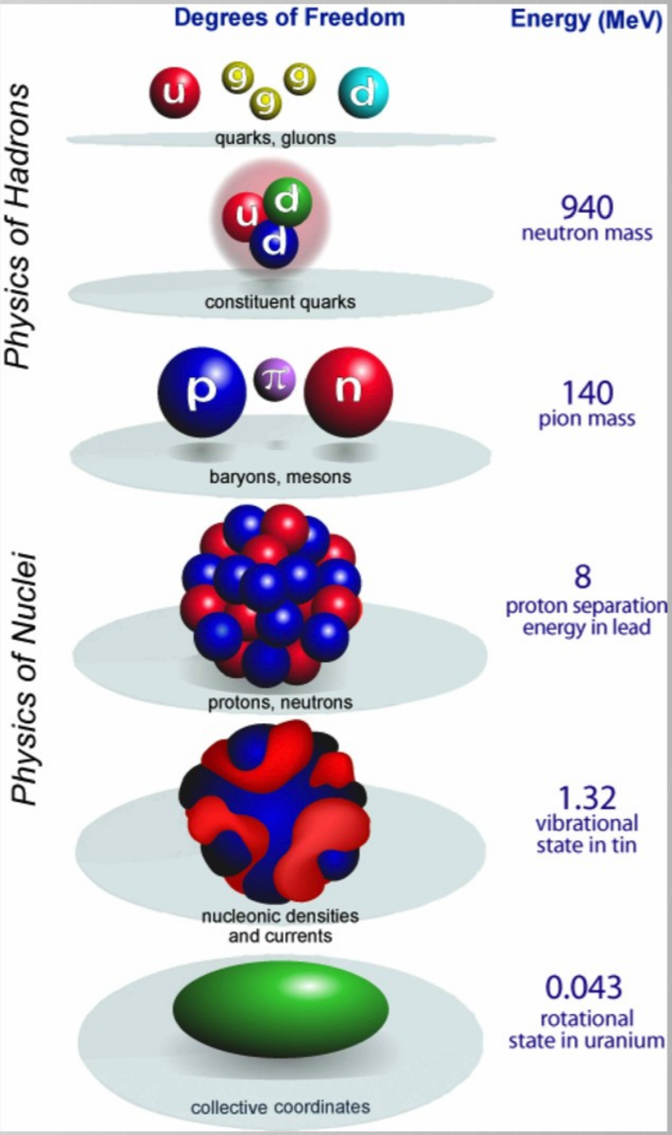

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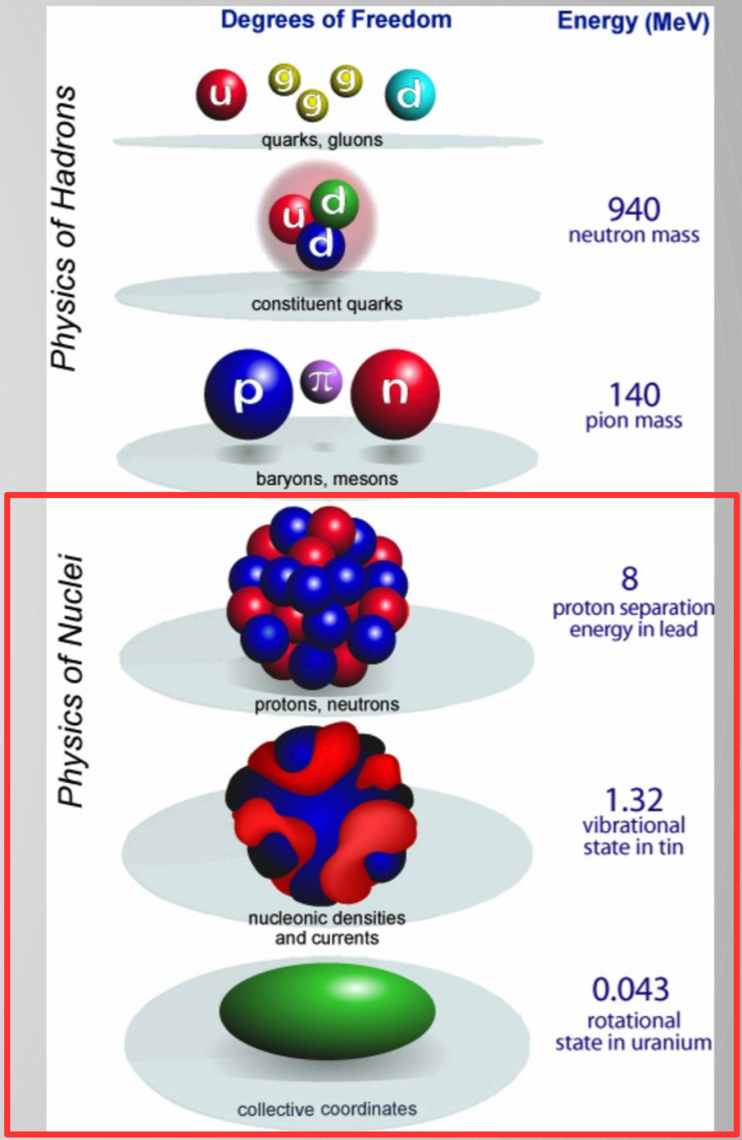

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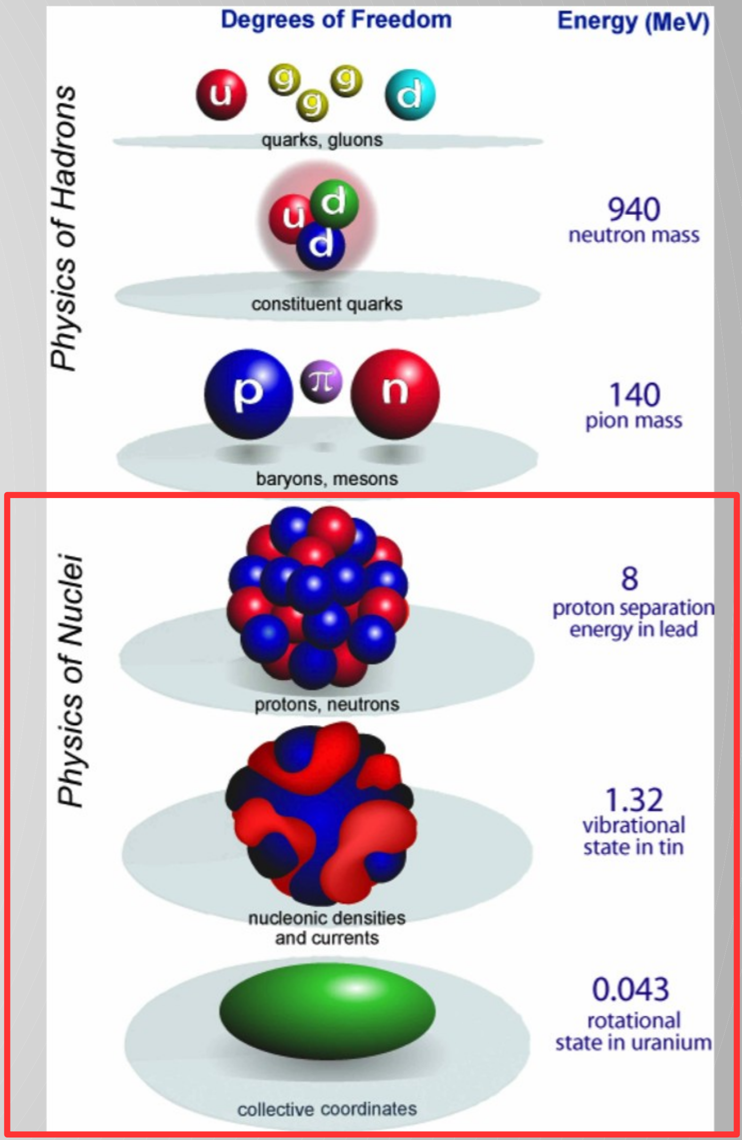
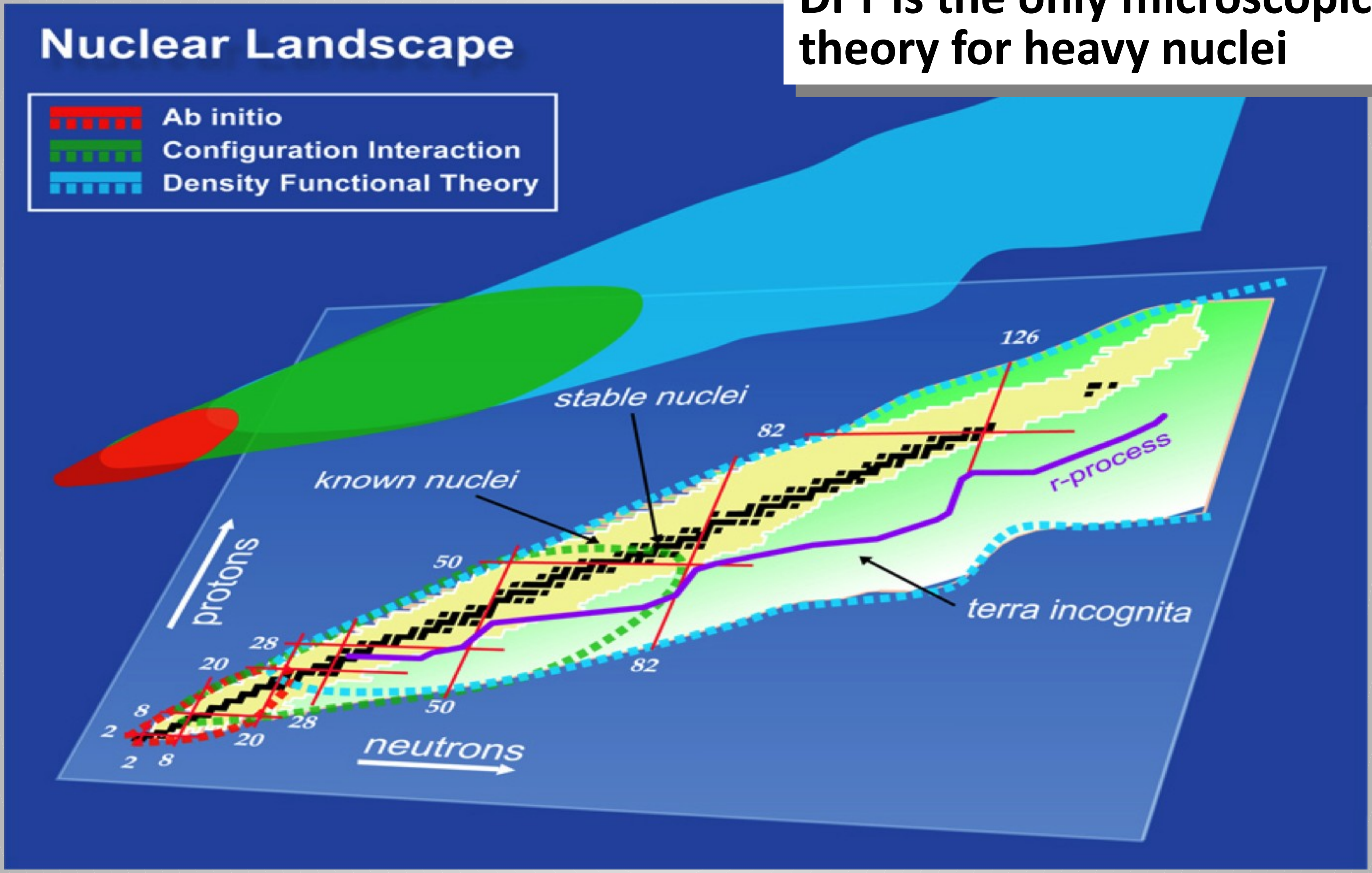
- Nuclear density functional theory (DFT)
  - Built on effective nuclear forces between protons and neutrons
  - Uses densities of nucleons as fundamental degrees of freedom
  - Relies on symmetry breaking



The Realm of Nuclear DFT

DFT is the only microscopic theory for heavy nuclei



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- Examples: Skyrme (zero-range) and Gogny (finite-range) forces

Reviews: RMP **75**, 121 (2003), Prog. Part. Nucl. Phys. **64**, 120 (2010)
Skyrme: PRC **5**, 626 (1972); Gogny: PRC **21**, 1568 (1980)

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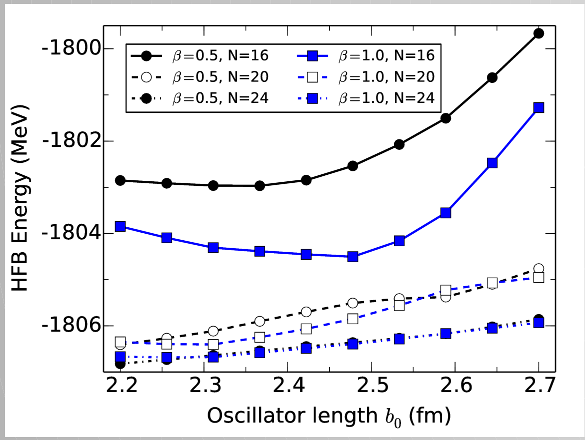

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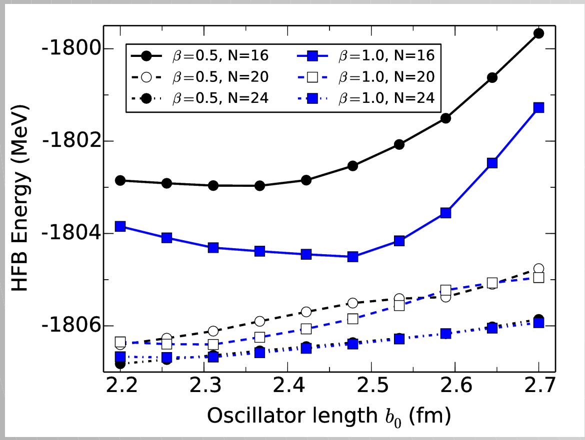

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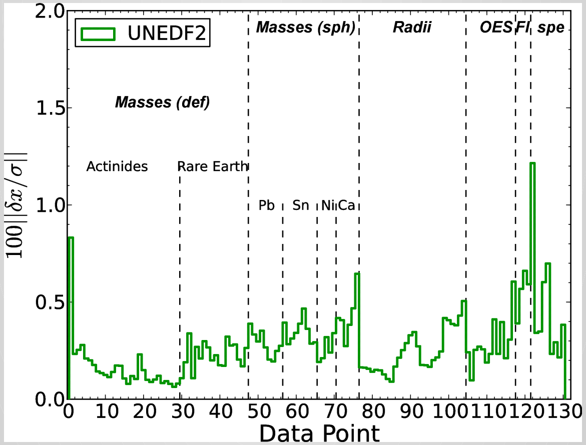

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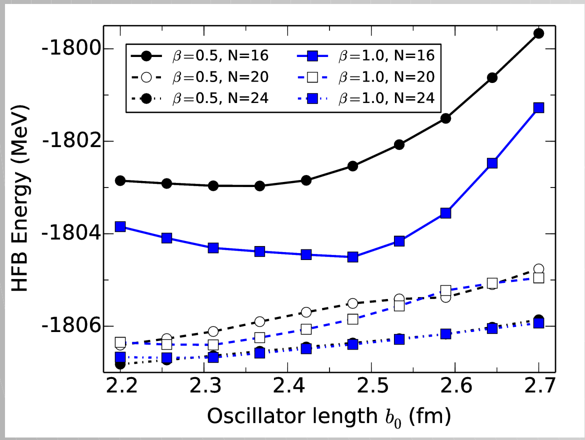
  - Systematic errors caused by the choice of the functional



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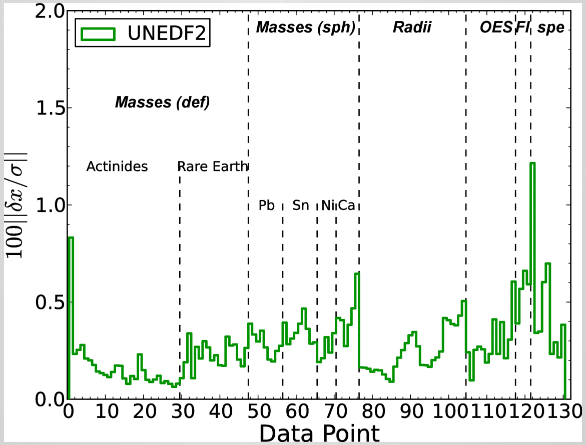

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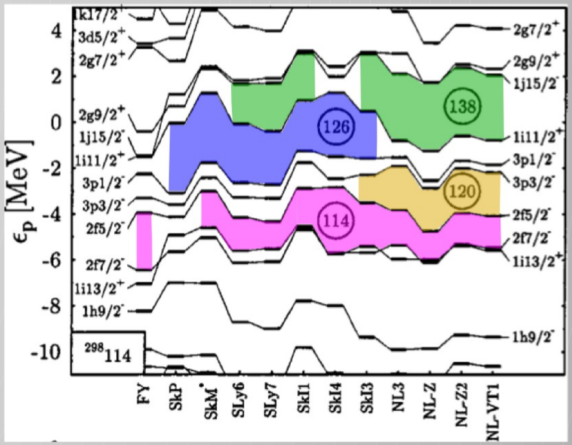

Systematic errors
*From PRC **61**, 034313 (2000)*

Skyrme Energy Density

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- Starting from the Skyrme effective force, write the energy of the system as the integral (over space) of the Skyrme EDF

$$E = \int d^3\boldsymbol{r} \left[\mathcal{E}_{\mathrm{kin}}(\boldsymbol{r}) + \mathcal{E}_{\mathrm{Cou}}(\boldsymbol{r}) + \mathcal{E}_{\mathrm{pair}}(\boldsymbol{r}) + \sum_{t=0,1} \chi_t(\boldsymbol{r}) \right]$$

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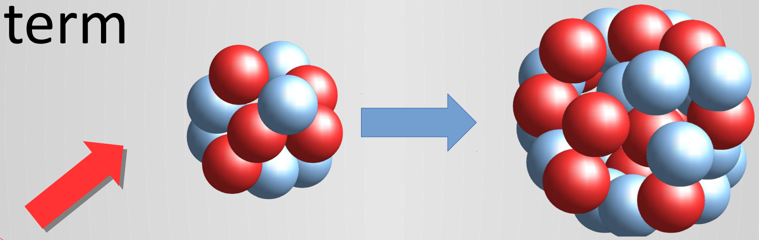

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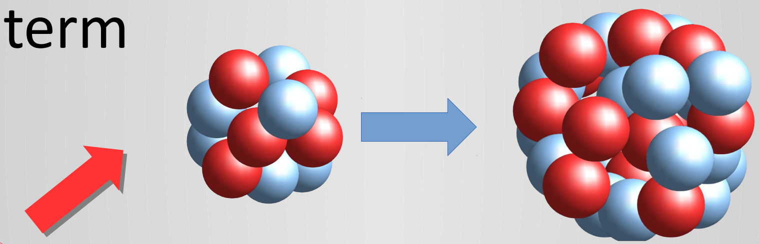

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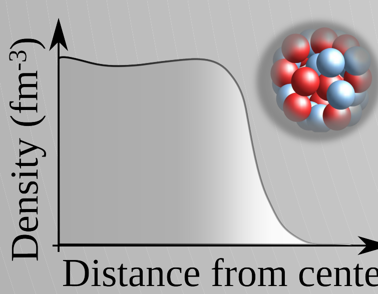

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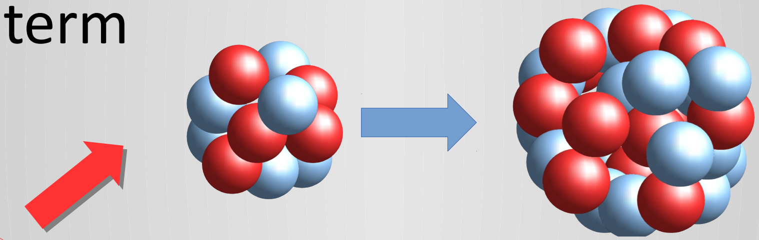

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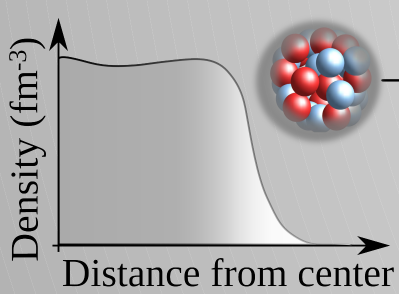

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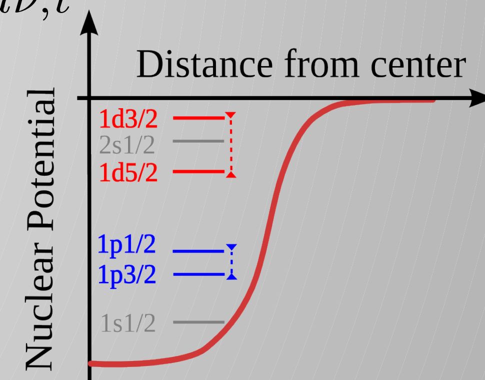

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Skyrme mass model: PRC **62**, 024308 (2000), PRC **88**, 061302(R) (2014); Gogny mass model: PRL **102**, 242501 (2009); FRLDM: PRL **108**, 052501 (2012), Atom. Data and Nucl. Data Tab. **59**, 185 (1995); UNEDF: PRC **82**, 024313 (2010), PRC **85**, 024304 (2012), PRC **87**, 054314 (2014)

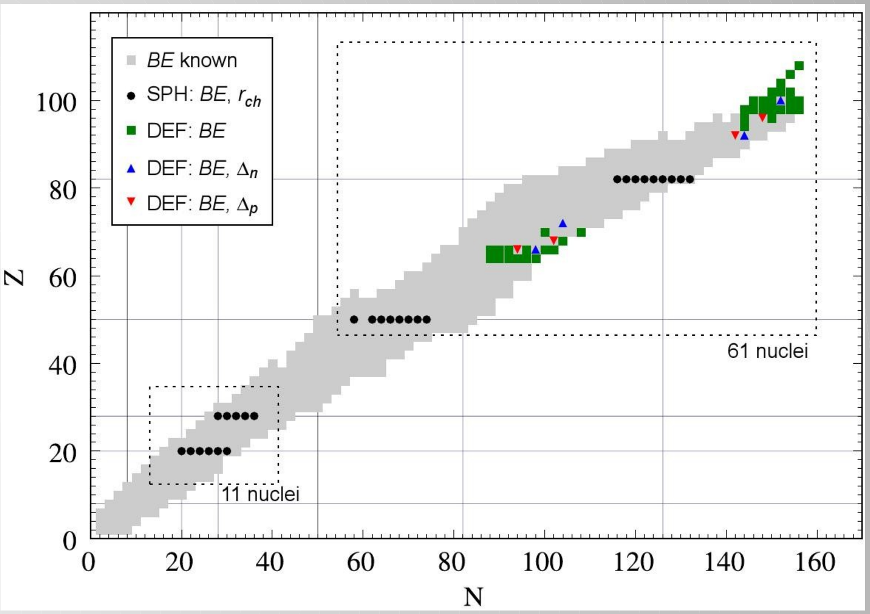
The UNEDF Protocol

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

- Fit at deformed HFB level
- Composite χ_2

$$\chi_2 = \frac{1}{n_d - n_x} \sum_{t=1}^{T} \sum_{i=1}^{n_T} \left(\frac{y_{it}(\boldsymbol{x}) - d_{it}}{\sigma_t} \right)^2$$

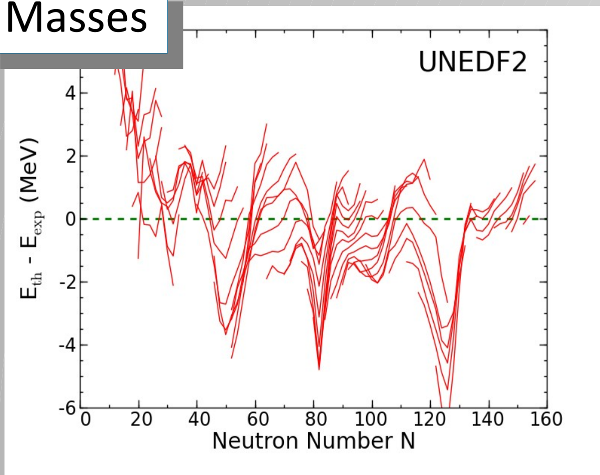
- Supplement "best-fit" with full covariance and sensitivity analysis
  - Provide sensitivity on data points
  - Covariance matrix allows uncertainty propagation



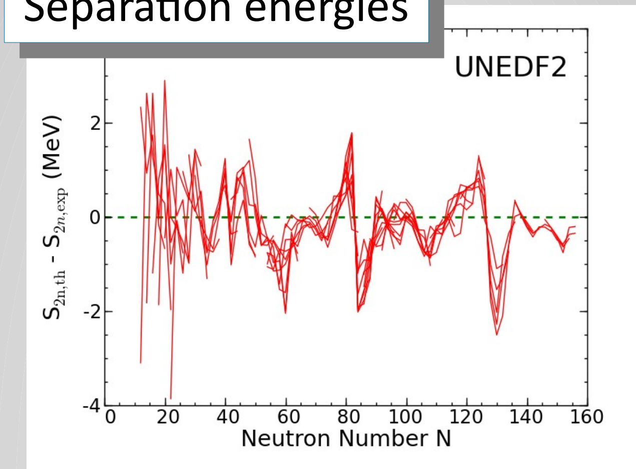
	UNEDF0	UNEDF1	UNEDF2
Number of parameters n_x	12	12	14
Type of data t	Masses, r.m.s. radii, OES (*T=3*)	Masses, r.m.s. radii, OES, E* fission isomer (*T=4*)	Masses, r.m.s. radii, OES, E* fission isomer, s.p. splittings (*T=5*)
Number of data points n_d (total)	108	115	130

The UNEDF Family

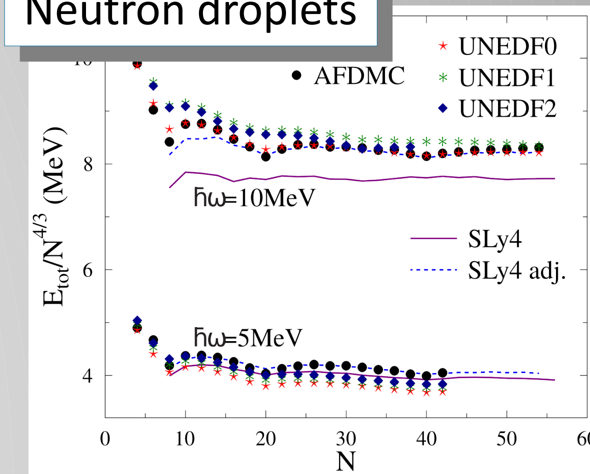
Masses



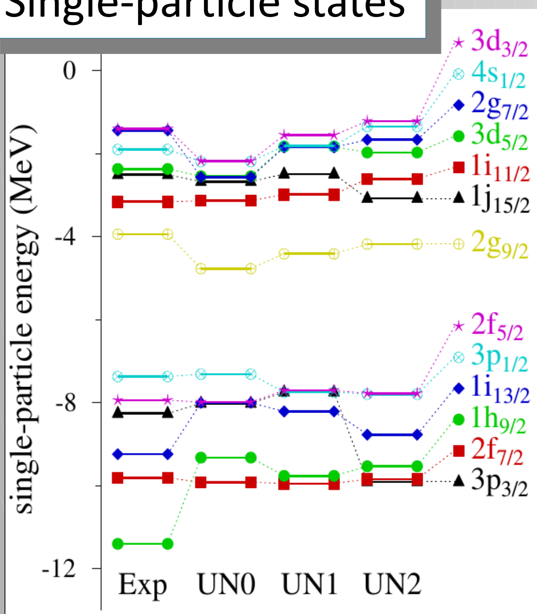
Separation energies



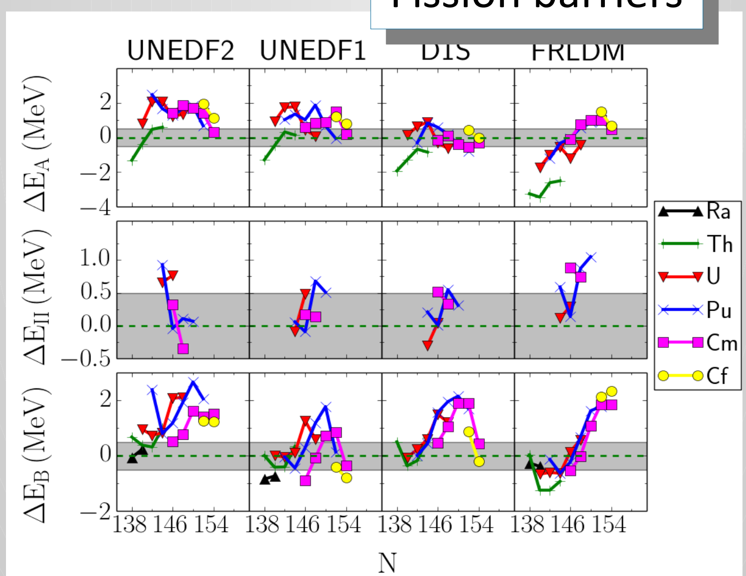
Neutron droplets



Single-particle states

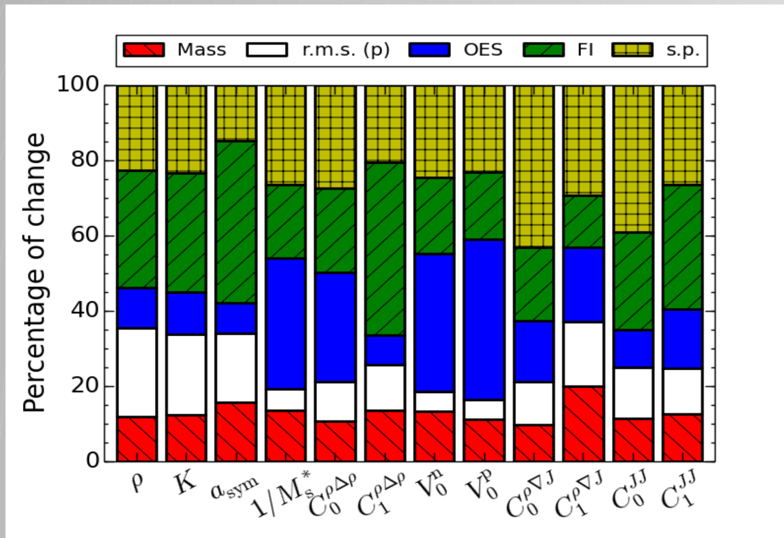


Fission barriers

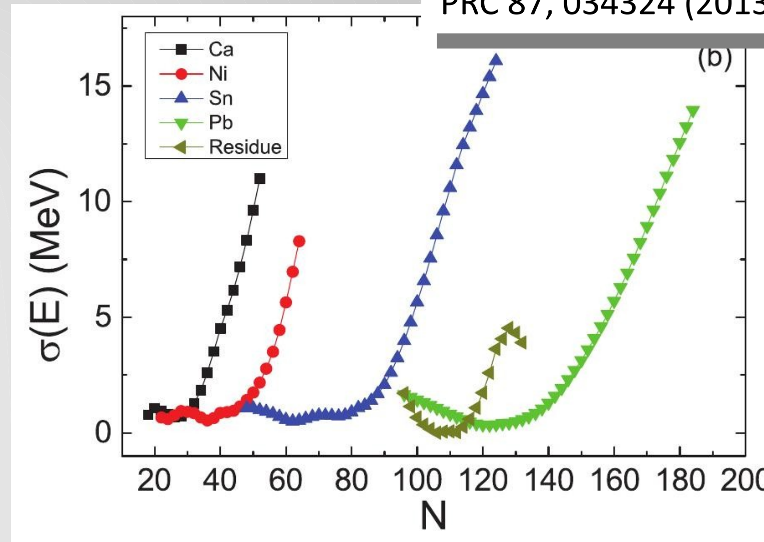


- UNEDF functionals are all-round functionals
- Quality degrades when more constraints added
- Skyrme form too limited

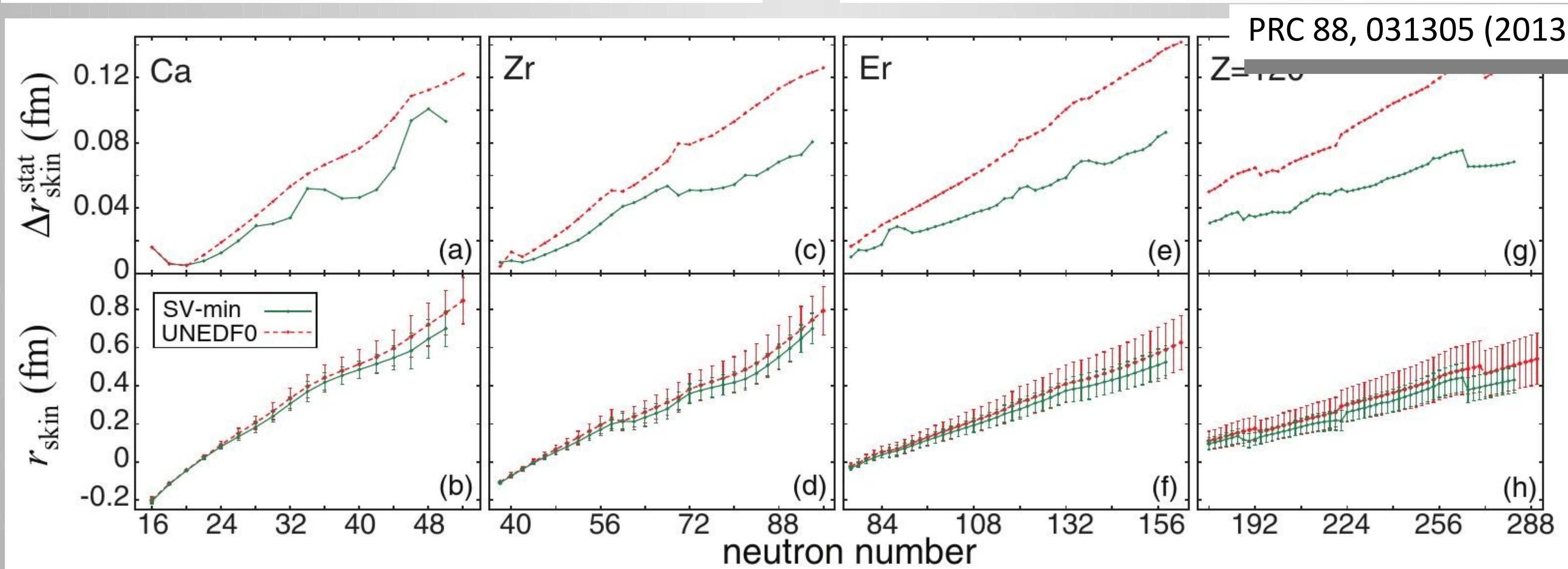
Covariance Analysis



PRC 87, 034324 (2013)



PRC 88, 031305 (2013)



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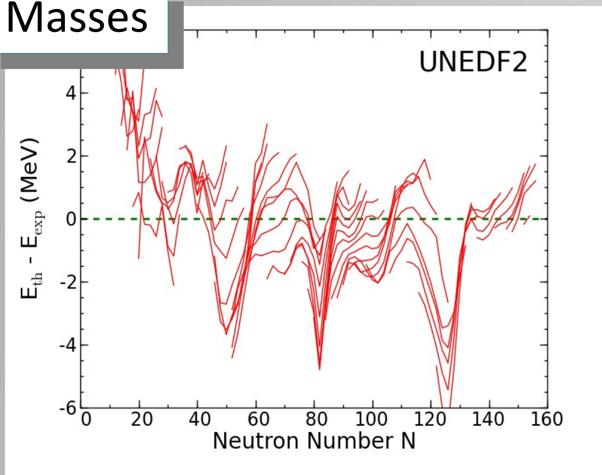

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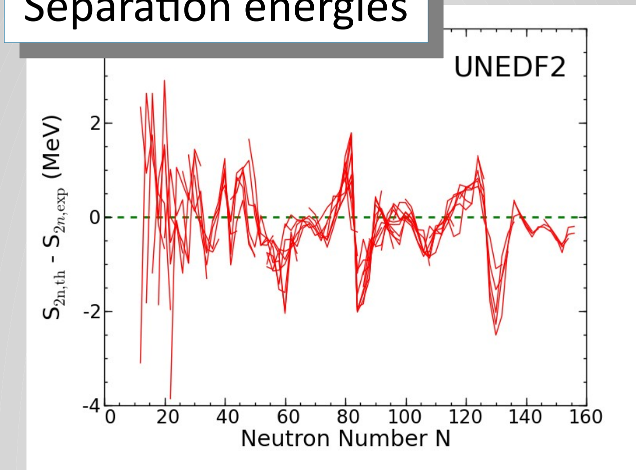

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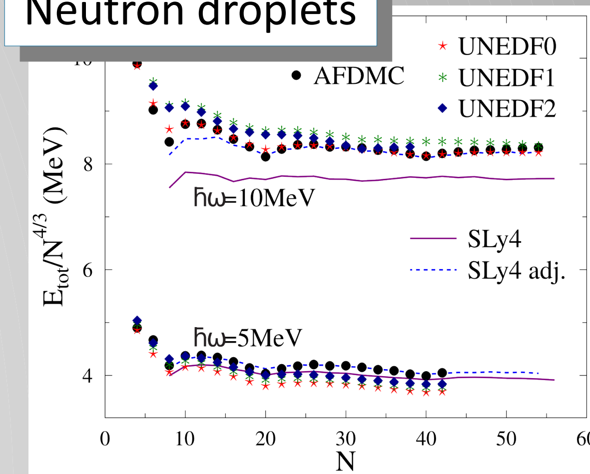

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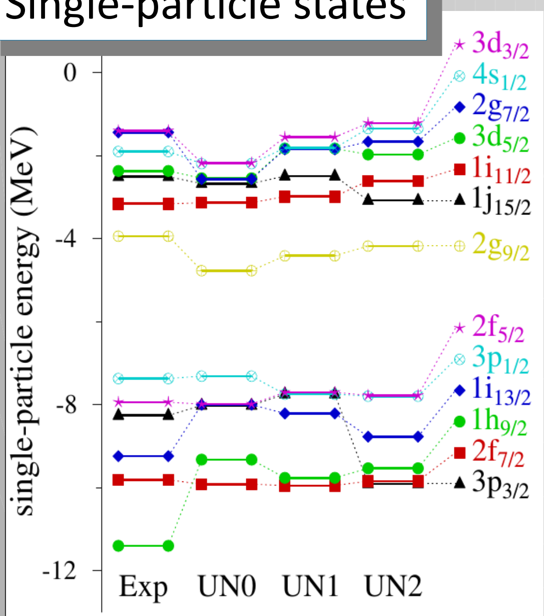

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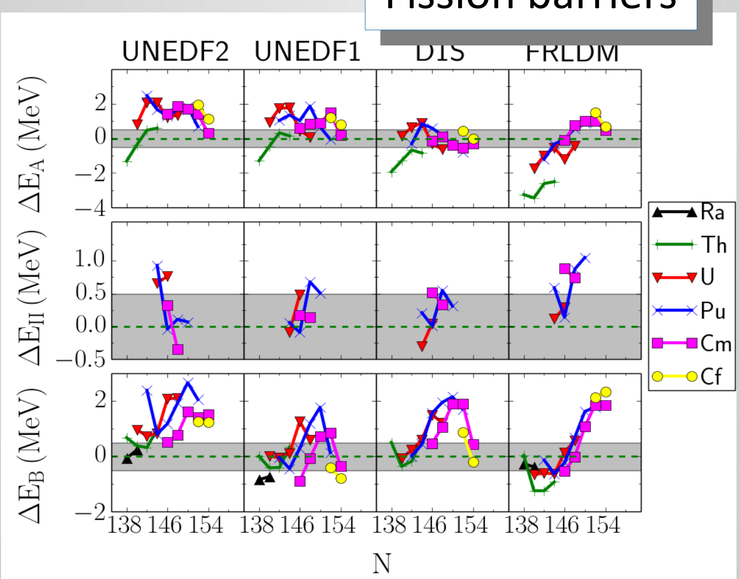

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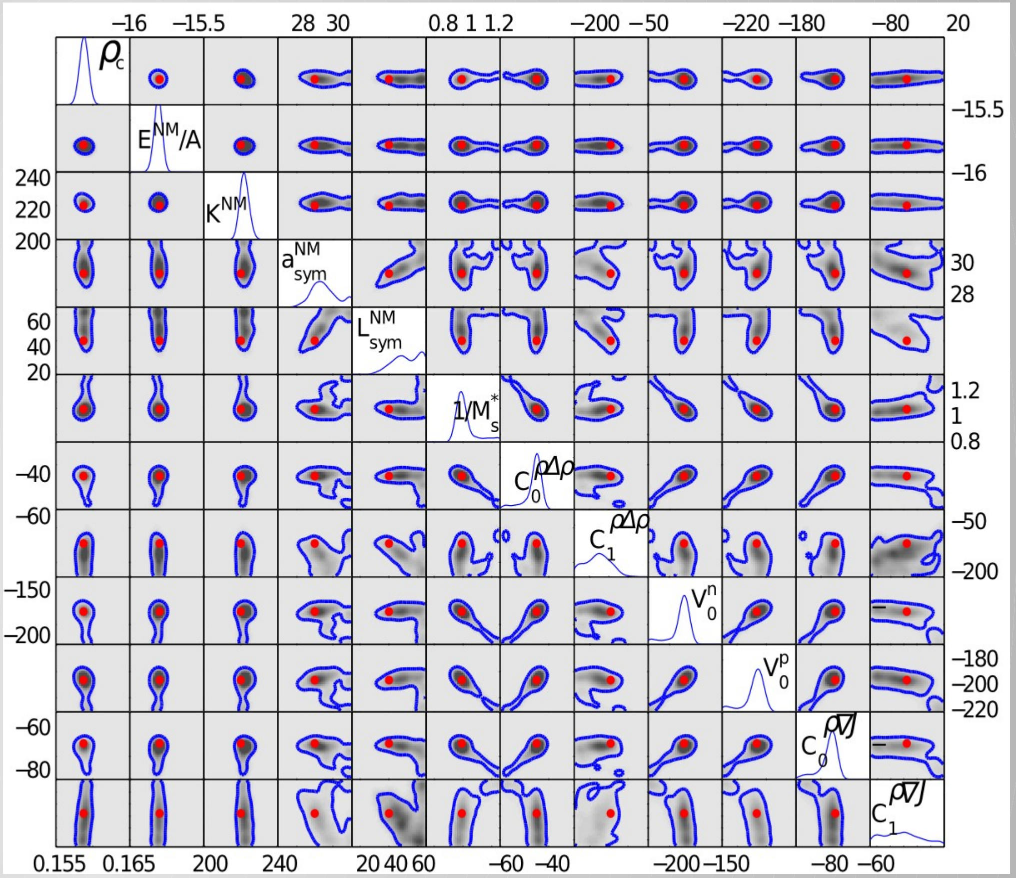

Bivariate posterior distribution for the UNEDF1 Skyrme functional. *arXiv:1407.3017, arXiv:1406.437*

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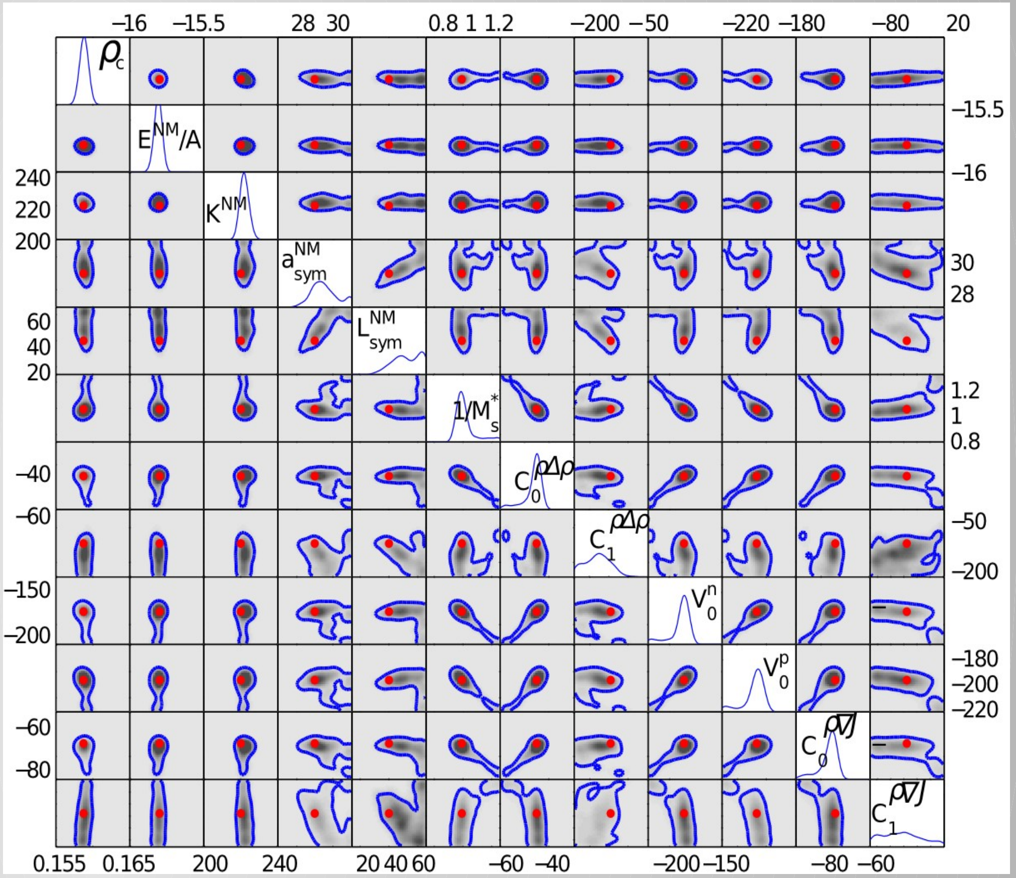

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UQ work: ~5 M CPU hours

Propagating Uncertainties

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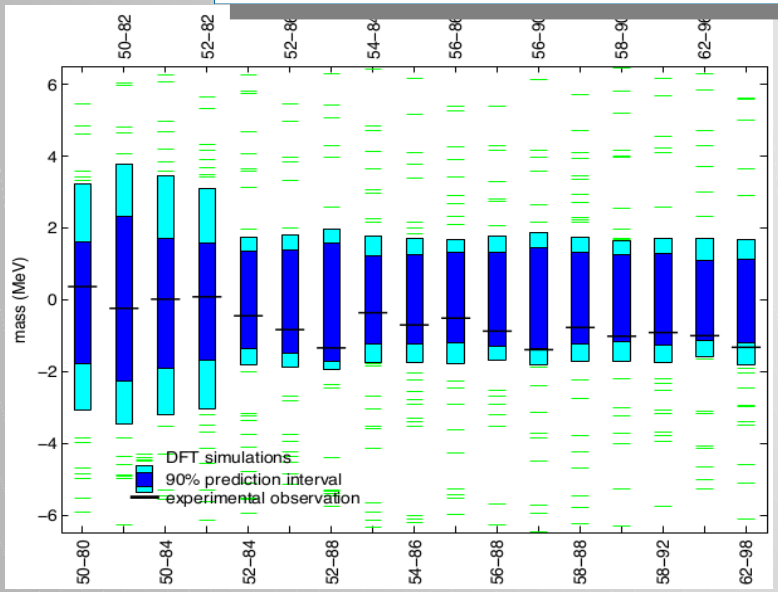
Masses of neutron-rich nuclei



Propagating Uncertainties

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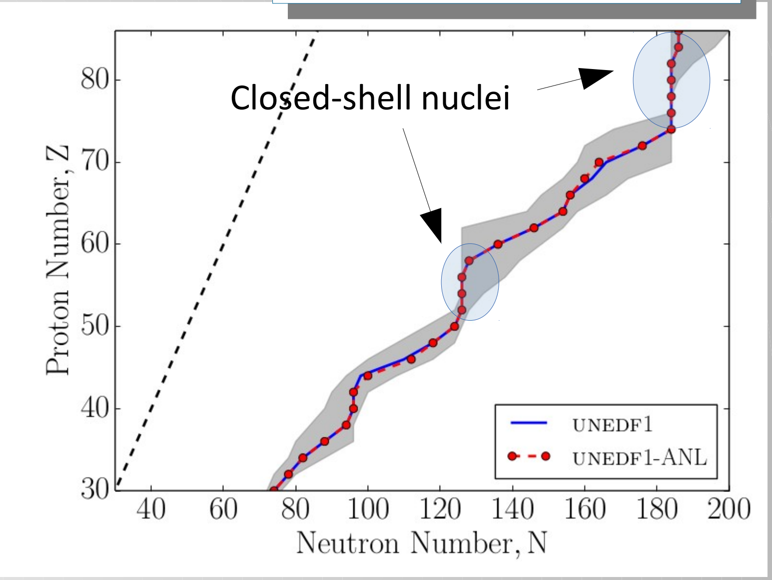
Two-neutron driplines



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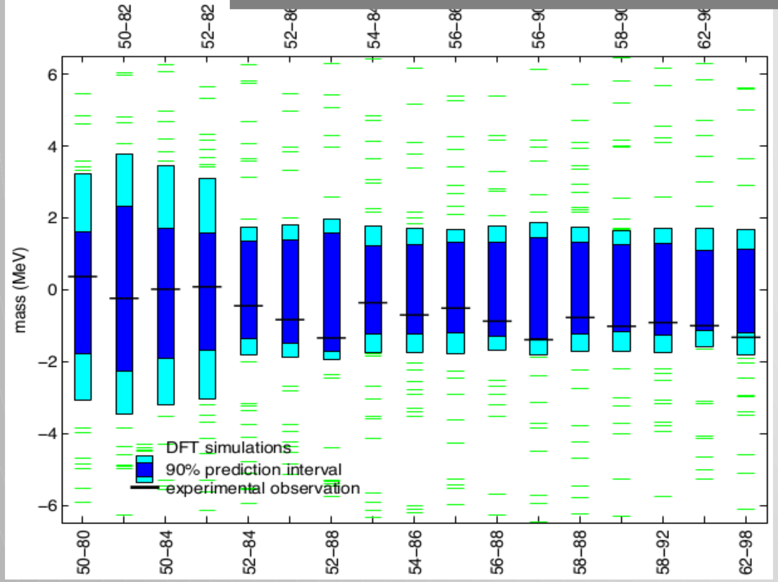

Propagating Uncertainties

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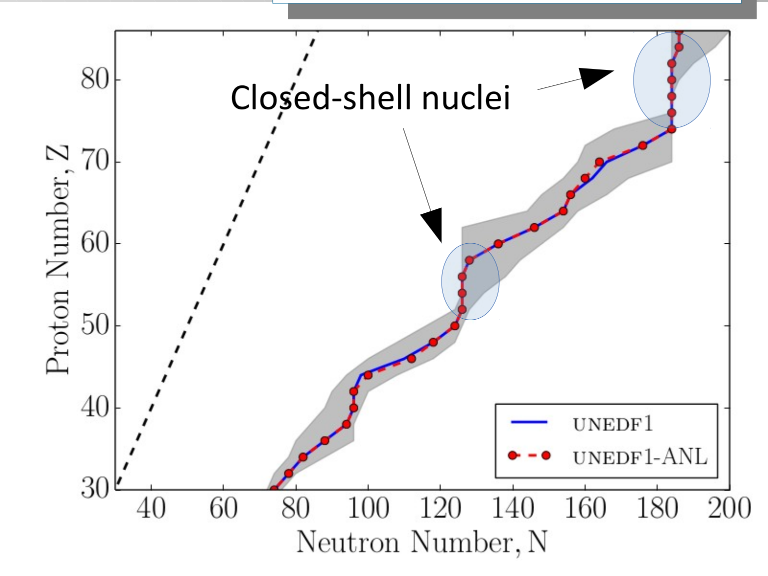
- Large statistical errors in fission barriers translate into orders of magnitude uncertainties for half-lives

Two-neutron driplines



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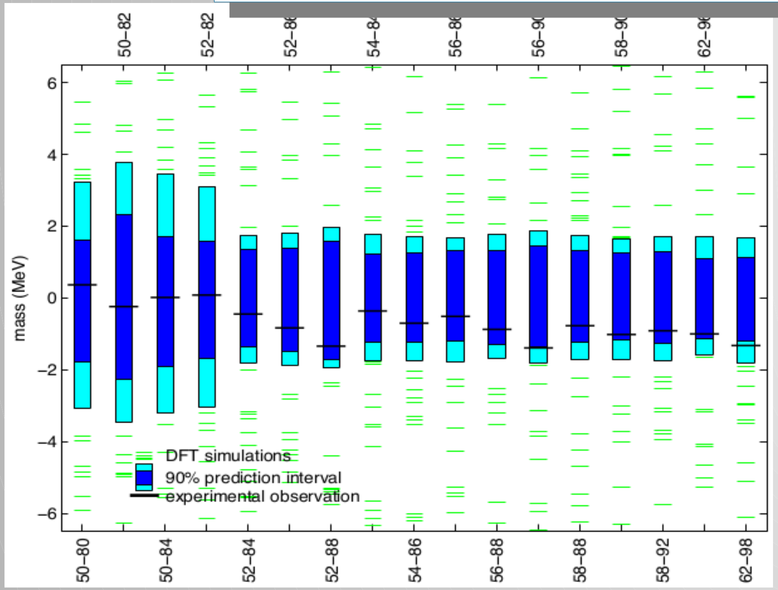
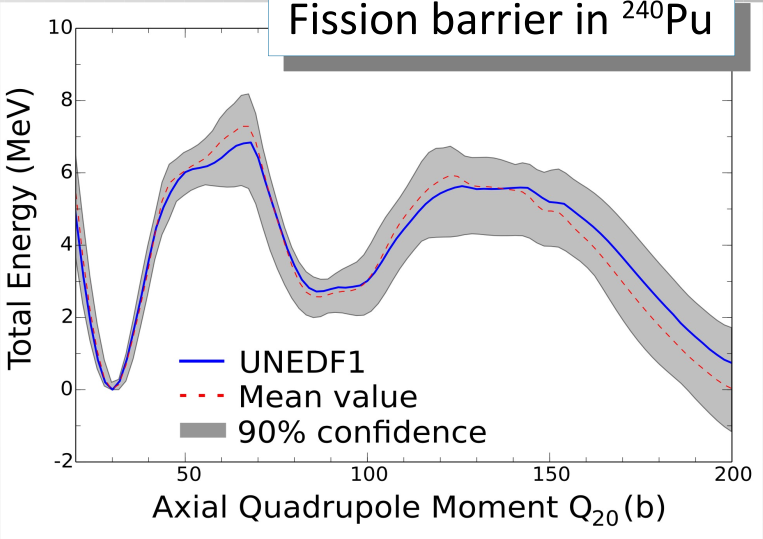


Fission barrier in ^{240}Pu



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- Challenges
  - Improve the connection between the EDF and theory of nuclear forces
  - Propagate uncertainties in complex problems such as decays, spectroscopy

Lawrence Livermore
National Laboratory