Computational Nuclear Structure

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Techniques for Solving Nuclear DFT Equations

Basis Expansion Methods (1/2)

Basis expansion techniques are based on configuration space representation of operators: one introduces a "convenient" basis of the Hilbert space of *single-particle* states $|a\rangle$, $\langle \boldsymbol{r}|a\rangle \equiv \phi_a(\boldsymbol{r})$.

Solutions to the DFT equations are then expanded on that basis, for example

- Hartree-Fock s.p. orbitals, i.e., the eigenstates $|\alpha\rangle$ of the HF Hamiltonian, are written

$$|\alpha\rangle = \sum_a C_{a\alpha}|a\rangle; \tag{1}$$

- In the HFB theory, the matrix of the Bogoliubov transformation is written

$$\begin{pmatrix} U_\alpha \\ V_\alpha \end{pmatrix} = \sum_a \begin{pmatrix} U_{a\alpha} \\ V_{a\alpha} \end{pmatrix} |a\rangle. \tag{2}$$

Basis Expansion Methods (2/2)

Why use basis expansion methods?

- DFT is remapped into a pure linear algebra problem, which can be solved by successive matrix diagonalizations, or by the conjugate gradient method using optimized libraries;
- Basis techniques can be adapted to almost any geometry, while more direct methods become very costly for complex nuclear shapes.

Diasadvantages

- The spatial part of s.p. states belongs to $\mathcal{L}_2(\mathbb{R})$: basis expansion techniques are exact only in the infinite limit. *Every numerical implementation leads to truncation errors*.
- There are few basis that combine all the necessary properties: analyticity, good convergence with the number or states, etc.

The Harmonic Oscillator Basis

The Harmonic oscillator is by far the most popular basis used in nuclear DFT calculations...

- It is analytical for the three main systems of coordinate, Cartesian, cylindrical and spherical;
- Moshinksy transformations allow to neatly, and exactly, separate the center-of-mass motion from the relative motion;
- The HO potential is a good approximation of the deeper part of the nuclear mean-field.

...but it is not perfect (of course)

- Basis function behave like Gaussians at $r \to +\infty$, while realistic nuclear wave functions should fall off like e^{-kr}: the HO basis yields the wrong asymptoptic behavior of wave functions;
- The HO depends on a number of parameters: the frequency ω_0, the ratio of frequencies in cylindrical or Cartesian coordinates, the number of shells, the number of states, etc.

Coordinate Space Representation

In coordinate space, the HFB equations take the form

$$\int d^3\boldsymbol{r}' \sum_{\sigma'} \begin{pmatrix} +h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') & +\Delta(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') \\ -\Delta^*(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') & -h^*(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') \end{pmatrix} \begin{pmatrix} U(E,\boldsymbol{r}'\sigma') \\ V(E,\boldsymbol{r}'\sigma') \end{pmatrix} = \begin{pmatrix} E+\lambda & 0 \\ 0 & E-\lambda \end{pmatrix} \begin{pmatrix} U(E,\boldsymbol{r}\sigma) \\ V(E,\boldsymbol{r}\sigma) \end{pmatrix} \quad (3)$$

These equations can be solved directly by numerical integration for each energy E, with the following caveats

- Boundary conditions must be specified for the U and V components;
- In the general case, the eigenspectrum is both discrete (for $|E| < |\lambda|$), and continuous;
- Direct integration techniques for Ordinary Differential Equations (ODE) must be used (Runge-Kutta, Numerov, etc.)

Pros and Cons of the Coordinate Space Representation

Better physical accuracy and numerical precision...

- The numerical accuracy of solving the HFB equations in coordinate space is much higher than basis expansions, which yields numerically nearly exact results.
- Since equations are solved in a box (typically $R \approx 20$ fm), the decription of the continuum is much better.

... but only affordable in spherical nuclei for local functionals

- Implementations of the HFB equations for local functionals in spherical symmetry are very fast (a few seconds), but extensions to axial symmetry are much more expensive (a few dozens of CPUS for half a day), and 3D codes do not exist;
- Finite-range pseudopotentials (or functionals of the non-local density) are much more difficult to handle: not yet done.

Benchmarking Basis Expansion Against Direct Integration

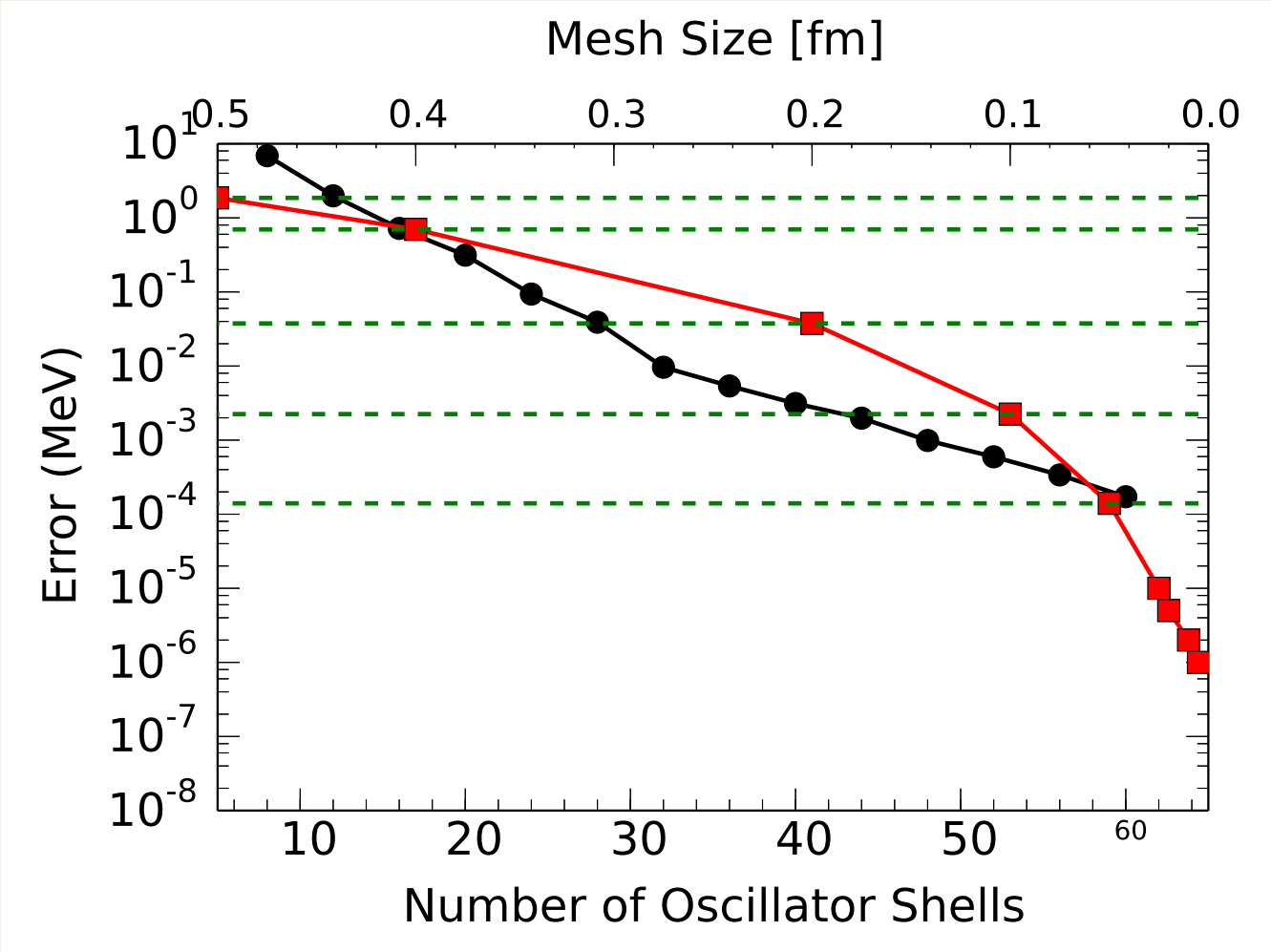


Figure 1: Convergence of a HF calculation in ^{208}Pb with a Skyrme functional as a function of the number of HO shells (black dots) and mesh size (red square).

Public DFT Solvers (1/3)

In spherical symmetry, 5 solvers are available in CPC:

- **HOSPHE** – Uses a HO expansion to solve the HFB equations; implements Skyrme functionals and general EDF with up to 6^{th} order derivatives couplings; pairing forces are simple density-dependent delta (DD) forces [1];
- **HFBRAD** – Uses the direct numerical integration of the HFB equations in coordinate space; implements only Skyrme functionals and DD pairing forces [2].
- **RMF** – Uses finite element analysis (FEA) to solve the relativistic Hartree equations (meson-echange formulation) [3];
- **RHB** – Uses FEA to solve the relativistic Hartree-Bogoliubov equations (meson-echange formulation); the pairing channel is treated with the Gogny force [3].
- **DIRHBS** – Solves the RHB equations (covariant DFT with point coupling model) in a HO basis; pairing include zero- and finite-range forces (Gogny, momentum separable) [4].

Public DFT Solvers (2/3)

In axial symmetry, 2 solvers are available:

- **HFBTHO** – Solves the HFB equations in the cylindrical HO basis or in the transformed HO basis obtained by applying a local scale transformation on the HO functions [5]. In its latest release, it implements general Skyrme functionals, can do multi-constrained calculations (up to $\lambda = 8$ including odd multipole moments), finite-temperature HFB calculations, etc. [6]. An experimental version (not yet published) also implements the density matrix expansion of chiral potentials.
- **DIRHBZ** - Solves the HFB equations in the cylindrical HO basis; allows constraints on axial quadrupole moment $\hat{Q}_{20}$; parity is conserved; included in the package DIRHB, hence includes the same features as DIRHBS, in particular with respect to pairing forces. [4].

Public DFT Solvers (3/3)

For non-conserved axial symmetry, 3 solvers are available:

- **Ev8** – Uses the imaginary time method to solve the HF+BCS equations on a lattice of points; In its latest version (under review), includes general Skyrme functional including those with tensor forces [**?**, 7];
- **HFODD** – The most versatile DFT solver; solves the HF, HF+BCS, HFB equations in the HO basis for Skyrme forces or functionals, Gogny and Yukawa forces; breaks all geometrical symmetries; includes isospin mixing and projection, angular momentum projection of HF states, multi-constrained calculations (including constraints on angular momentum), finite-temperature, etc. Based on a MPI/OpenMP programming model. [8, 9, 10, 11, 12, 13, 14].
- **DIRHBT** - Solves the HFB equations in the Cartesian HO basis; included in the package DIRHB, hence includes the same features as DIRHBS [4].

Benchmarking DFT Solvers

	HOSPHE	HFBTHO	HFODD
E_{tot} [MeV]	−2445.930 216	−2445.930 216	−2445.930 215
$E^{(\text{n})}_{\text{kin}}$ [MeV]	2614.806 852	2614.806 852	2614.806 852
$E^{(\text{p})}_{\text{kin}}$ [MeV]	1438.160 641	1438.160 641	1438.160 641
E_{Skyrme} [MeV]	−6498.897 708	−6498.897 708	−6498.897 706
E_{SO} [MeV]	−109.091 691	−109.091 691	−109.091 691
$r^{(\text{n})}_{\text{rms}}$ [fm]	5.519 846	5.519 846	5.519 846
$r^{(\text{p})}_{\text{rms}}$ [fm]	5.249 812	5.250 015	5.250 015

Table 1: Benchmark of the three solvers HOSPHE, HFBTHO and HFODD for a spherical Hartree-Fock calculation in ^{208}Pb with the SLy5 Skyrme functional in a full spherical basis of $N_{\text{max}} = 16$ shells with oscillator length $b = 2.0$ fm.

Related Technology

In addition to the DFT solvers themselves, several codes related to DFT in one way or another are available

- **skyrme_rpa** – The code solves the spherical HF equations in coordinate space with a Skyrme force, and uses the results to solve the RPA equations by matrix diagonalization [15]. The code is fully self-consistent: the same Skyrme force used for the mean-field is used for the residual interaction.
- **Sky3D** – The code solves the time-dependent Hartree-Fock equations for Skyrme forces. The initial density $\rho(t = 0)$ is obtained by solving the 3D HF equations in a Cartesian mesh with no symmetry assumption. Numerical techniques involve Fast Fourier Transforms to evaluate derivatives [16].

Applications of Nuclear DFT Solvers

What can you do with... a spherical DFT solver

In spherical symmetry, DFT equations can be solved

- very quickly (typically a few seconds);
- nearly exactly in coordinate space.

Spherical DFT solvers are, therefore, very useful to

- Benchmark approximations to the many-body problem, see your computational projects...
- Study the precision of numerical truncation schemes

Doubly-closed shell nuclei and nuclei along several semi-magic isotopic lines are spherical

- Study of the isovector channel of the EDF/pseudopotential
- Analysis of low-lying spectrum using (Q)RPA

... but about 95% of all atomic nuclei are deformed already in their ground-state.

What can you do with... an axially-symmetric DFT solver

Nearly all nuclei are deformed, and all of those are axially deformed in their ground-state.

Axially-symmetric DFT solvers based on basis expansions are still very fast: a few minutes to obtain the HFB solutions for a heavy nucleus [6].

Applications

- *Large-scale static calculations*: nuclear binding energies, separation energies, Q-values, r.m.s. radii, etc.
- Collective rotational bands are built upon static (often, axially-) deformed DFT solutions: axially-symmetric solvers are key to *nuclear γ spectroscopy*
- Recently, new technology (Finite Amplitude Method) allows fast calculations of the dipole, quadrupole, etc. response functions in deformed nuclei: *giant resonances, β-decay*, etc.

Illustration: Mass Table

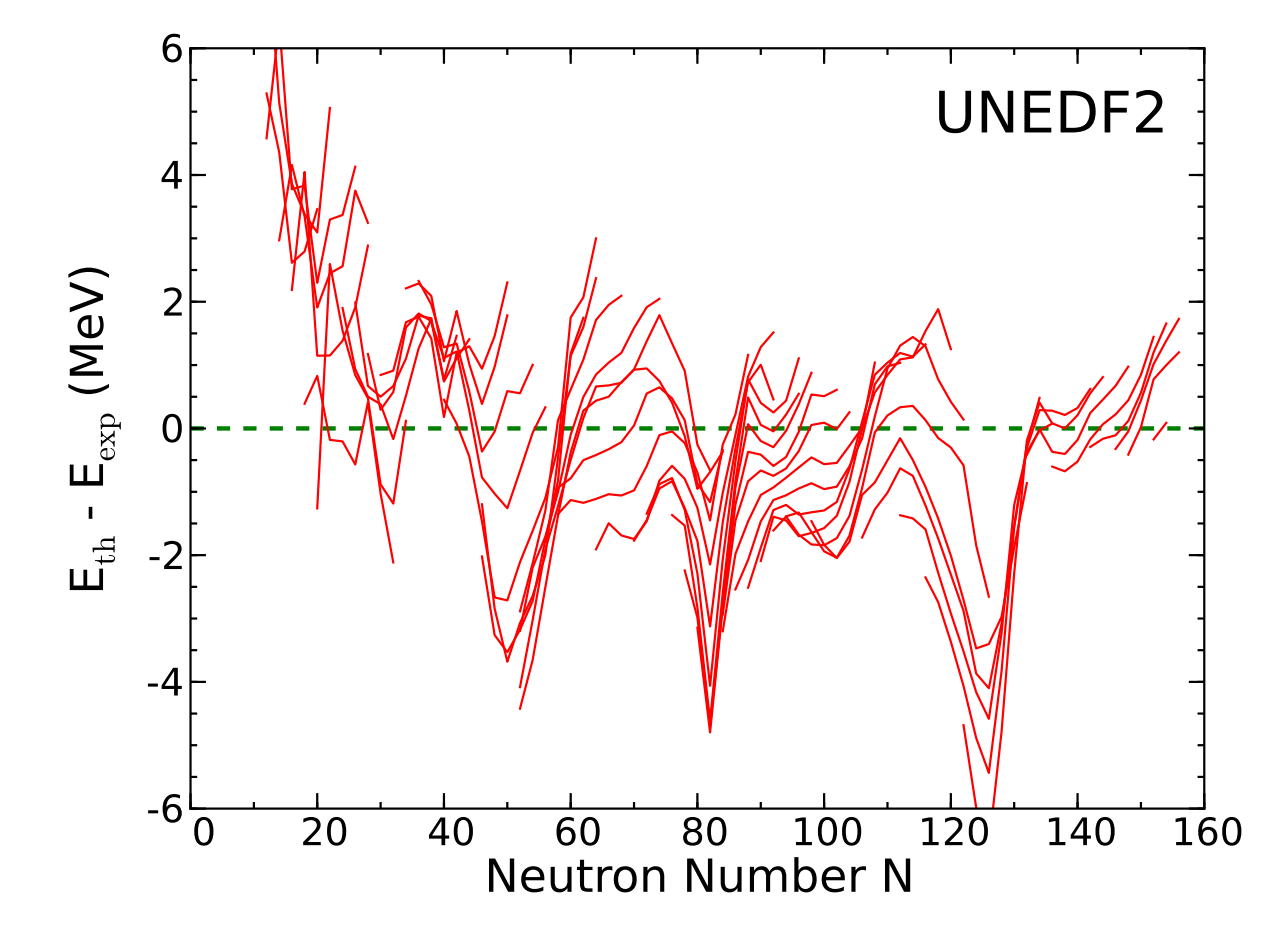


Figure 2: Deviations between calculated and measured nuclear binding energies with the UNEDF2 parametrization of the Skyrme EDF [17].

What can you do with... a symmetry-unrestricted DFT solver

Triaxiality - Nuclei sometimes exhibit static triaxial shapes

- Triaxiality effects lower fission barriers by a couple of MeV;
- Triaxiality is also relevant to understand shape coexistence around closed-shell nuclei.

Time-odd terms - Remember that half of the Skyrme EDF depends on densities built from the spin density s. This part of the EDF vanishes automatically in static ground-states of even-even nuclei but:

- Time-odd channels are in principle active in odd-even nuclei (small effect, a few dozens keV on g.s. energies);
- State-of-the-art theory of collective inertia requires time-odd densities, effect unknown;
- The description of Gamow-Teller transitions, rotational states, chiral bands, etc., also require time-odd terms.

Illustration: Potential Energy Surface for Fission

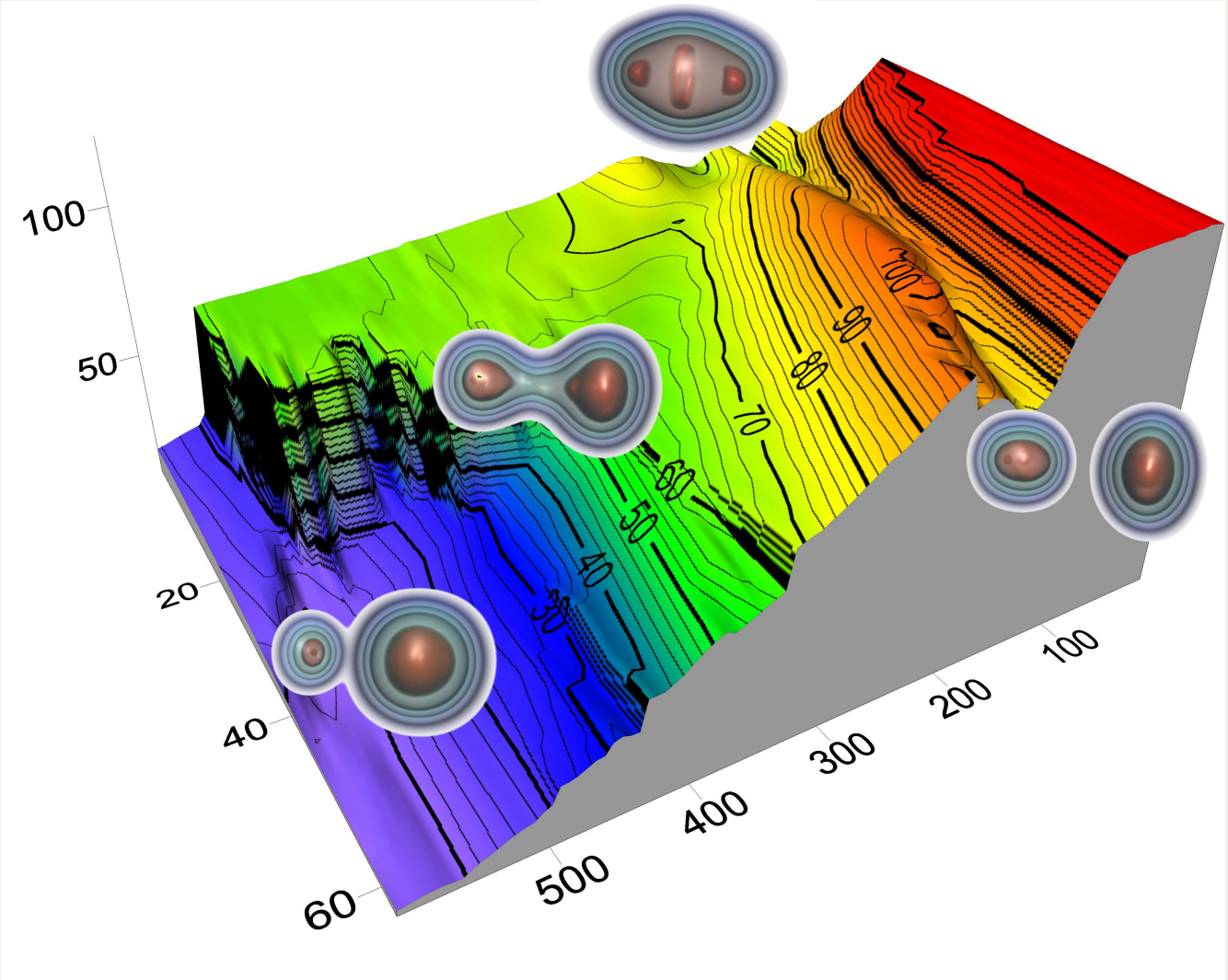


Figure 3: Potential energy surface of ^{240}Pu with the SkM* EDF as a function of axial quadrupole and axial octupole degrees of freedom.

Optimization of Energy Functionals

EDF Optimization

DFT solvers are also the basic tool to determine the parameters of nuclear EDF.

Optimization Problem - We define a model (=nuclear EDF) depending on n_x parameters $\boldsymbol{x} = (x_1, \ldots, x_n)$. We need to fit these parameters on a set of n_d data points. There are n_T different types of data, n_t points per type T. Examples of such data types include: binding energies, r.m.s. radii, separation energies, etc.

- For non-relativistic and relativistic EDF, we have $n_x \approx 10 - 20$;
- The number of data points varies from $n_d \approx 20$ (historical Skyrme forces) to $n_d > 2000$ (nuclear mass models)

For the model, we build the χ_2 function

$$\chi_2 = \frac{1}{n_d - n_x} \sum_{t=1}^{n_T} \sum_{j=1}^{n_t} \left(\frac{y_{tj}(\boldsymbol{x}) - d_{tj}}{\sigma_t} \right)^2 \tag{4}$$

UNEDF Parametrizations

The model is the Skyrme EDF; it depends on all the coupling constants $\boldsymbol{x} \equiv C_t^{uu'}$, including two coupling constants for the pairing functional. References are [18, 19, 17, 20, 21].

The output of the model is obtained by solving the HFB equations with a DFT solver (here, HFBTHO): $y_{tj} \equiv E_{\mathsf{HFB}}$, or $y_{tj} \equiv R_{\mathsf{nuc}}$, etc.

Name	n_T	n_d	Types
UNEDF0	3	108	masses, radii, odd-even staggering
UNEDF1	4	115	masses, radii, odd-even staggering, fission isomer excitation energies
UNEDF2	5	130	masses, radii, odd-even staggering, fission isomer excitation energies, spin-orbit splittings

Computational Cost of EDF Optimization

Each function evaluation of the χ_2 requires $130 \times 6 = 780$ cores (with OpenMP); 1 multi-threaded HFB calculation takes about 5 minutes on modern CPUs.

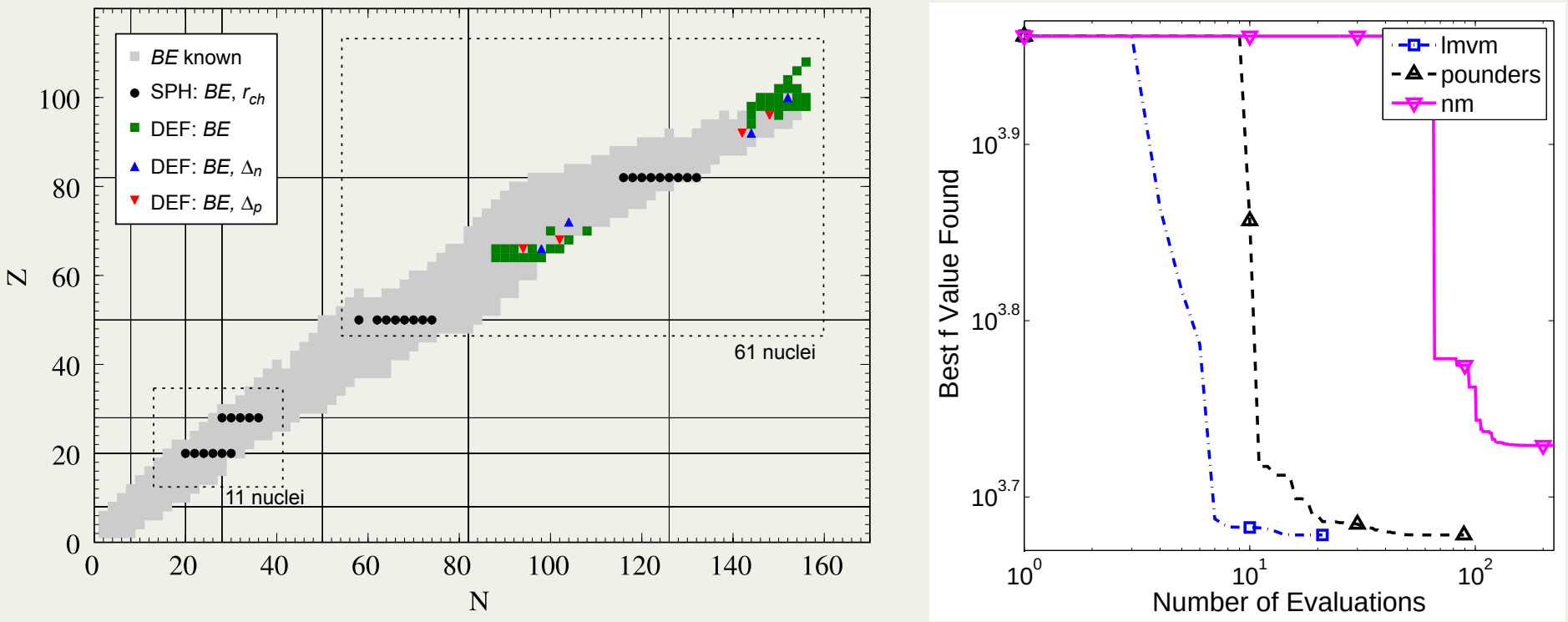


Figure 4: Left: where the data comes from; right: quality of the optimizer POUNDerS [17].

Using Statistical Methods to Probe the Robustness of EDF Parametrizations

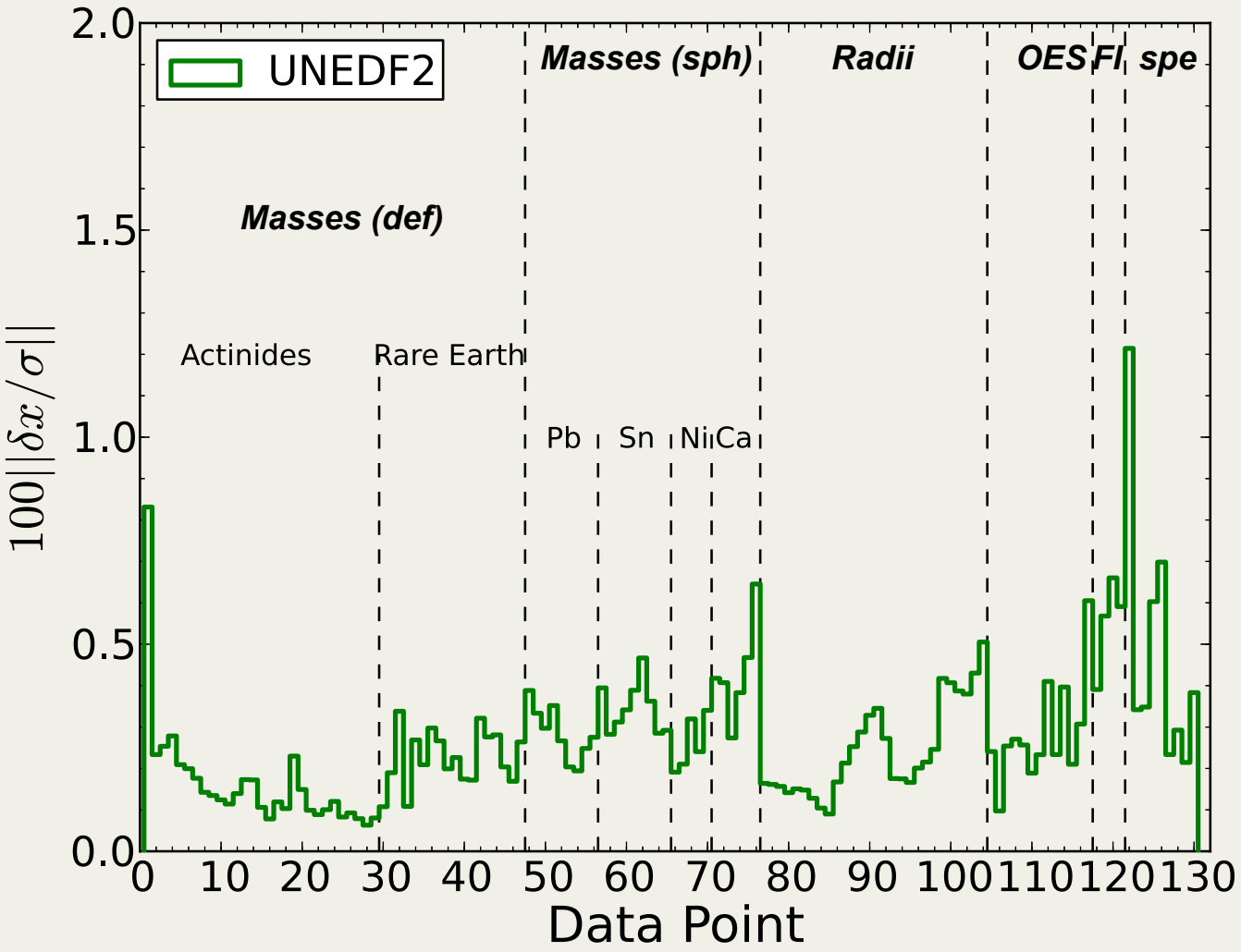


Figure 5: Sensitivity of a Skyrme EDF parametrization to specific experimental input data for the fit [17].

Benchmarking EDF against Ab Initio Calculations

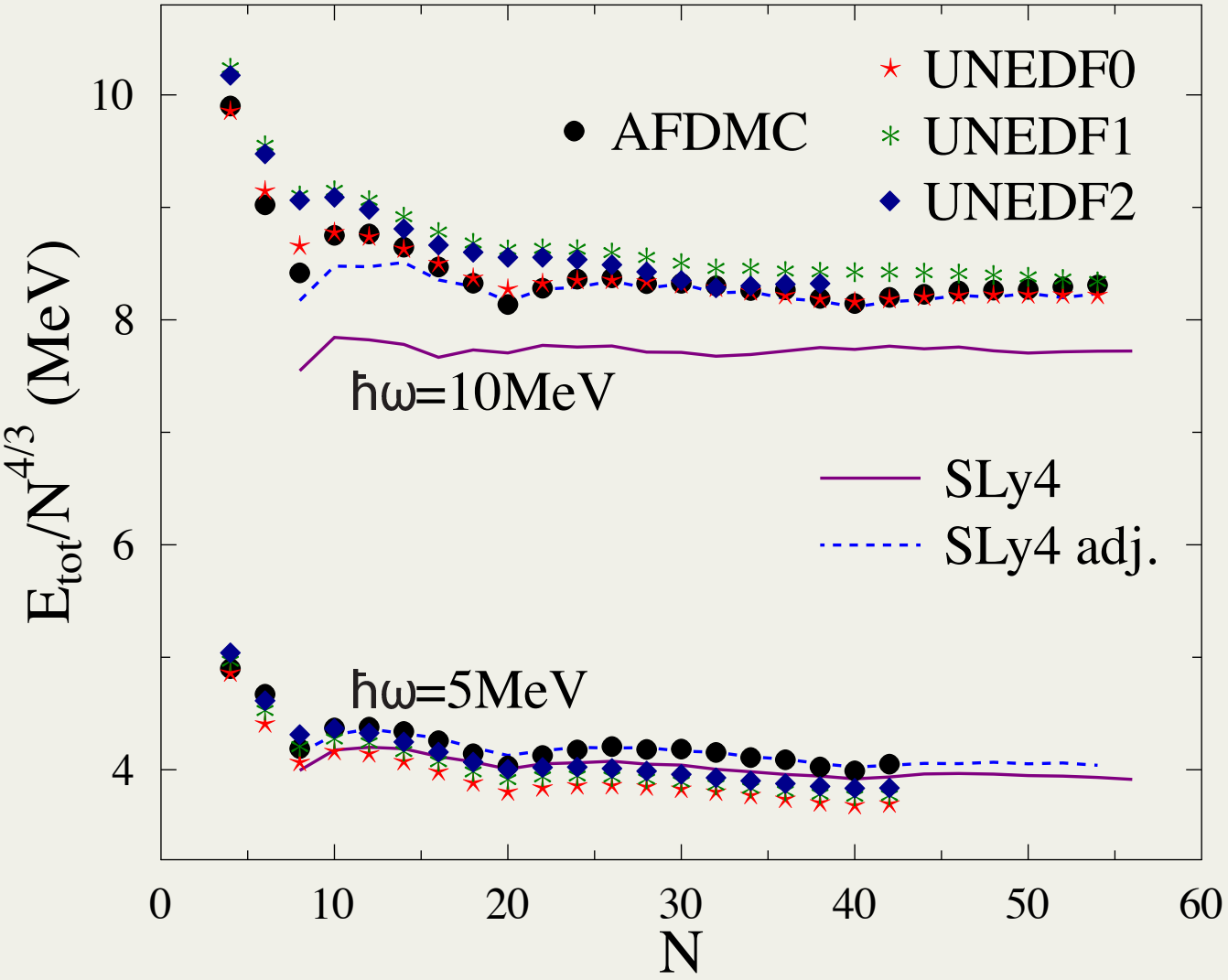
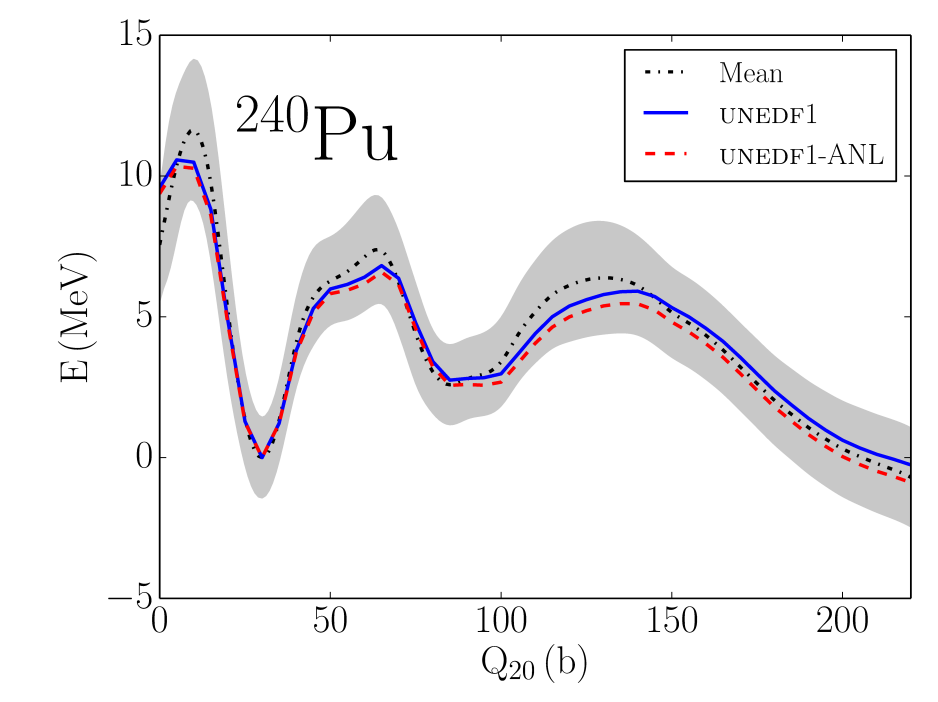


Figure 6: Benchmark of recent Skyrme EDF on neutron drops [17].

Uncertainty Quantification

Next step: take existing EDF parametrizations and try to estimate the uncertainties of calculations resulting from the fit of EDF parameters.



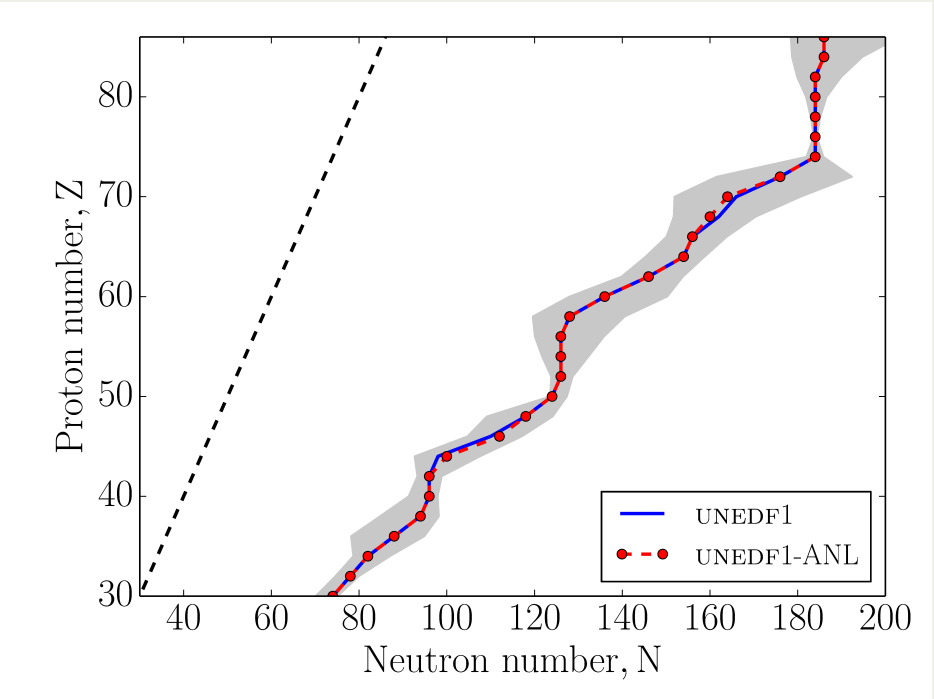


Figure 7: Uncertainty quantification for theoretical predictions of neutron drip lines and fission barriers.

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