Microscopic nuclear mass table with high-performance computing

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Abstract. We overview the methodology behind the large-scale mass table calculations based on the nuclear density functional theory (DFT) with Skyrme energy density functionals (EDFs). The calculations employing massively parallel computers are done in a large configuration space of an axially deformed harmonic oscillator. Nuclear mass tables tabulating global nuclear properties such as binding energies, radii, shape deformations, and pairing gaps are obtained for several Skyrme EDFs augmented by a mixed-type pairing functional, using an approximate particle number projection before variation. Specialty visualization tools have been developed to analyze the results. As an illustrative example of our current capabilities, we show some results for a wide range of even-even nuclei with $Z \leq 120$ and $N \leq 300$.

1. Introduction

Experiments employing beams of short-lived nuclei have dramatically expanded our knowledge of the nuclear landscape, including the remote regions of nuclei far off the valley of stability [1]. Modern radioactive ion beam facilities enable explorations of very exotic nuclei as one moves towards, and sometimes approaches, the particle drip lines where the nuclear binding ends. In this endeavor, of most interest are neutron-rich nuclei which are of critical importance for our understanding of a plethora of nuclear and astrophysical phenomena, as well as superheavy systems at the limits of nuclear mass and charge. From a theoretical point of view, the description of these species is a demanding task, as it requires the understanding and control of three crucial aspects of the nuclear many-body problem: interactions, many-body correlations, and coupling to the continuum of scattering and decay channels [2].

There is a well-delineated path towards a comprehensive description of the nucleus at the nucleonic level across the nuclear chart that merges three approaches: ab initio, configuration-interaction, and nuclear DFT. For complex nuclei with many valence particles, and mass table calculations throughout the nuclear chart, ab initio and configuration interaction methods become intractable due to exploding dimensions of the configuration space. Here the DFT becomes the tool of choice.

The modern nuclear DFT is based on the self-consistent mean-field approach rooted in the self-consistent Hartree-Fock-Bogoliubov (HFB), or Bogoliubov-de Gennes, problem [3]. The three most prominent nuclear DFT schemes are: the Skyrme-HFB method based on local
densities and currents [3, 4, 5], the Gogny-HFB approach using the finite-range Gogny force [6, 7], and the relativistic mean-field model [8, 9]. All those schemes have been used to produce global nuclear mass tables, see Refs. [10, 11, 12, 13] and references quoted therein.

To take advantage of the steady increase in computing power, partnerships have been created in which physicists collaborate with mathematicians and computer scientists on a specific science challenge. In low-energy nuclear theory research, new paradigms have been opened up by the SciDAC Universal Nuclear Energy Density Functional (UNEDF) project [14, 15]. Some of the unique computational nuclear DFT infrastructure developed under UNEDF has recently been used to optimize the nuclear EDF [13, 16] and carry out large-scale nuclear mass table calculations [11, 12]. In this work, we briefly discuss such calculations and their content.

In our systematic calculations, we employ Skyrme EDFs. Their general form is more or less prescribed by a low momentum expansion [5]. Since the coupling constants of the nuclear EDF cannot yet be computed by means of ab-initio methods, it is customary to adjust these to experimental data using least-square optimization techniques [17, 13, 16]. As the parameters of currently used EDFs are primarily constrained by global properties of nuclei near the valley of stability and some nuclear matter parameters, dramatic extrapolations are involved when extending mass tables into unexplored regions, e.g., towards the neutron drip line. To assess corresponding statistical and systematic errors, it is inevitable to compare a variety of different functionals to get a robust prediction for observables and information on their theoretical uncertainties. In combination with that it is helpful to use linear regression techniques to obtain estimates on extrapolations uncertainties [17, 18]. Because of the number of nuclear configurations involved and complexities of the HFB problem, to optimize EDFs and calculate mass tables is a serious undertaking that requires a significant computational effort and resources. To this end, highly optimized codes and access to massively parallel supercomputers are needed to perform calculations in a manageable time.

This paper is organized as follows. Section 2 briefly reviews the Skyrme-HFB model. The computational framework employed, i.e., the HFB solver and adaptation to the supercomputer infrastructure, is discussed in Sec. 3. Results of systematic calculation of mass tables for even-even nuclei are reported in Sec. 4. Finally, Sec. 5 contains conclusions and prospects for future work.

2. The Skyrme-Hartree-Fock-Bogoliubov Approach

This section briefly outlines the self-consistent Skyrme-Hartree-Fock-Bogoliubov framework employed in this study. (For an in-depth presentation of the HFB theory, we refer the reader to Refs. [3, 19, 5] and references therein.) In the nuclear DFT, the total binding energy of the system can be written as a spatial integral:

$$E[\rho, \tilde{\rho}] = \int d^3 r \mathcal{H}(r),$$

(1)

where $\rho$ and $\tilde{\rho}$ are, respectively, the one-body density and pairing matrices, and $\mathcal{H}(r)$ is the quasi-local energy density. In practical applications, one considers local proton and neutron densities and currents built from single-particle wave functions, namely: particle density, kinetic density, spin-orbit density, current and spin density, as well as pairing densities describing nucleonic superconductivity.

The energy functional (1) can be decomposed into several terms. The key piece in the Skyrme-HFB approach is the Skyrme energy functional, which represents the effective nuclear interaction between nucleons and can be partly derived by considering a low momentum expansion of the density matrix [20, 21, 22]. Another crucial ingredient in a mean-field description of nuclear structure is pairing [23, 24]. A widely used mean-field approach to pairing is that provided by the HFB method, where pairing correlations are described by introducing the concept of
Bogoliubov quasiparticles [19]. Nuclear superconductivity is explicitly included by adding a pairing functional based on a zero-range two-body force combined with a density dependence [25]. The EDF also contains the kinetic term, the Coulomb term (consisting of the direct Hartree energy treated exactly and the exchange term in Slater approximation), and the correlation term that accounts for dynamical correlations due to, e.g., symmetries that are spontaneously broken on a mean-field level. How to account for such correlation energy is still an area of intense research. Meanwhile, it is often assumed that all correlations are already built into the EDF through its density dependence. Such a strategy has been recently pursued during the optimization of the functional UNEDF1 [16].

A fundamental consequence of the pairing ansatz is that the HFB states are not eigenstates of the particle-number operator. To restore the broken particle number symmetry and avoid artificial pairing collapse in the regions of the low single-particle density, we use the approximate Lipkin-Nogami scheme [26, 27], which – in most cases – yields results that are close to those obtained by means of the exact projection before variation [28].

![Figure 1](image.png)

**Figure 1.** The potential energy surface of the deformed nucleus $^{152}$Sm as a function of the quadrupole deformation $\beta_2$. Open circles mark three regions of nuclear shapes (spherical, oblate and prolate) where deformation-constrained HFB calculations are performed. The local minima (dots) are obtained by unconstrained HFB calculations initiated from the neighboring constrained solutions.

3. **Computational Framework**

The centerpiece of the present calculation is the HFB solver hfbtho [29]. The code solves the non-linear HFB equations in configurational space by expanding self-consistent eigenstates in a large basis of the deformed harmonic oscillator. The axial symmetry of nuclear mean fields is imposed to reduce the dimension and complexity of the problem.

To cure the incorrect asymptotic behavior of harmonic oscillator wave functions when dealing with weakly bound neutron-rich nuclei near particle drip lines, an alternative approach based on the local scaling transformation of basis vectors was developed in Ref. [30]. Under UNEDF, the original hfbtho solver has been replaced by that based on the modified Broyden’s method [31]. The Broyden’s scheme guarantees stable and fast convergence of self-consistent iterations; this is crucial for large-scale nuclear structure calculations.

The application of such advanced numerical techniques and further optimization of the hfbtho solver carried out in Refs. [13, 16] have resulted in significant performance improvements. For instance, a ground state calculation of $^{120}$Sn on a single processor, using
a large transformed harmonic oscillator basis of 20 oscillator shells (1,771 basis states) can be done in about 1.5 minutes. To reduce the speed of a single HFB run is essential, as the number of nucleonic configurations that need to be computed during the EDF optimization process and mass table calculations can easily reach several millions.

As the general majority of nuclei are known to be axially and reflection symmetric in their ground states, in our study we consider only axial and parity-conserving intrinsic shapes. In spite of this simplification, one still has to explore configurations associated with different shapes (spherical, prolate, and oblate), since the ground-state shape is not known a priori [32]. This makes it necessary to scan the nuclear energy surface of each isotope in a wide range of shape deformations. The procedure is shown schematically in Fig. 1 for the deformed nucleus $^{152}$Sm. To find the ground-state minimum, we divide the potential energy surface into three regions: spherical, prolate, and oblate. In each region, we calculate the total energy by constraining the total quadrupole moment $Q_2$ of the nucleus. If a local minimum is found, we carry out unconstrained minimization to pin down its energy, and the ground-state energy is eventually obtained by taking the lowest-energy solution.

As one HFBTHO run representing the single nuclear configuration can be performed on a single processor, mass table calculations are embarrassingly parallel. For the present large-scale mass table calculations, the HFBTHO solver has been extended with a minimal MPI communication in order to run in a parallel regime across the nodes. The scaling of the mass table calculation with the number of processors implies that a simple master-slave parallel architecture is sufficient.

The calculations were done in a wide range of nuclei in order to include all nuclei between the neutron and proton drip line for a given EDF parameterization. We used JAGUAR or KRAKEN Cray XT5 supercomputers housed at Oak Ridge National Laboratory’s Leadership Computing Facility and the University of Tennessee’s National Institute for Computational Sciences. Figure 2 shows all 4,508 even-even nuclei initially included in the mass table calculations. Using 9,060 processors of JAGUAR, computation of the entire even-even mass table took about 2 hours. The fast turnaround time is crucial, as the selected nuclear observables stored in the mass table are further used as input data for the EDF optimization [13, 16]. If odd-$A$ nuclei are added to the table, several one-quasiparticle states around the Fermi level need to be considered for each nucleus to find the lowest-energy state [33]. Considering 6 blocking candidates (3 particle-like states and 3 hole-like states) and 50 constrained calculations for each configuration, the full nuclear mass table, corresponding to 5,000 even-even, 5,000 odd-$Z$, 5,000 odd-$N$, and 5,000 odd-odd nuclei, requires

$$N_{\text{HFB}} \approx 5,000 \times (1 + 6 + 636) \times 50 \approx 12 \cdot 10^6$$

HFB runs distributed over hundreds of thousands of nodes.

4. Large-Scale Nuclear Mass Tables

Nuclear properties obtained in large-scale DFT simulations can be directly confronted with specific experimental data. However, theoretical mass tables can also be used to search for systematic trends, especially in the regions where experimental data are not available. To facilitate analysis, specialty visualization tools have been developed to analyze various nuclear observables and compare predictions across different models. In this way, one can estimate systematic model errors and assess robustness of extrapolations.

As an illustrative example, Fig. 3 summarizes the results of systematic calculations of ground-state quadrupole deformation $\beta_2$ for all particle-bound even-even nuclei up to $Z = 120$ using the Skyrme EDFs SkM$^*$ [34], SkP [4], SLy4 [35], SV-min [17], UNEDF0 [13] and UNEDF1 [16]. To complete the picture, Fig. 3 also displays results from other published models; namely the Skyrme-HFB-21 model [36], Gogny D1S model [37], and finite-range droplet model FRDM [38]. While all models show similar global systematic trends (e.g., large quadrupole deformations in
Figure 2. Computing nuclear mass table on JAGUAR XT5 supercomputer. The problem is embarrassingly parallel, as a single HFB run can be carried out on one slave node without communicating with other tasks. Simulations were performed using the SkM* EDF [34] for 4,508 even-even nuclei (gray circles). 2,342 of those nuclei (marked by dark dots) are predicted to be particle stable, i.e., they have negative proton and neutron chemical potentials $\lambda_p$ and $\lambda_n$, respectively. The neutron-rich nuclei beyond the neutron drip line ($\lambda_n > 0$) are unstable to the ground-state neutron decay. The proton-rich nuclei beyond the proton drip line ($\lambda_p > 0$) are ground-state proton emitters. Image of JAGUAR courtesy of the National Center for Computational Sciences, Oak Ridge National Laboratory.

mid-shell nuclei), there are important local differences both in predictions for the location of the neutron drip line and deformations of neutron-rich and superheavy nuclei. Those differences are going to impact simulation involving the neutron-rich matter, especially in the context of astrophysical r-process and modeling nuclear reactions taking place in advanced fission reactors.

5. Conclusions

High-performance computing transforms the nuclear many-body problem in a profound way: it provides answers to questions that neither experiment nor analytic theory can address. Nuclear theorists seek to replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that delivers maximum predictive power with well-quantified uncertainties. To this end, advanced algorithms and extensive computational resources are needed.

This paper shows how global nuclear properties across the nuclear landscape can be rapidly computed using the nuclear density functional theory in its Skyrme-HFB version. Such calculations are crucial for interpreting experimental data, assessing importance and feasibility of planned measurements, predicting nuclear properties in the regions that are impossible to access experimentally (thus providing crucial nuclear physics input for astrophysics and applications), and defining future research directions at major experimental radioactive ion beam facilities worldwide.
Figure 3. Ground-state quadrupole deformations $\beta_2$ of all even-even nuclei, from proton to neutron drip line up to proton number $Z = 120$, using the Skyrme EDFs SkM* [34], SkP [4], SLy4 [35], SV-min [17], UNEDF0 [13] and UNEDF1 [16]. Skyrme-HFB calculations were performed using the mixed pairing [25] and the Lipkin-Nogami procedure [30]. Results from other mass models are shown for comparison: Skyrme model HFB-21 [36], Gogny D1S model [37], and FRDM microscopic-macroscopic model [38].

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