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Witold Nazarewicz
Michigan State University

Nicolas Schunck
Lawrence Livermore National Laboratory

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Large-Scale Mass Table Calculations

M. Stoitsov[1,2,3], W. Nazarewicz[1,2,4], and N. Schunck[1,2]
[1] *Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996*
[2] *Physics Division, Oak Ridge National Laboratory, P.O.Box 2008, Oak Ridge, Tennessee 37831, USA*
[3] *Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia-1784, Bulgaria*
[4] *Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681, Warsaw, Poland*

Systematic self-consistent nuclear mass calculations, based on the nuclear density functional theory, represent a rich scientific agenda that is closely aligned with the main research directions in modern nuclear structure and astrophysics, especially in the context of the radioactive nuclear beam physics. The status of large-scale mass calculations carried out under the UNEDF project and the development of the mass-table visualization software are briefly discussed.

1. Introduction

The new data on nuclei far from stability provided by radioactive beam facilities indicate that there are many gaps in our present theoretical understanding. The challenge is to predict properties of exotic nuclei with large neutron-to-proton asymmetry, and to explain the origins of these properties. New ideas and progress in computer technology have allowed nuclear theorists to understand bits and pieces of nuclear structure quantitatively. Nuclear masses play a key role in this enterprize.

The nuclear Density Functional Theory (DFT)[1] is a well-established approach to the calculation of nuclear ground-state properties in a microscopic framework. Its main ingredient is the energy density functional (EDF) that depends on densities and currents representing distributions of nucleonic matter, spins, momentum, and kinetic energy, as well as their derivatives (gradient terms). The current empirical EDFs have proven remarkably successful in predicting a broad range of nuclear properties. Among them, Skyrme-like functionals, built from local densities, are particularly useful.

Mass calculations with the Skyrme DFT achieve a quite remarkable rms deviation of the order of ∼700 keV with respect to the existing mass measurements[2]. However, even these relatively simple functionals remain rather poorly constrained[3,4,5]. For example, existing parametrizations of the Skyrme functional differ significantly in their prediction of nuclear masses when extrapolating from the regions where data are available; there are also significant uncertainties regarding shell structure, i.e., single-particle states. A long-term goal and the main objective of the Universal Nuclear Energy Density Functional (UNEDF) collaboration[6] is an improved reliability for the nuclear DFT that avoids uncontrolled phenomenological parameterizations.

Even if one had a "perfect" energy density functional, the nuclear DFT problem still poses serious conceptual and numerical challenges[3]. The spontaneous symmetry breaking on the mean-field level, phenomena related to various kinds of nucleonic superfluidity, and coupling to the scattering continuum and low-lying decay channels in weakly bound nuclei, just to mention a few, imply that the theoretical treatment of the problem is nontrivial. In addition, about one million nuclear configurations with different deformations and blocking quantum numbers have to be considered in order to predict properties of the ground- and low-lying excited states of all particle-bound nuclei, including odd-A and odd-odd systems. This is, by itself, a very challenging numerical task which can be properly addressed only by invoking the unprecedented numerical capabilities of current leadership class computers.

In this paper, we summarize our recent efforts in performing large-scale mass table calculations based on the nuclear DFT with Skyrme functionals and using the DFT solver HFBTHO[7] and the Cray XT4 supercomputer (Jaguar) at the Oak Ridge National Laboratory (ORNL). In Sec. 2 we briefly review the main characteristics of HFBTHO and provide some useful benchmark results. The strategy adopted to calculate the DFT mass table is discussed in Sec. 3. Section 4 introduces web-based visualization tools facilitating the analysis of huge sets of data coming from our large-scale calculations. Summary and conclusions are given in Sec. 5.

2. Benchmarking the DFT solver

The DFT solver used in the present paper is an upgraded version of the published HFBTHO code[7]. It solves the axial Skyrme Hartree-Fock-Bogolyubov (HFB) equations by using the basis expansion technique with Harmonic Oscillator (HO) and/or Transformed HO (THO) wave functions. Due to the nonlinearity of HFB equations, the problem is solved self-consistently by using the modified Broyden method[8]. In addition to axial symmetry, both time-reversal and parity are assumed to be self-consistent symmetries of HFBTHO. In practice, these symmetry constraints are sufficient to describe ground-state properties of the great majority of nuclei.

The current HFBTHO solver is fairly flexible, and it is relatively easy to use with the novel functionals. The major advantage of HFBTHO is its speed. On a standard PC laptop, it takes typically about 3 minutes of CPU time to compute a nucleus using a basis of $N=$ 20 THO shells. Of course, the speed of the solver comes with a price. Apart from the symmetry restrictions mentioned above, the description of the continuum through discretized HFB eigenstates is not too accurate, especially in the context of weekly bound nuclei[9].

The HFBTHO solver has been carefully tested against a variety of Skyrme-HFB solvers such as HFBRAD[10], HFODD[11], and the recently published axially-symmetric coordinate-space solver HFB-AX[12]. Sample benchmark HFBTHO results for various nuclear characteristics, compared to those of HFODD, are given in Tables 1 and 2 together with a colore outline facilitating the comparison. They nicely illustrate the precision and reliability of HFBTHO.

Table 1. Comparison between HFBTO and HFODD results for spherical ^{208}Pb and ^{120}Sn, and deformed ^{168}Er.

Nucleus:	^{208}Pb		^{168}Er		^{120}Sn	
Code:	HFBTHO	HFODD	HFBTHO	HFODD	HFBTHO	HFODD
Basis:	2D-HO	3D-HO	2D-HO	3D-HO	2D-HO	3D-HO
N_0	14	14	14	14	14	14
N_{st}	680	680	680	680	680	680
$b_\perp = b_z$	2.2348121	2.2348121	2.1566616	2.1566616	2.039048	2.039048
λ_n	−8.114**078**	−8.114**02**	−6.93605**9**	−6.93605**8**	−8.015208	−8.015208
λ_p	−8.810**477**	−8.810**445**	−7.15648**6**	−7.15647**7**	−8.25**1999**	−8.24**5192**
Δ_n	0	0	0.3945**72**	0.3945**78**	1.24464**4**	1.24464**5**
Δ_p	0	0	0.3906**02**	0.3906**05**	0	0
E_n^{pair}	0	0	−1.71**6979**	−1.71**7024**	−12.4263**88**	−12.4263**97**
E_p^{pair}	0	0	−1.5286**16**	−1.5286**43**	0	0
R_n	5.61975**6**	5.61975**7**	5.357578	5.357578	4.7330**88**	4.7331
R_p	5.4600**78**	5.4600**90**	5.22553**8**	5.22553**9**	4.5962**94**	4.5963
Q_n	−0.00000**1**	6.6E-11	11.47391**8**	11.47392**0**	−0.000000**1**	6.6E-11
Q_p	−0.00000**1**	4.7E-11	7.88022**1**	7.88022**4**	−0.000000**1**	6.6E-11
E_n^{kin}	2525.99**2765**	2525.99**1925**	1974.61**4008**	1974.61**3824**	1338.2104**78**	1338.2105**01**
E_p^{kin}	1334.85**5572**	1334.85**4465**	1118.31**3683**	1118.31**3442**	829.438**221**	829.438**221**
E_{so}	−96.375**045**	−96.375**003**	−80.1868**09**	−80.1868**26**	−49.0023**07**	−49.0023**16**
E_{dir}^C	827.607**375**	827.607**885**	602.810**248**	602.810**352**	366.326**962**	366.326**917**
E_{exc}^C	−31.2484**79**	−31.2484**62**	−25.93591**0**	−25.93590**5**	−19.08958	−19.08958
E_{tot}	−1634.14**8867**	−1634.14**8120**	−1357.658**500**	−1357.658**322**	−1018.141**626**	−1018.141**673**

3. Large-Scale Calculations of Nuclear Ground States

Around 3000 even-even nuclei are expected to exist between the proton and neutron drip lines within the range $2 \leq N \leq 190$ and $2 \leq Z \leq 110$. They are either spherical ($\beta = 0$), prolate ($\beta > 0$), oblate ($\beta < 0$), or they exhibit shape coexistence. In order to determine ground-state equilibrium deformations, constrained calculations are first carried out for each even-even nucleus on a β-deformation grid of $-0.5 \leq \beta \leq 0.5$ with a step of $\Delta\beta = 0.05$. The resulting deformation energy curves define the regions where the energy has a minimum. Around each local minimum, the unconstrained HFB calculations are performed and the ground-state configuration is associated with the solution having the lowest energy. This procedure requires

Table 2. Comparison between HFBTHO and HFODD results for one-quasineutron configurations in ^{121}Sn

state:	$2d_{3/2}(\Omega{=}1/2)$		$3s_{1/2}(\Omega{=}1/2)$		$h_{11/2}(\Omega{=}3/2)$	
code:	HFBTHO	HFODD	HFBTHO	HFODD	HFBTHO	HFODD
N_0	14	14	14	14	14	14
$N_{\rm st}$	680	680	680	680	680	680
$b_\perp = b_z$	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697
$E_{\rm qp}$	1.007644	1.008	1.611961	1.612	1.388951	1.387
λ_n	−7.749566	−7.7494	−7.696179	−7.6962	−7.972801	−7.9742
$E_n^{\rm pair}$	−9.294443	−9.2964	−10.397019	−10.3983	−8.703141	−8.7035
Δ_n	1.057516	1.0576	1.120611	1.1207	1.037402	1.0373
r_t	4.689535	4.6895	4.690459	4.6905	4.689510	4.6895
β	−0.025699	−0.0256	0.000000	0.0001	0.015789	0.0147
Q_t	−0.862706	−0.8604	0.000000	0.0036	0.530038	0.4921
$E_n^{\rm kin}$	1360.437867	1360.442751	1362.407077	1362.409601	1358.912567	1358.886614
$E_p^{\rm kin}$	827.317590	827.317961	827.123364	827.123676	827.195176	827.191207
$E_{\rm so}$	−50.483676	−50.485916	−50.922860	−50.923940	−49.607742	−49.592026
$E_{\rm dir}^C$	365.743676	365.743774	365.621013	365.621031	365.736277	365.735680
$E_{\rm tot}$	−1024.707275	−1024.707272	−1024.301233	−1024.301252	−1024.415866	−1024.416901

the HFB equations to be solved about 180,000 times (which is the number of nuclei times the number of deformation points on the grid).

In the HFB theory, the ground-state of an odd nucleus is a one-quasiparticle excitation. The corresponding vacuum can be associated with the ground state of the neighboring even-even nucleus. Since the quantum numbers of the quasiparticle excitation that has the lowest total energy are not known beforehand, we select as blocking candidates all one-quasiparticle states with quasiparticle energies below the energy cutoff $E_{1qp,cut}$, which is not smaller than 2 MeV for heavy nuclei and not bigger than 8 MeV for very light systems. For most nuclei, we take $E_{1qp,cut}{=}25/\sqrt{A}\,$MeV. The blocked HFB calculations are carried out for each blocking configuration in the uniform filling approximation which preserves the time reversal symmetry. The configuration having the lowest energy is associated with the ground-state of the odd-A nucleus. Two-quasiparticle states of odd-odd nuclei are handled by a double blocking procedure: for each blocked one-quasineutron state, we solve the HFB equations by considering all possible one-quasiproton states within the energy range given above, and the lowest-energy state is the predicted ground state of an odd-odd system. The total number of different configurations to be taken into account across the mass table is of the order of one million.

In spite of the high efficiency and excellent speed of the HFBTHO solver, one mass-table run described above would take almost 12 CPU-years, if executed on a single processor. However, with the help of massively parallel computers such as the Cray XT4 Jaguar machine at ORNL, the entire calculation is accomplished in a single 24 CPU hour run involving 3,000 processors. The combination of highly optimized fast DFT solvers, teraflop architectures, and massively parallel computation algorithms paves the way to the complete DFT mass table in less than a day.

4. Data Visualization Tools: Mass Table Explorer

One of the bottlenecks in large-scale calculations is a massive amount of data produced in a single run. Specialty tools must be developed to analyze and exploit those rich data. Under the UNEDF project, a web server has been dedicated to collecting, sorting, and visualizing the output of mass table calculations that can be freely accessed at the address `http://massexplorer.org` . This website contains links to the raw datafiles, and more useful data will become available as the UNEDF project is progressing. The website *massexplorer.org* also offers two useful applications aimed at facilitating the visualization of nuclear structure data.

The first application, called Mass Table Explorer (MTeX), has been developed with the Java technology. It offers a powerful and portable graphical package that can be freely downloaded and runs under almost every operating system (Linux, Unix, Windows, Macintosh...). MTeX can help with the visualization, manipulation, and access to the numerical values and graphical representations of data without prior knowledge of the storage format. It has some flexibility as far as the comparison between different mass table data sets is concerned, and is capable of integrating additional user-supplied data files.

The second visualization tool, named WebMassExplorer, is being developed using different scripts combined with the Ajax remote scripting framework. It is meant to be run on the *massexplorer.org* server by executing the scripts from within the browser without performing a page refresh. Such technology should work on all major browsers such as MS IExplorer, Firefox, Safari, or Opera. The output is displayed in the browser as an image file that can be further copied and manipulated. This utility makes it possible to perform online DFT "calculations" by utilizing all the pre-calculated mass table datasets available. The range of plots that can be produced is very broad and is based on combinations of some basic components:

- FILTERS: predefined filters for neutrons or protons (one- and two-particle separation energies, pairing gaps, proton-neutron energies, Q-values), arbitrary (custom) filters and functions of N and Z applied to different (N, Z) range and data sets;
- CHARTS: 2D and 3D nuclear data charts with options modifying the data and color grid, plotting $N = Z$ line and surfaces;
- PLOTS: highly customizable 2D plots of various physical characteristics: energies, rms radii, deformations, pairing properties, contributions from different terms of the functional to the total energy, etc. for up to 3 different Skyrme datasets;
- GAPS: plots of differences between nuclear characteristics across different mass table sets, calculates rms differences and maximal deviations, also

including experimental data.

5. Conclusions

We presented the status of large-scale DFT mass table calculations, including the description of the highly optimized DFT solver used, the computational strategy employed, and post-processing applications developed to visualize massive amounts of theoretical data obtained. Some recent applications of our mass tables include, among others, studies of valence neutron-proton interactions[13], systematics of one-quasiparticle states in odd nuclei[14], and the global survey of odd-even binding energy differences [15].

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