Towards the universal nuclear energy density functional

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Abstract. The UNEDF SciDAC project to develop and optimize the energy density functional for atomic nuclei using state-of-the-art computational infrastructure is briefly described. The ultimate goal is to replace current phenomenological models of the nucleus with a well-founded microscopic theory with minimal uncertainties, capable of describing nuclear data and extrapolating to unknown regions.

1. Introduction
An understanding of the atomic nucleus is crucial for a complete nuclear theory for element formation, for properties of stars, and for various societal applications. The “Universal Nuclear Energy Density Functional” (UNEDF) SciDAC-2 collaboration \cite{1} carries out a comprehensive study of all nuclei based on the most reliable theoretical approaches, the most advanced algorithms, and extensive computational resources, with a view of scaling to the petaflop platforms and beyond. We 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.

In order to ensure close alignment of the necessary applied mathematics and computer science research with the necessary physics research, partnerships have been formed consisting of computer scientists and applied mathematicians linked with specific physicists. In this short overview, we describe one research task under UNEDF aiming at development of the optimized nuclear energy density functional and the related computational infrastructure to solve self-consistent, nonlinear equations of the nuclear energy Density Functional Theory (DFT). Our goal is to combine the best knowledge of the nuclear Hamiltonian with newly developed many-body techniques to construct a novel class of energy functionals. These functionals, validated by using the relevant data, will then be applied to predict nuclear properties and describe nuclear reactions.

Currently used energy density functionals, such as popular zero-range Skyrme functionals, are characterized by 10-15 coupling constants adjusted to selected experimental data. In spite
of their simplicity, they offer a remarkably effective and robust description of atomic nuclei. Over the past few years, however, it has become clear that commonly used functionals suffer from various deficiencies that make it impossible to obtain a consistent and highly quantitative description of nuclear properties. From the point of view of DFT practitioners, the challenges by the UNEDF roadmap are, therefore, threefold: (i) How can we compute the properties of all atomic nuclei within a reasonable timescale? (ii) Given a mathematical form of the functional, how can we optimize its parameters to a set of experimental data? (iii) What mathematical form should the energy functional take?

2. Nuclear energy density functional

Within the DFT, the total binding energy of the nucleus is given by

$$E = \int d^3r \mathcal{H}(r),$$  \hspace{1cm} (1)

where the energy density $\mathcal{H}(r)$ is a functional of the nucleonic intrinsic density matrices and their derivatives. A representative example is the commonly used nuclear Skyrme energy functional:

$$\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau + \sum_{t=0,1} \left( U^\rho_1 \rho_1^2 + U^\omega_1 \rho \tau + U^J_1 J_1^2 + U^\Delta \rho \Delta \rho + \sum_{t=0,1} \rho_t \nabla \rho_t \nabla \rho_t + U^\rho \rho \nabla J_t \cdot J_t + U^\rho J_{t} \nabla \rho_{t} \nabla \rho_{t} \right) + \sum_{t=0,1} U^{\tilde{\rho} \tilde{\rho} \rho} \tilde{\rho} \rho,$$  \hspace{1cm} (2)

where the isospin index $t$ labels iso-scalar ($t = 0$) and iso-vector ($t = 1$) particle $\rho_t$, pairing $\tilde{\rho}_t$, kinetic $\tau_t$, and spin-current $J_{t}$ local densities, respectively. In the most general case, the amplitudes $U^{m}_{t}$ with $m = \{ \rho \rho, \tilde{\rho} \tilde{\rho}, \rho \tau, J^2, \rho \Delta \rho, \nabla \rho \nabla \rho, \rho \nabla J, J \nabla \rho \}$ are functions of $\tau_t$, $\rho_t$, $\tilde{\rho}_t$, $J_{t}$, and possibly their derivatives.

The requirement that the total energy (1) be minimal under a variation of the particle and pairing densities leads to the Hartree-Fock-Bogoliubov (HFB; or Bogoliubov-de Gennes) equations. They form a self-consistent set of non-linear integro-differential equations which has to be solved iteratively.

3. DFT solvers

The computational cost of HFB iterative convergence schemes can become very expensive, especially when the size of the model space, largely determined by the imposed symmetries or the number of many-body configurations processed simultaneously, is huge. Of particular interest is the coordinate-space formulation of HFB, which has an advantage to treat arbitrarily complex intrinsic shapes, including those seen in fission or heavy-ion fusion. A number of coordinate-space DFT solvers have been developed over the years, and their performance strongly depends on the size and symmetries of the spatial mesh employed. Of particular interest is the recently developed 2D solver HFBAX [2] based on B-splines that contain a number of enhancements resulting in a significant numerical speedup of the code. Figure 1 shows the neutron density distribution of a deformed exotic nucleus $^{110}$Zr calculated with HFBAX in a 2D spacial box of dimension $A \times B$ fm. Under UNEDF, efforts are under way to develop a new-generation 3D DFT solver based on the multi-resolution wavelet analysis under the MADNESS framework [3].

The configuration-space DFT solvers are based on the expansion of HFB eigenstates in a discrete basis, such as the harmonic oscillator basis. The codes that use the basis expansion technique can be very versatile. For example, the 3D DFT solver HFODD [4] is capable of treating arbitrary shapes, which is of particular importance when studying complex configurations such as high-spin states or nuclear fission. In many problems of physical
interest, however, symmetry-restricted solvers are sufficient. The HFBTHO solver [5] is a highly optimized equivalent of HFODD that is restricted to axially-symmetric shapes. It is particularly adapted to large-scale nuclear mass calculations, since the vast majority of atomic nuclei are axially-deformed in their ground-states.

4. Large scale nuclear mass table
Calculating the entire nuclear mass table is a challenge of its own. Around 10,000 nuclei are expected to exist between the proton and neutron limits of stability, representing about 600,000 many-body configurations for which a DFT solution needs to be found. They are either spherical (quadrupole deformation \( \beta = 0 \)), prolate (\( \beta > 0 \)), or oblate (\( \beta < 0 \)). In order to determine the ground-state equilibrium deformation, constrained calculations are first carried out for every nucleus on a \( \beta \)-deformation grid. The resulting energy curves define the regions within which the local minima are found. The ground-state configuration is assigned to the lowest-energy minimum.

In the nuclear DFT, the ground-state of an odd-mass nucleus is represented by the blocking of a one-quasi-particle excitation out of a paired HFB vacuum representing a neighboring even-even system [6]. The quantum numbers of the quasi-particle excitation that yield the lowest total energy are not known beforehand; hence, one must select several blocking candidates in a given energy window around the Fermi level. In HFBTHO, the quasi-particle calculations are carried out for each configuration within the so-called equal-filling approximation, which preserves the time-reversal symmetry. Odd-odd nuclei are handled by a double-blocking procedure: for each blocked one-quasi-neutron state, we solve the DFT equations by considering all possible one-quasi-proton states within the energy cutoff range, and the lowest-energy final state is assigned to the ground-state of the 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 of HFBTHO, computing the entire mass-table would take almost 12 CPU years on a single processor. However, with the help of massively parallel computers such as the Cray XT5 Jaguar and Kraken, the entire calculation is accomplished in a single 14-CPU-hour run involving 9,000 processors. As an illustrative example, Figure 2 shows the result of a large-scale HFBTHO mass-table run with the SLy4 Skyrme functional [7] and a zero-range pairing force covering all even-even, odd-even and odd-odd nuclei with neutron number \( 2 \leq N \leq 190 \) and proton number \( 2 \leq Z \leq 110 \). For some recent applications of mass-table results, see Refs. [8, 9].

5. DFT solvers enhancements
The complexity of the large-scale nuclear mass table problem cannot be resolved by a trivial increase in the number of processors used. To find converged DFT results for the multitude of nuclear configurations is a challenging task that requires the development of efficient DFT solvers, optimized for leadership-class architectures.

One of the crucial enhancements, proposed and analyzed in detail in Ref. [10], is the use of the modified Broyden mixing for the numerical solution of nonlinear equations in many variables to nuclear self-consistent calculations. (The size of the Broyden vector in our calculations ranges from \( \sim 300,000 \) in HFBTHO to \( \sim 3,000,000 \) in HFODD.) This method provides impressive performance improvements against the conventional linear mixing procedure. For example, using linear mixing, one is left with almost 30% unconverged cases assuming the standard accuracy requirements. With the Broyden method, all nuclei in the mass table of figure 2 are resolved. Other recent enhancements include the application of the augmented Lagrangian method for constrained DFT calculations [11] and parallelization of HFODD on the Jaguar Cray XT5.
6. Optimization of the functional

Recent progress in code development and hardware architectures make it possible to undertake a global parameter search and statistical analysis of energy functionals.

For values of $p$ parameters $\theta$, our simulators compute $T$ observables $\{s_{t,n}(\theta)\}_{t=1}^T$ for nucleus $n$. Given an experimental data set $\{d_{t,n}\}_{t,n=1}^{T,N}$, corresponding to different nuclear properties (such as binding energies, radii, and moments), our objective is to find the parameters $\theta$ so that the theoretical output approximates the experimental data. To this end, we solve the nonlinear least squares problem $\min_{\theta \in \mathbb{R}^p} \{ f(\theta) = \sum_{t,n} (d_{t,n} - s_{t,n}(\theta))^2 / \sigma_{t,n}^2 : \theta \in \mathbb{R}^p \}$, where $\sigma_{t,n} > 0$ reflects the relative accuracy of the experimental data. The optimization procedure is based on updating a quadratic model $q(\theta) = f(\hat{\theta}) + (\theta - \hat{\theta})^T g + \frac{1}{2}(\theta - \hat{\theta})^T H(\theta - \hat{\theta})$ approximating $f(\theta)$ near the calculated solution $\hat{\theta}$.

Since the Hessian $H$ is positive semi-definite at a solution, we can conduct sensitivity and correlation analysis at $\theta$ as a byproduct of the optimization. Under certain statistical assumptions, $H$ can be used to approximate the covariance $\text{Cov}(\theta) \approx H^{-1}$, and hence the correlation matrix $R_{ij} = \text{Cov}(\theta)_{ij} / \sqrt{\text{Cov}(\theta)_{ii} \text{Cov}(\theta)_{jj}}$. Such an analysis is a standard approach in other domains of physics, but could not be addressed in nuclear structure until very recently due to the extremely high cost of the function evaluations.

7. New generation nuclear energy density functionals

A straightforward empirical generalization of the standard Skyrme functional is obtained by replacing all coupling constants $U_{lm}^{\mu}$ in (2) with density-dependent functions. In this way, the standard set of parameters is extended, thus increasing the flexibility of the functional. Another
extension of the DFT currently pursued, which retains the general functional structure (2) but offers novel density dependence, comes from the Density Matrix Expansion method applied to the long-range part of chiral nucleon-nucleon interactions [12].

8. Visualization tools
One of the bottlenecks in large-scale calculations is the massive amount of data produced in mass-table runs. Specialized tools must be developed to analyze and exploit this rich theoretical output. To this end, a web server has been dedicated to collecting, sorting, and visualizing the data produced by UNEDF mass-table runs. It can be freely accessed at http://massexplorer.org. This web site contains links to the raw data files, and more useful data will become available as the UNEDF project progresses.

9. Conclusions
Finding the nuclear energy density functional for atomic nuclei capable of describing stable and short-lived nuclei and their reactions requires the unique combination of innovative theoretical tools that can link microscopic interactions to energy functionals, significant code development with special emphasis on massively parallel algorithms, and state-of-the-art optimization techniques that can efficiently cope with the high computational cost of function evaluations. The UNEDF SciDAC project will develop key computational codes and algorithms for reaching the goal of solving the nuclear quantum many-body problem, thus paving the road to the comprehensive model of the nucleus.

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