Building a universal nuclear energy density functional

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Abstract. This talk describes a new project in SciDAC II in the area of low-energy nuclear physics. The motivation and goals of the SciDAC are presented as well as an outline of the theoretical and computational methodology that will be employed. An important motivation is to have more accurate and reliable predictions of nuclear properties including their binding energies and low-energy reaction rates. The theoretical basis is provided by density functional theory, which the only available theory that can be systematically applied to all nuclei. However, other methodologies based on wave function methods are needed to refine the functionals and to make applications to dynamic processes.

1. Motivation
In this talk I will describe the motivation for forming the UNEDF SciDAC and the physics that the project will address. Our goal is to make a reliable theory of the properties of nuclei that will be useful in other disciplines needing that information. Reactor safety design, nuclear waste burning, and simulation of nuclear weapons are technical areas where more reliable information is sought. There are also questions in fundamental science that require better knowledge of nuclear properties. In astrophysics there is much to be learned in studying the environments of nucleosynthesis. Some of the fundamental symmetries have their most stringent tests in nuclei. Demanding that the theory be reliable requires that it be global in scope so that it can be tested with all the available information. And to be useful for our contemplated applications we need a qualitative improvement in accuracy.

The domain we deal with is shown in Fig. 1, the chart of the nuclides. Each nucleus is identified as a box positioned according to its proton and neutron numbers. The isotopes found in nature are shown in black. The wider yellow band shows nuclei that have been produced in the laboratory and for which at least one property has been measured. The much wider green area shows where nuclei can exists, at least for a short time as a measurable bound system. For longer times, radioactive decay converts these nuclei to a more stable one closer to the black stability line.

The most fundamental property for which we need a reliable theory for is the energy of the nucleus, commonly expressed as the binding energy with respect to separated nucleons. The nuclei in yellow have known binding energies, but nuclei certainly were formed outside of this region as intermediates in the astrophysical processes that formed the heaviest elements. Nucleosynthesis took place partly in a very neutron-rich environment, permitting nuclei to accrete neutrons and go into the unknown green region of the chart. These processes probably
took place in an environment having a temperature of the order of a hundred KeV. This sets the scale of the desired accuracy we would like to achieve for binding energies. Also needed for modeling these processes is information about the radioactive decay rates for nuclei in the green region. Interactions with neutrons is also a important subject for nuclear technology and engineering. Here is a quotation from the report made last year:

“For some intermediate mass nuclei (e.g., $^{23}$Na or $^{56}$Fe) inelastic scattering cross-section accuracies of the order of 10% are needed. Moreover, there exists a general need to improve the knowledge of inelastic scattering for actinides. Relevant experiments have proven particularly difficult. It would be worthwhile for the basic science community to investigate whether current challenges could be met with new and innovative measurement techniques.”

–from the report, “Nuclear Physics and Related Computation Science R&D for Advanced Fuel Cycles,” 2006.

Obviously, theory becomes important when measurements are difficult or impossible. However, such a high accuracy in cross sections is very likely beyond what we can achieve.

The fission process may also play a role in nucleosynthesis. It is very likely that the neutron-rich environment that produces uranium and thorium also produces heavier elements that immediately fission and leave a trace only in the fission products that become stable mid-mass

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**Figure 1.** The nuclear landscape showing nuclei as a function of their neutron and proton numbers. Black squares represent stable nuclei and nuclei found in nature. The yellow area shows the region of nuclei that have been produced and studied in the laboratory. The green area show the theoretical limits of bound nuclei.
nuclei.

2. Practical theory

Now I want to turn to methodologies and the envisaged role of the SciDAC project. At a fundamental level the theory would contain the degrees of freedom of quantum chromodynamics, but these are largely hidden from view in low-energy nuclear physics. For our purposes, we believe that the physics of nuclei can be treated by nonrelativistic quantum mechanics. The particles are nucleons that interact via a force that is quite complex but still largely known. While the theory is easily formulated, it requires solving the Schrödinger wave equation. This is computational challenge beyond any imaginable computer resource. The difficulty is that the wave function depends on all of the coordinate variables as once. Thus, a nucleus of 10 nucleons (such as $^{10}$B), has a wave function with 30 variables, three spatial dimensions times ten coordinates, way too many to include in a numerical representation of the function.

The same difficulty confronts any discipline that deals with quantum-mechanical many-particle systems, most notably the theory of electrons in molecules or ordinary matter. Density functional theory was developed as a way to sidestep the wave function problem, and it proved to be spectacularly successful. I will describe the history of the development of the theory. It is this history that we wish to duplicate in nuclear physics.

There are two parts to density functional theory, a conceptual part and practical part. The conceptual part provides the motivation for a search for practical theories, but doesn’t give much guidance on the final form of the theory. It is encapsulated in the Hohenberg-Kohn theorem which states: 1) any quantum system can be characterized by its density; and 2) its energy can be calculated by minimizing some function of the density function. At one stroke we have reduced the number of variables from the 3N-dimensional wave function to an ordinary function in 3 dimensions, the particle density $n(\vec{r})$. There are two warnings that should be mentioned. The first is that the theorem applies only to situations where the ground state is a unique state. The other is that the functional is unknown and could be very complicated, depending on the values of $n(\vec{r})$ at all spatial points at once.

The practical theory was proposed by Kohn and Sham in 1965 [1]. They proposed using as variables orbital wave functions, one orbit per particle in the system. Each orbital $\phi_i$ is an ordinary function in three-dimensional space, $\phi_i : \mathbb{R}^3 \rightarrow \mathbb{C}$. The index $i$ labels the particle. This more complicated than the density function, but it is still a tremendous simplification compared to the full many-particle wave function. The functional to be minimized in the Kohn-Sham theory has the structure

$$\int d^3r \left( \frac{\hbar^2}{2m} \sum_i^N |\nabla \phi_i|^2 + V[\phi] \right).$$

The relation to the density is $n(r) = \sum_i^N |\phi_i(r)|^2$. The first term is the quantum-mechanical kinetic energy and provides the essential quantum mechanics to the theory. Notice that it requires the gradients of the orbitals. The second term incorporates all the interaction effects, and is the part that is modified when changes are made to the functional. The simplest functional, called the local density approximation, assumes that $V$ is an ordinary function of the density at the same point, $V(r) = V(n(r))$. For ab initio theory, the function $V$ is calculated from first-principles theory of an infinite system of uniform density.

Another aspect of the development of computational chemistry should be mentioned. Its community was very organized in assessing candidate computational methodologies. Molecules were grouped into sets for testing purposes. It was thus easy to see the performance of any candidate theory under consideration.

[1] More precisely, a set of two functions in 3D space, one function for each possible spin.
Figure 2. DFT in quantum chemistry. The bar graph compares the performance of various theories of chemical energies. The baseline theory is Hartree-Fock. Next is the density functional theory proposed by Kohn and Sham in 1965, called the "local density approximation". On the left are DFTs with improved functionals found more than 20 years later.

Fig. 2 shows the performance of various theories for one of the sets of molecules, taken from ref. [2]. The first is the Hartree-Fock theory, the oldest orbital-based theory and the baseline theory for comparisons. The average error for the molecules in the data set is 3 eV. This is far too inaccurate for chemistry purposes, which seeks theory at "chemical accuracy" equated to the thermal energy at room temperature, less than a tenth of an eV. The second bar shows the performance of DFT with the functional originally proposed by Kohn and Sham, called the "Local Density Approximation." It does better than Hartree-Fock, but still not good enough for chemistry. It actually took more than 20 years of study before functionals were found that make a significant improvement. The new functionals, called "Generalized Gradient Approximations," give an order-of-magnitude improvement over the baseline theory. This is enough to make the theory very practical and useful not only in chemistry but in condensed matter physics and materials science.

In nuclear physics, a primitive DFT was actually proposed in the early days of the science and was quickly developed into the Liquid Drop Model. This model remains a baseline theory for nuclear binding energies in the same way that Hartree-Fock does for chemistry. Readers are invited to explore the predictive power of the liquid drop model on an interactive web site constructed for the UNEDF project, see http://unedf.org/. Fig. 3 shows the chart of the nuclides showing the results of a fit at the web site. One can see bands due to shell effects that are completely missing from the model. The performance of the model is shown as the first bar in Fig. 4. Note that the energy scale is MeV rather than eV.

More modern DFT’s were first introduced in the 1970’s. They had the form of the LDA functionals as in Kohn-Sham theory, but with adjustable parameters. These theories have been under study since then, with slow progress [3]. One impediment until the 2000’s has been availability of computer resources, but this is no longer a problem for solving LDA functionals. It is only very recently that global studies of the performance of nuclear DFT have been published. The second bar in Fig. 4 shows the performance of one these, the so-called Skyrme
Figure 3. Liquid drop model performance on the chart of nuclides. This figure was generated at http://unedf.org to display the error tendencies in binding energy fits. The model underbinds the nuclei shown in blue and overbinds the ones in red.

parameterization of the DFT. It is much better than the liquid drop model, but not good enough to be useful for needed predictions. Also shown on the Figure is the performance of a hybrid model, combining the liquid drop with terms derived from Kohn-Sham orbital energies [4]. While it does fairly well, it has many more phenomenological parameters which cast a shadow on the theory as a predictive tool.

3. A new start
To make a useful predictive theory, UNEDF’s goal is making an order-of-magnitude improvement in the DFT. How do we approach such an ambitious endeavor? The heart of the project is the functional itself. Clearly we need to go beyond the confines of LDA. There are many ways to generalize the functional, and we must rely on fundamental theory and the findings of ab initio calculations to guide us. So the Schrödinger physics that can be carried out for light nuclei becomes part of the computational toolkit in the UNEDF.
Figure 4. Nuclear binding energy status. The baseline for the theory of nuclear binding energies is the liquid drop model, which has an average (rms) error of 3 MeV. Next to its performance is shown that of a DFT with a functional of the Skyrme type. On the right is a hybrid model including features of the liquid drop together with energy corrections from orbital effects.

The computational tools for DFT itself need considerable improvement. Even at the LDA level, existing codes have difficulty treating the most demanding situations, namely a fissioning nucleus at its scission point. More sophisticated functionals might go beyond the LDA with nonlocal interactions such as exchange. This would demand at least an order of magnitude more computational effort, but one within the purview of our SciDAC.

All descriptions of dynamics require an extension of the DFT, and this raises questions of methodology that need to be resolved. First, there is more than one theoretical approach to treat dynamics, and it is not yet clear which is most reliable for a global theory. Leading contenders are the time-dependent DFT and the Generator Coordinate Method. Although these extensions have been known for a long time, the systematics studies to assess their accuracy have been lacking. Also, the computer demands are orders of magnitude more severe for dynamics. In a theory of dynamics, the orbitals depend on additional variables besides the particle number and spatial position. Instead of $\phi_i(\vec{r})$ we need to calculate $\phi_i(\vec{r}, X)$, where $X$ might represent time or some variable parameter of nuclear shape. Additional variables of course require multiplicative factors on computer storage and arithmetic operations. Finally, the codes for the extensions need much more development on the computer science side.

An overall picture of the UNEDF project showing the different aspects and their relationships is shown in Fig. 5.

4. Present status and near-term goals
In the initial phase of UNEDF, a number of tasks need to be accomplished in preparation for later work. Here are the ones that we are emphasizing for the first year.

The performance of present theories and functionals must to be evaluated. As mentioned
Universal Nuclear Energy Density Functional

Inter-Nucleon 
NN, NNN Interactions
AV18, EFT, \( v_{\text{low-k}} \)

Theory of Light Nuclei
Verification: NCSM\( \Rightarrow \)GFMC\( \Rightarrow \)CC
Validation: nuclei with \( A \leq 16 \)

Density Functional Theory
improved functionals
remove computationally-imposed constraints
global properties of nuclei with \( A > 16 \)

Dynamic Extensions of DFT
LACM, GCM, TDDFT, QRPA, CI, CC
Level densities

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

Figure 5. The plan for building a universal nuclear energy density functional. On top in the nuclear interaction as we know from scattering experiments and the symmetries of QCD. Below that is the \textit{ab initio} theory of light nuclei using the Schrödinger equation. It serves both to refine knowledge of the interaction and to provide a theoretical testing ground for advanced functionals. The middle box indicates the central goal of the SciDAC, to find advanced functionals and developed the codes to make use of them. Dynamical processes are important but require extensions of the DFT. This is indicated on the leftmost lower box. Finally, a major application of the improved theory will be low-energy reactions as shown in the box to the right.
earlier, it is only recently that systematic studies of nuclear properties have been carried out with DFT. These studies are essential for assessing the reliability of the theories. UNEDF is actively engaging in this activity, and publications have already begun to appear under UNEDF auspices. An example has just appeared in Physical Review Letters concerning the properties of the lowest excited state of nuclei [5]. That state is very important in energy exchanges such as inelastic scattering of neutrons. The quoted study applied one of the DFT extensions to the entire data set of known even-even nuclei, and calculated the energy and the transition strength. The results for the transition strength are shown in Fig. 6. Each point represents a nucleus, positioned with $x$ and $y$ coordinates according to experimental and theoretical transition strength. Theoretical agreement is shown by points on the dashed line. One sees that the theory works quite well for the largest transition strengths. These nuclei are the heavy, deformed nuclei such as uranium and other actinides. This agreement is good news for the DFT, suggesting that it is reliable for nuclear shapes and for properties such as fission that depend on shape. One also sees much disagreement on the low side of the graph. Those points represent spherical and soft nuclei that do not have large transition strengths. Getting comparable accuracy for them sets a scale for the UNEDF challenge.

An important task UNEDF is to build codes needed for the DFT, but first a fundamental computational question must be answered, to decide on the numerical representation of the orbitals. They are functions of position in three-dimensional space, and they might be represented on a 3-D spatial mesh as in lattice QCD, or expanded in a basis, as is often done in quantum chemistry, or represented by wavelets. We have made it a near-term goal to compare several representations with a view to selected the most efficient to use for the SciDAC codes to

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**Figure 6.** Performance of an extension of the DFT for excited states in even-even nuclei. The graph shows theoretical values of the transition strength as a function of the experimental values for almost all of the nuclei for which it is known. Points on the dashed line represent perfect agreement. One sees that the theory does well for nuclei with large transition strengths but is poor for nuclei having small transition strengths.
be developed. This work is still at an early stage, comparing storage and arithmetic requirements to calculate orbitals of a fixed external potential. Also it is noteworthy that this work involves a close collaboration between physicists and scientists supported by the Office of Advanced Scientific Computing Research.

As mentioned earlier, the Schrödinger theory of light nuclei will be used in the search for improved functionals. There are several methods in use to calculate the wave-function-based properties of light nuclei, and UNEDF is supporting an effort to verify the computational methodologies in use. Some years ago a comparison was made for $^4\text{He}$, but this is too small a nucleus to be helpful for the DFT search [6]. In the present comparison, a number of nuclei with atomic mass numbers in the range 6-12 are being calculated. This is below the atomic mass numbers where the DFT is commonly applied, but it is the best compromise at present for a meeting point.

5. Institutional Issues
It is obviously that scale of the UNEDF project so large that only the collaborative environment of SciDAC makes it tenable to succeed. Nevertheless, theorists are not used to working in large groups and it cannot be taken for granted that there will be the needed teamwork.

One problem is how to get tasks done that are necessary to the project as a whole but are seen as unappealing. The benchmarking of existing theory is an example. It is more rewarding to find a new theory than to measure the failings of one that is already on the books!

Another problem is communication between members of the collaboration. This is particularly acute for the collaboration between between theorists and computer scientists. There is a limited amount of travel that can be done for physical subcollaboration meetings, and teleconferencing will have to be better facilitated.

These are issues that undoubtedly arise in other SciDAC projects and become resolved in the course of time.

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