SciDAC
Scientific Discovery through Advanced Computing

understanding our universe

Building a Universal Nuclear Energy Density Functional

A Low-Energy Nuclear Physics National HPC Initiative

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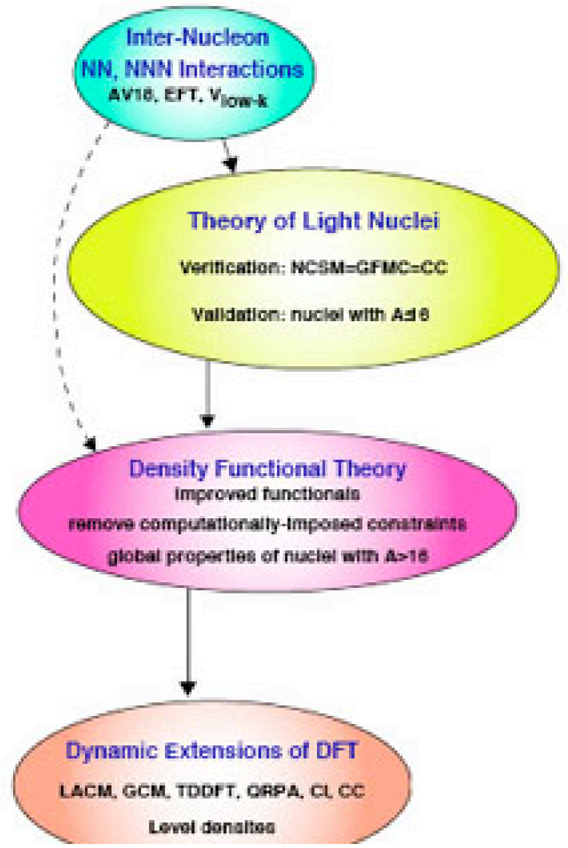
There are approximately 3,000 known nuclei, most of them produced in the laboratory. It is estimated that additionally up to approximately 6,000 nuclei could in principle still be created and studied in the foreseeable future. An understanding of the properties of these elements is crucial for a complete nuclear theory, for element formation, for properties of stars, and for present and future energy and defense applications. We plan a comprehensive study of all these nuclei, based on the most accurate knowledge of the strong nuclear interaction, the most reliable theoretical approaches, and a massive use of the computer power available at this moment in time, with the view of scaling to the petaflop computers to become available in the near future.Until recently such an undertaking was hard to imagine, and even at the present time such an ambitious endeavor would be far beyond what a single researcher or a traditional research group could carry out. This project will involve theoretical physicists, computer scientists, and students from universities and national laboratories. Our long-term vision is to arrive at a comprehensive and unified description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons. 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.

The Energy Density Functional (EDF) is at the heart of the project. EDF theory has been spectacularly successful in condensed matter physics and chemistry, as was recognized in the Nobel Prize awarded to Walter Kohn in 1998. In fact, it was the combined work of many dedicated researchers that

Universal Nuclear Energy Density Functional



A. Project Overview

Building a universal nuclear energy density functional

Goal: reliable theory of low-energy nuclear physics

Participation: 8 universities and 4 DOE laboratories

UNEDF is new in SciDAC II

Sponsorship:

--NNSA $1M/yr
--DOE NP $1M/yr
--ASCR $1M/yr

B. Science Lesson

We deal with the quantum mechanics of protons and neutrons that interact with nuclear forces

The Holy Grail is the wave function $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, ...)$

$$\Psi : \ R^{3N} \to C$$

Practical theory is based on orbitals $\phi_i(\vec{r}_i) \ i = 1, ..., N$

$$\phi : \ R^3 \to C$$

Orbitals are computed by minimizing the energy functional.

We do not yet have the ultimate functional.

Some important quantities require further computer-intensive processing of the orbitals.

C. Parallel Programming Model

UNEDF is an umbrella for a diverse set of codes at various stages of parallelization.

Typical coding is F90 + MPI + python data manipulation

All codes run on NERSC.

Wave function methods are already highly parallelized: GFMC, MFD, CC

Density functional methods are in the initial stages of parallelization:
HFODD, EV8, PROMESSE, FastDFT

Model A: distribute the 5000 nuclei to different processors.
Good for production runs with simple functionals.

Model B: parallelize the orbital solver

D. Computational Methods

MFD: sparse matrix linear algebra

DFT: conjugate gradient solvers, linear algebra

FastDFT: fftw

E. I/O Patterns and strategy

I/O is an issue for DFT: 1GB generated per processor

Checkpoint/Restart is needed particularly for time-dependent DFT.

F. Visualization

Needed for outreach, not for science or code verification.

G. Performance

Performance is largely limited by memory. Degradation starts at the cache-RAM interface.

H. Tools

I. Status and Scalability

J. Roadmap

In two years we want to have a DFT solver that will deal with orbital data sets >1GB and run efficiently on the leadship-class machines.