Adaptive Multiresolution 3D Hartree-Fock-Bogoliubov Solver for Nuclear Structure

G. Fann[1], W. Nazarewicz[2], J. Pei[3], Y. Shi[2], W. S. Thornton[4] and R. J. Harrison[4,5]

[1)] Oak Ridge National Laboratory, Oak Ridge, TN 37831 [2)] Facility for Rare Isotope Beams, Michigan State University, East Lansing, MI 48824, USA [3)] State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China [4)] Stony Brook University, Stony Brook, NY 11794, USA [5)] Brookhaven National Laboratory, Upton, NY 11973, USA

A solver for the Hartree-Fock-Bogoliubov equations is a key element of any density functional theory framework to enable a quantitative understanding of complex nuclear structures and its extensions to complex nuclei. This work highlights NUCLEI's close collaborations between domain scientists, applied mathematicians, and computer scientists to develop a new adaptive multiscale solver to enable scalable and high accuracy simulations of complex many-body open systems on leadership-class systems.

Physics Problems

Multiple scales and complex topologies arise in complex many-body open quantum systems such as

- triaxial and reflection-asymmetric nuclei,
- weakly bound halo states,
- cluster configurations,
- nuclear fragments from heavy-ion fusion reactions,
- cold Fermi gases, and
- pasta phases in a neutron star crust.

Systems, with symmetry breaking and complex and changing topologies, can be described within nuclear density functional theory (DFT) framework. See Sagert's poster for an example of MADNESS in a periodic crust simulation.

Hartree-Fock-Bogoliubov

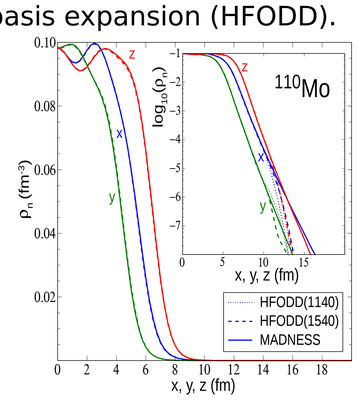
Self-consistent solutions of Hartree-Fock-Bogoliubov (HFB or Bogoliubov-de Gennes) equations are a key element of any DFT framework. The HFB equations define “quasi-particles” which approximate ground-states of many-body systems beyond HF + BCS theory. For a two-component system (↑ and ↓) with corresponding HF Hamiltonian h, chemical potentials λ and a pairing potential δ, the HFB equation is

$$\begin{bmatrix} h_\uparrow - \lambda_\uparrow & \delta \\ \bar{\delta}^t & -h_\downarrow + \lambda_\downarrow \end{bmatrix} \begin{bmatrix} u_i \\ v_i \end{bmatrix} = E_i \begin{bmatrix} u_i \\ v_i \end{bmatrix}$$

Benchmarking

Comparisons were made between the **MADNESS-HFB** solver against 2D coordinate-space solver using B-splines (HFB-AX) and a 3D solver based on the harmonic-oscillator basis expansion (HFODD).

Single-particle density distributions for ^{110}Mo illustrates (see semilog inset) the superior asymptotic properties of the **MADNESS-HFB** solutions to DFT over conventional techniques using 1140 and 1540 harmonic-oscillator basis functions.



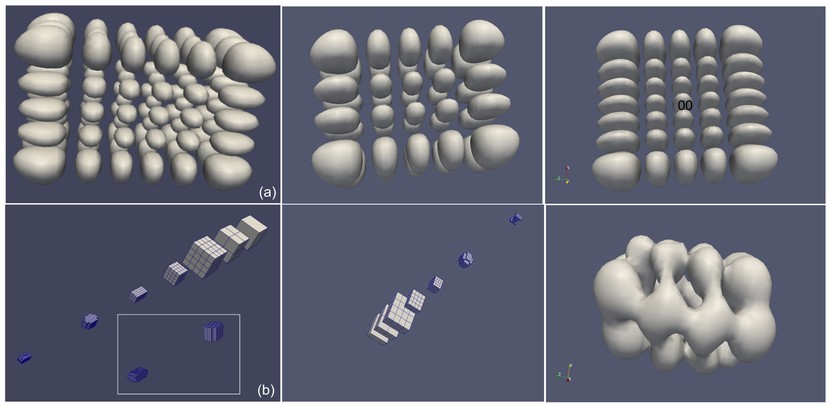
Funding: This material is based on work supported by the U.S. Department of Energy, Office of Science, SciDAC NUCLEI, Office of Science, Divisions of Advanced Scientific Computing Research, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory. This is a part of the SciDAC NUCLEI Project (PI: J. Carlson, LANL).

Computational Problems

Solutions for the needed 3D solutions in DFT, within a large and asymmetric domain without symmetry, require orders of magnitude more computational resource than 2D simulations. **MADNESS-HFB** introduced an adaptive and variational pseudo-spectral framework for solving self-consistent equations of nuclear DFT, without symmetry restrictions, on massively parallel computers. The new framework solves multi-scale physics challenges in nuclear and atomic physics problems involving many-particles systems, by combining the eigensolution of an HFB equation and a corresponding set of Lippman-Schwinger equations (with $k^2 = -2E$), with improved asymptotic behavior.

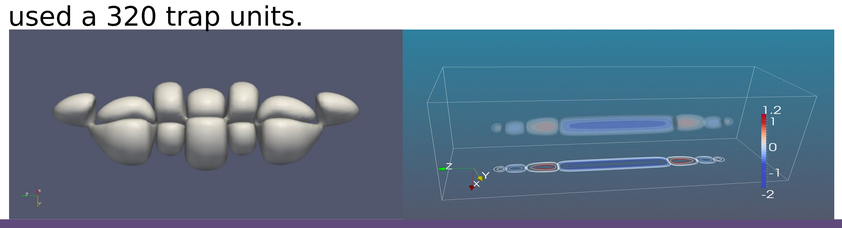
$$\left(\frac{-1}{2}\Delta + V\right)\psi = E\psi \;\rightarrow\; (\Delta + 2E)\psi = V\psi \;\rightarrow\; \psi = -2\int \frac{e^{-k|r-s|}}{4\pi|r-s|} V\psi\, dr$$

Complex Topologies



Examples of adaptive representations of wave-functions, for a given precision, are illustrated. Each wave-function and operator has its own adaptive spectral representation. For example, the modulus squared of the single-neutron corresponding to -5.214 MeV calculations for ^{110}Mo (a) with its corresponding spectral refinement structure (b). Examples of other wave-functions are pictured above.

An important example is the simulation of a Fermi gas and the superfluid phase in spin-imbalanced systems in an elongated trap, such as the Fulde-Ferrell-Larkin-Ovchinnikov phase that exhibits oscillating pairing gap using an asymmetric local density approximation. The transversal pairing field are indicative of the Larkin-Ovchinnikov phase. The simulation used a 320 trap units.

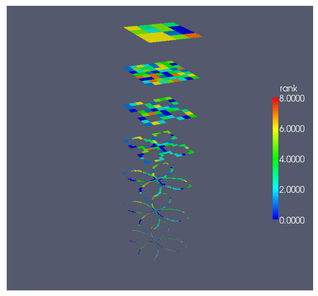


MADNESS

MADNESS is a general purpose numerical environment for deploying advanced scientific algorithms on petascale and beyond – emphasizing productivity and performance.

A fast prototyping, high level coding – a nearly symbolic programming object-oriented C++ environment:

$$E = \int \left(\frac{-1}{2}\Delta + V\right)\psi(r)\psi(r)\,dr + \int \frac{\psi(r_1)\psi(r_2)}{|r_1 - r_2|} dr_1 dr_2$$



The colors represent the nodes holding non-trivial blocks of coefficients of a function approximated in Alpert's multiwavelet basis.

```
real_function_3d Vnuc = real_factory_3d(world).f(V);
real_function_3d psi  = real_factory_3d(world).f(guess);

real_convolution_3d op = CoulombOperator(world, rlo, thresh);
real_function_3d rho = square(psi).truncate();
double two_electron_energy = inner(op(rho),rho);
double nuclear_attraction_energy = 2.0*inner(Vnuc,rho);

double kinetic_energy = 0.0;
for (int axis=0; axis<3; axis++) {
   real_derivative_3d D = free_space_derivative<double,3>(world, axis);
   real_function_3d dpsi = D(psi);
   kinetic_energy += inner(dpsi,dpsi);
}

double total_energy = kinetic_energy + two_electron_energy +
   nuclear_attraction_energy + nuclear_repulsion_energy;
```

A parallel runtime library is responsible for managing task scheduling and placement, as well as dependencies (futures) with user enabled load and memory balancing. All communication are asynchronously. All intra-node communication by performed by parallel threads. Interface to Intel TBB available.

Fast “mathematical O(N)” computation with guaranteed precision through the use of MRA in conjunction with compact nonlinear multiscale approximations for high-order (up to 32+) and accurate solutions of coupled 1-6D systems of time-dependent integral and differential equations with functional and a variety boundary conditions – solving systems with several trillions of variables.

- Controlled truncation for accuracy and sparsity, hierarchy of equations by scale (a la renormalization)
- Compact non-linear approximation of high-dimensional functions and integral operators (Green's functions)

$$f^n(x) = \sum_{i=0}^{k-1} s_{i0}^0 \phi_{i0}^0(x) + \sum_{n'=0}^{n-1}\sum_{l=0}^{2^{n'}-1}\sum_{i=0}^{k-1} d_{il}^{n'} \psi_{il}^{n'}(x) \qquad f(x_1,\ldots,x_n) = \sum_{l=1}^{min(M)} \sigma_l \prod_{i=1}^{d} f_i^{(l)}(x_i) + O(\epsilon)$$
$$\left\|f_i^{(l)}\right\|_2 = 1 \qquad \sigma_l > 0$$

Runs from Linux and Apple laptops to clusters and leadership class computers. Accelerators versions (GPU and Intel Phi) under development.

References:

- R.J. Harrison, G. I. Fann, T. Yanai, Z. Gan, G. Beylkin, “Multiresolution quantum chemistry: Basic theory and initial applications,” J. Chem. Phys. 121 11587 (2004)
- G. I. Fann, J. Pei, R.J. Harrison, J. Jia, J. Hill, M. Ou, W. Nazarewicz, W. A. Shelton, N. Schnuck, “Fast multiresolution methods for density functional theory in nuclear physics,” JPG, Phys. Conf. Ser. 180 012080 (2004)
- J.C. Pei, G.I. Fann, R.J. Harrison, W. Nazarewicz, Y. Shi, S. Thornton, “Adaptive multiresolution 3D Hartree-Fock-Bogoliubov solver for nuclear structure,” Phys. Rev. C 90 024317 (2014)
- R. Harrison, et. al., “MADNESS: A multiresolution adaptive numerical environment for scientific simulation,” arXiv:1507.01888v1, July 5, 1025.

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