Massively Parallel Adaptive 3-D DFT Solver for Nuclear Physics

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MADNESS applications in nuclear structures

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MADNESS

Multiresolution
Adaptive
Numerical
Scientific
Simulation

2011 R&D 100

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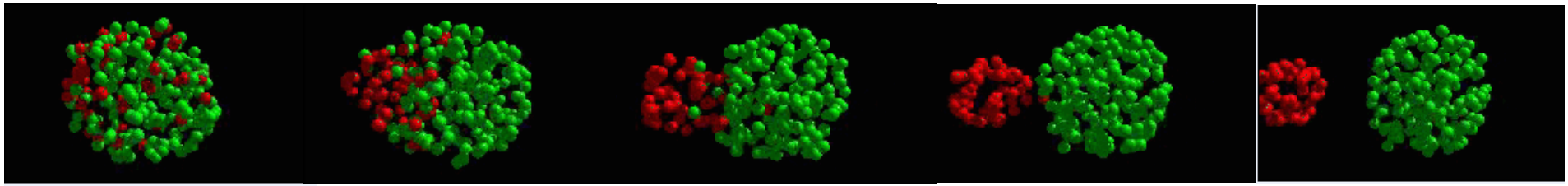
Some background

- *Most nuclear physics codes are based on the HO basis expansion method. Precision not guaranteed in case of weakly-bound or very large deformations.*
- *Not suitable for leadership computing, not easily parallelizable*
- *2D coordinate-space Hartree-Fock-Bogoliubov code was based on B-Spline techniques:* ***HFB-AX***
- *3D coordinate-space HFB is not available.*
  - *Developing* ***MADNESS-HFB****, adaptive pseudo-spectral based*
  - *No assumptions on symmetry, weak singularities and discontinuities*
- *Applications: complex nuclear fission, fusion process.*



HFB equation of polarized Fermi system

- A general HFB equation (tested with 2-D spline on 2008, 2009, 2010 benchmarks)

$$\begin{bmatrix} h_a(\boldsymbol{r}) - \lambda_a & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_b(\boldsymbol{r}) + \lambda_b \end{bmatrix} \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix} = E_i \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix}$$

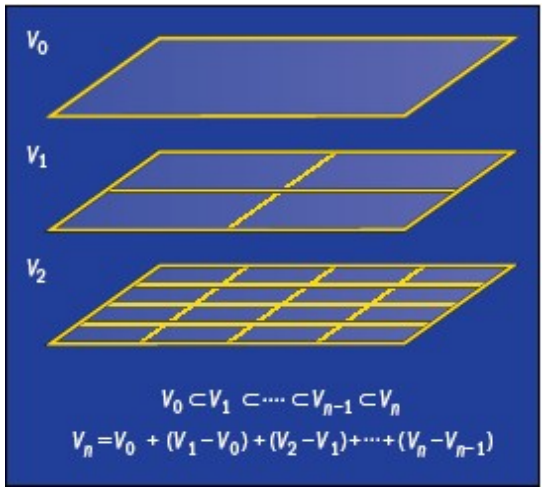
- Time-reversal symmetry broken: polarized system, odd-nuclei
- We are testing a 3-D Skyrme-HFB.
- 3D Skyrme: applies to any system with complex geometry shape:fission

$$h_a = -\frac{\hbar^2}{2m}\nabla \cdot (\nabla \alpha_a) + U_a + V_{\text{ext}}$$

- Effective mass is density dependent, with spin-orbit, Poisson solver for coulomb potential.

Mathematics

- Multiresolution



- Approximation using Alpert's multiwavelets

Function represented by 2 methods, spanning same approximation space:
1. scaling function basis
2. multi-wavelet basis

$$f^n(x) = \sum_{l=0}^{2^n-1} \sum_{i=0}^{k=1} s_{il}^n \phi_{il}^n(x)$$

$$f^n(x) = \sum_{i=0}^{k-1} s_{i0}^0 \phi_{i0}^0(x) + \sum_{n=0\ldots} \sum_{l=0}^{2^n-1} \sum_{i=0}^{k=1} d_{il}^n \psi_{il}^n(x)$$

- Low-separation rank: (e.g., optimized approx of Green functions with Gaussians: Beylkin-Mohlenkamp, Beylkin-Cramer-Fann-Harrison, Harrison)

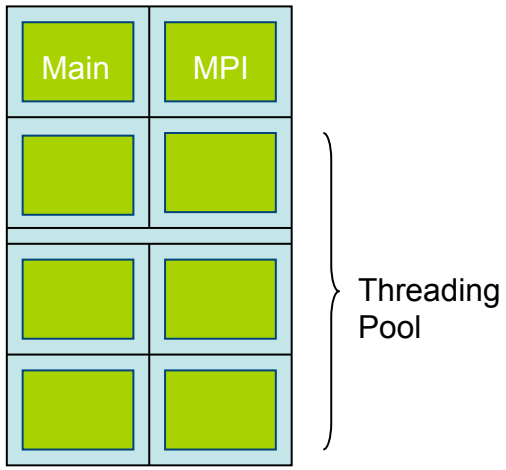
$$f(x_1, \ldots, x_n) = \sum_{l=1}^{M} \sigma_l \prod_{i=1}^{d} f_i^{(l)}(x_i) + O(\epsilon)$$

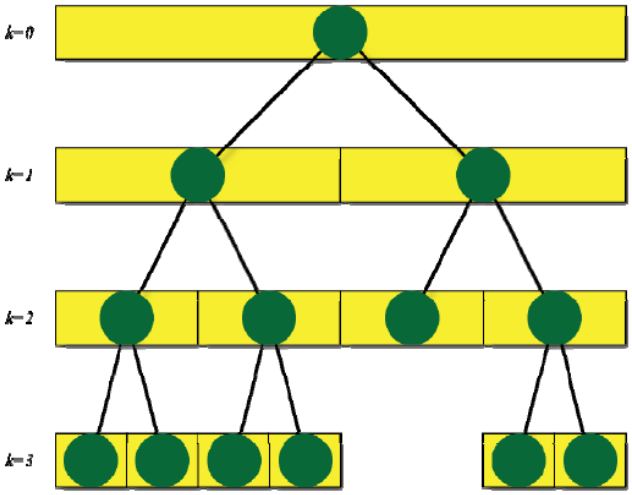
$$\left\| f_i^{(l)} \right\|_2 = 1 \qquad \sigma_l > 0$$

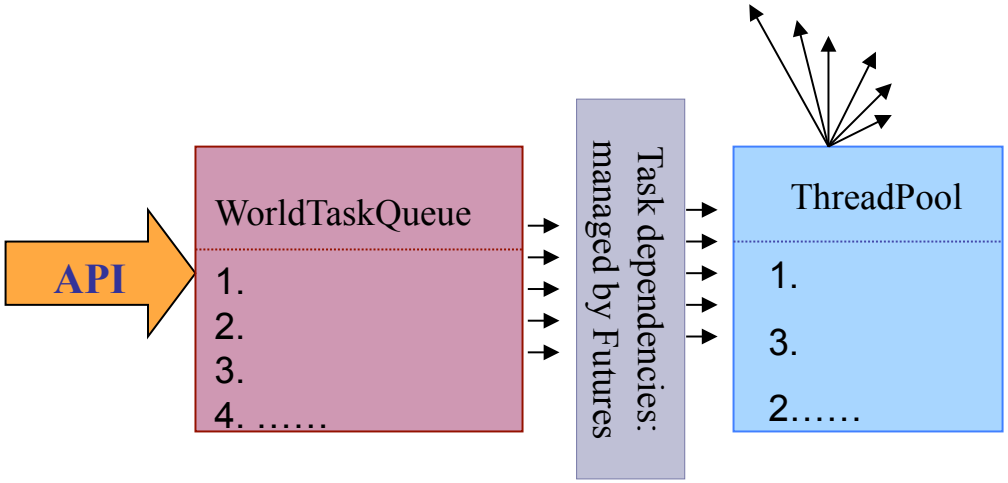
Parallel computing strategy

- MPI: node to node communication
- Distributed arrays and FUTURES
- Pthreads: multi-threading within one node

  threads per node: 10+main MPI +thread server = 12
- Load-balance: map tree to parallel hash table







Self-consistent HFB

- Initial Wavefunctions(u, v): deformed HO functions+random gauss
- Construct Hamiltonian: H(i, j);
  - time consuming, quadrature, L2-inner product
- Diagonalization: Hx=eBx; big problem for large system

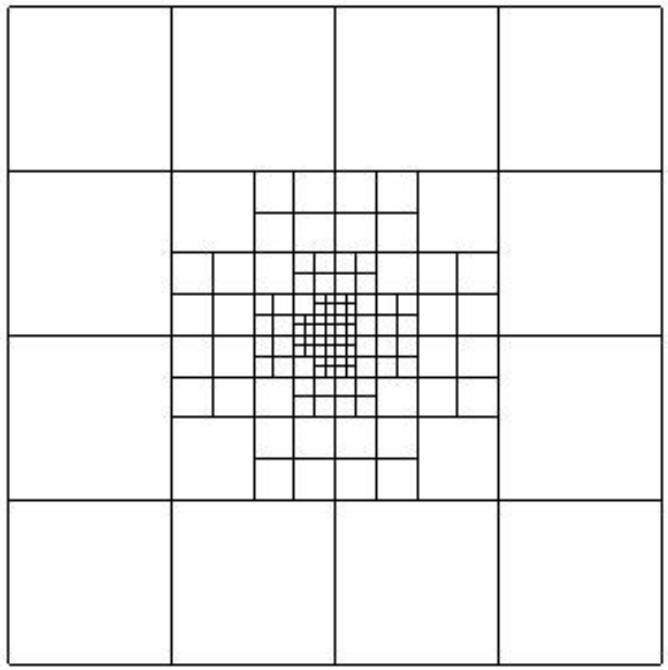
  (Parallel diag added)
- Transform from coefficients to wfs; used to be very time consuming
- Improve approximations by applications of BS Helmholtz kernel:

  u_new=apply(kernel, u), v_new=apply(kernel, v),
- Iteration until convergence: if error is small

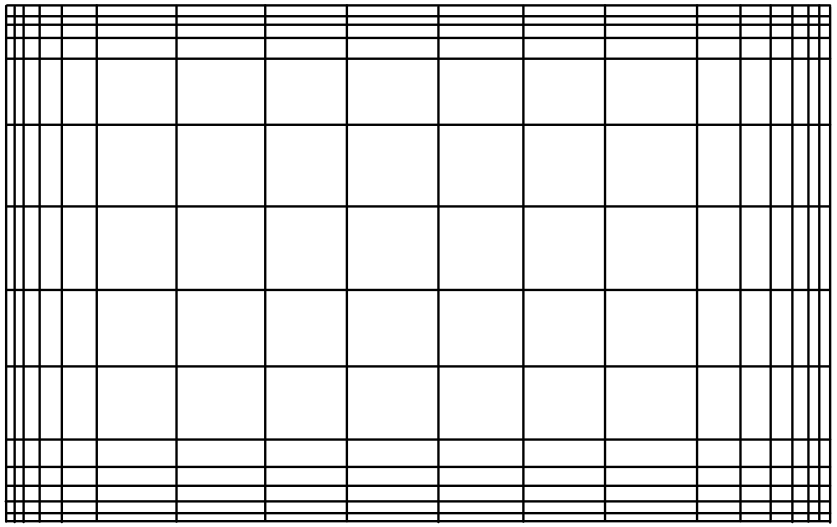
  error = norm(u_new-u)+norm(v_new-v)

Adaptive Representation of Quasi-Particle Wave Functions

MADNESS mesh



B-spline Mesh (focus on boundary condition; rectangle box for deformation)



Fixed mesh, not efficient

A 2-D slice of the 3-D support of the multiwavelet bases for the 2-cosh potential (left) and one of its wave-functions (right).

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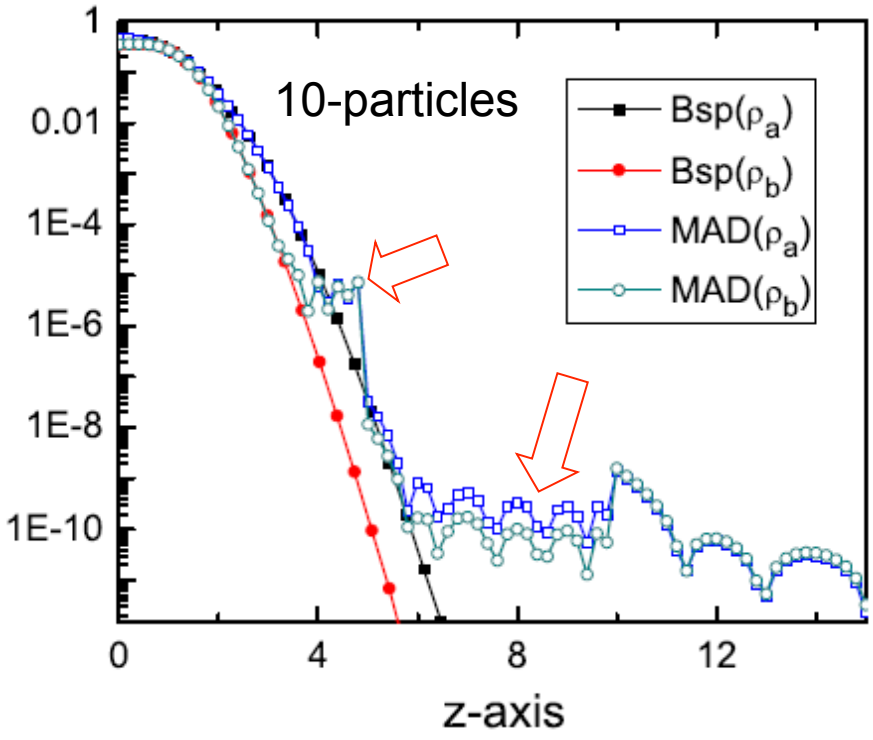
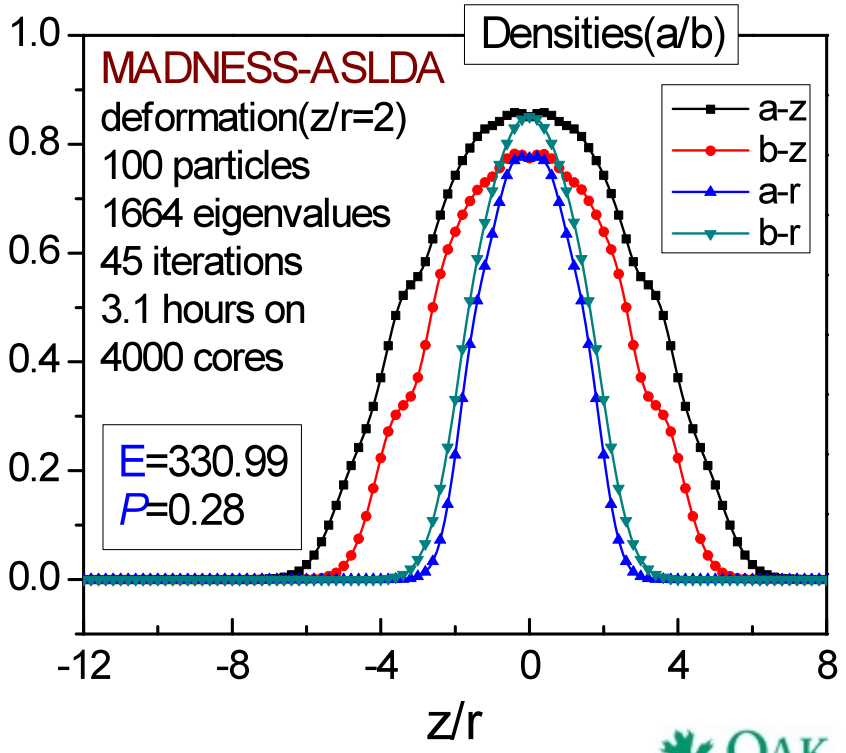
ASLDA Tests (from summer 2010)

- More complicated and time-consuming than SLDA
  in the calculation of local polarization (ρ_a/ρ_b) with thresh=1.e-4



Total energy:
E(bsp)=19.044
E(mad)=19.042

100 particles In a deformed trap



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Capabilities (recent additions)

Addition of parallel iterative complex Jacobi Hermitian diagonalizer

- full 64 bit addressing, thread safe (bypassing problems with 32 bit BLACS/Scalapack)
- fully distributed data

Boundary conditions: Dirichlet, Neumann, Robin, quasi-periodic, free, asymptotic, mixed : 1-6D for derivatives

Fast bandlimited tranformations (e.g. multiwavelets to/from FFT, JCP 2010)

New C++ standard compatibility (icc, gcc, pgcc)

Portable to PCs, Macs, IBM BGL, Cray, clusters

In SVN with autoconf, configure, …

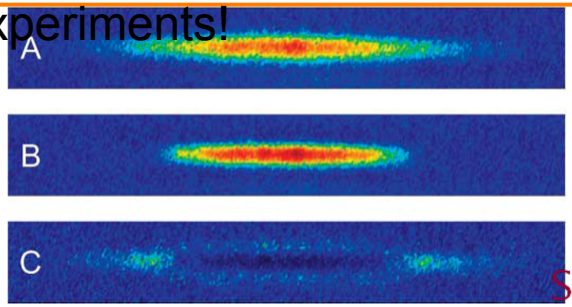
http://code.google.com/p/m-a-d-n-e-s-s/

Spin-orbit hamiltonian, nonlinear Schrodinger, molecular DFT, TDSE examples available in examples directory. Please ask us for HFB DFT code after this summer.

To extremely deformations (2010)

- Towards to 10^5 cold-atoms in an elongated trap

Finite-size effects indicated by experiments!

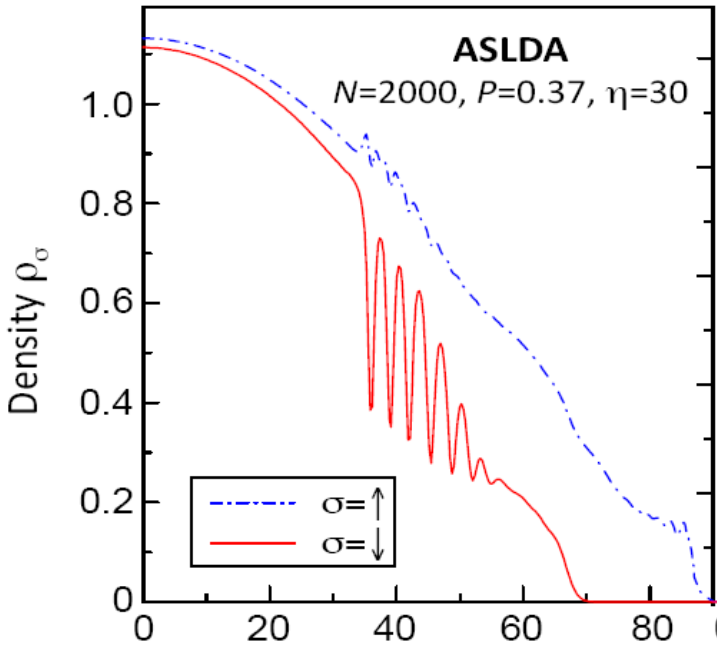


Science 311(2006)5

- MADNESS takes 3～4 hours for 100 particles on 2400 cores in an elongated trap.

Involving 2000 eigen-solutions

B-spline calculations:
extremely slow
(2 weeks, 140 cores)



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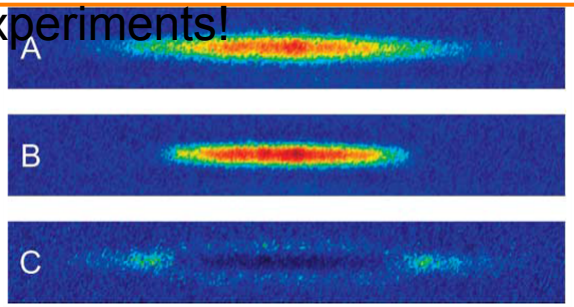

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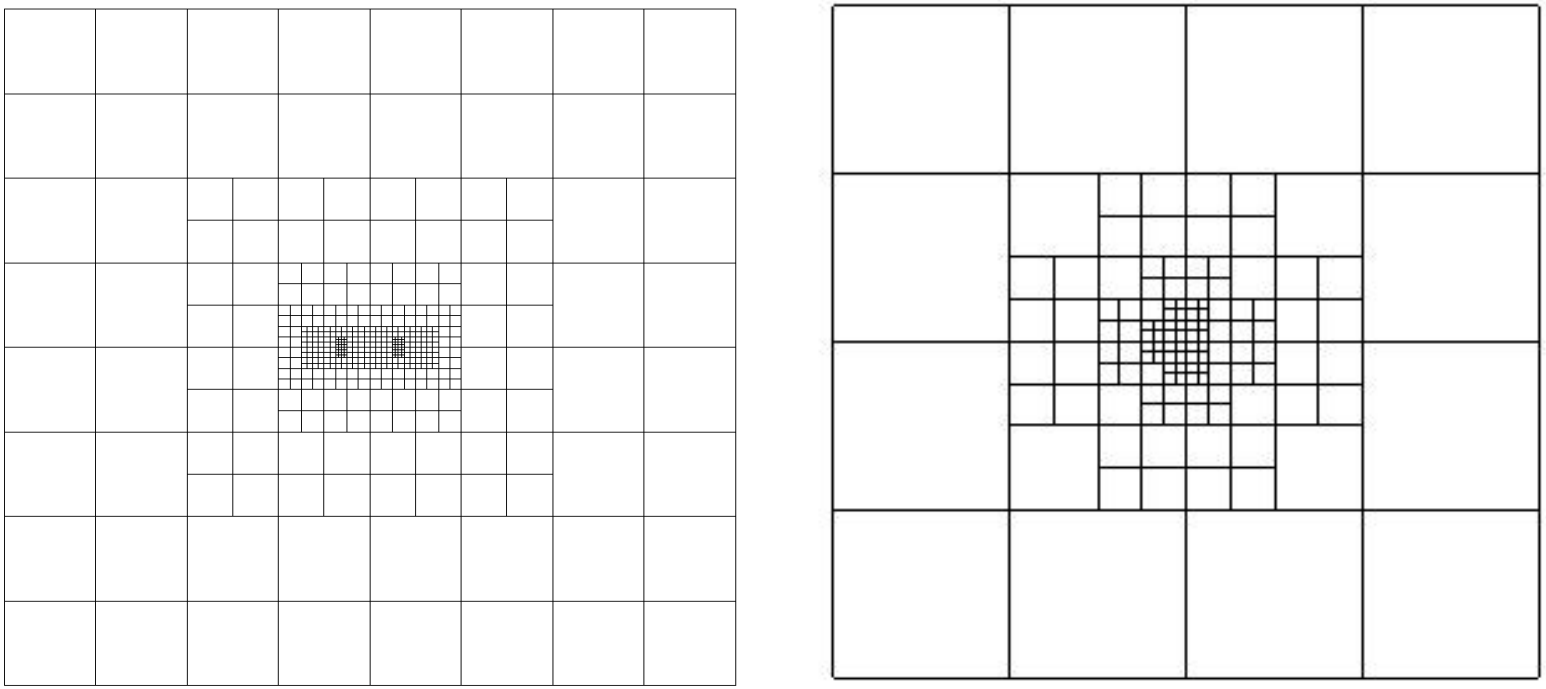
- deformation in z-direction 1/50.
- particle 1000 particles -> 10^5 wave fns
- ecut = 20

MADNESS: High-level composition

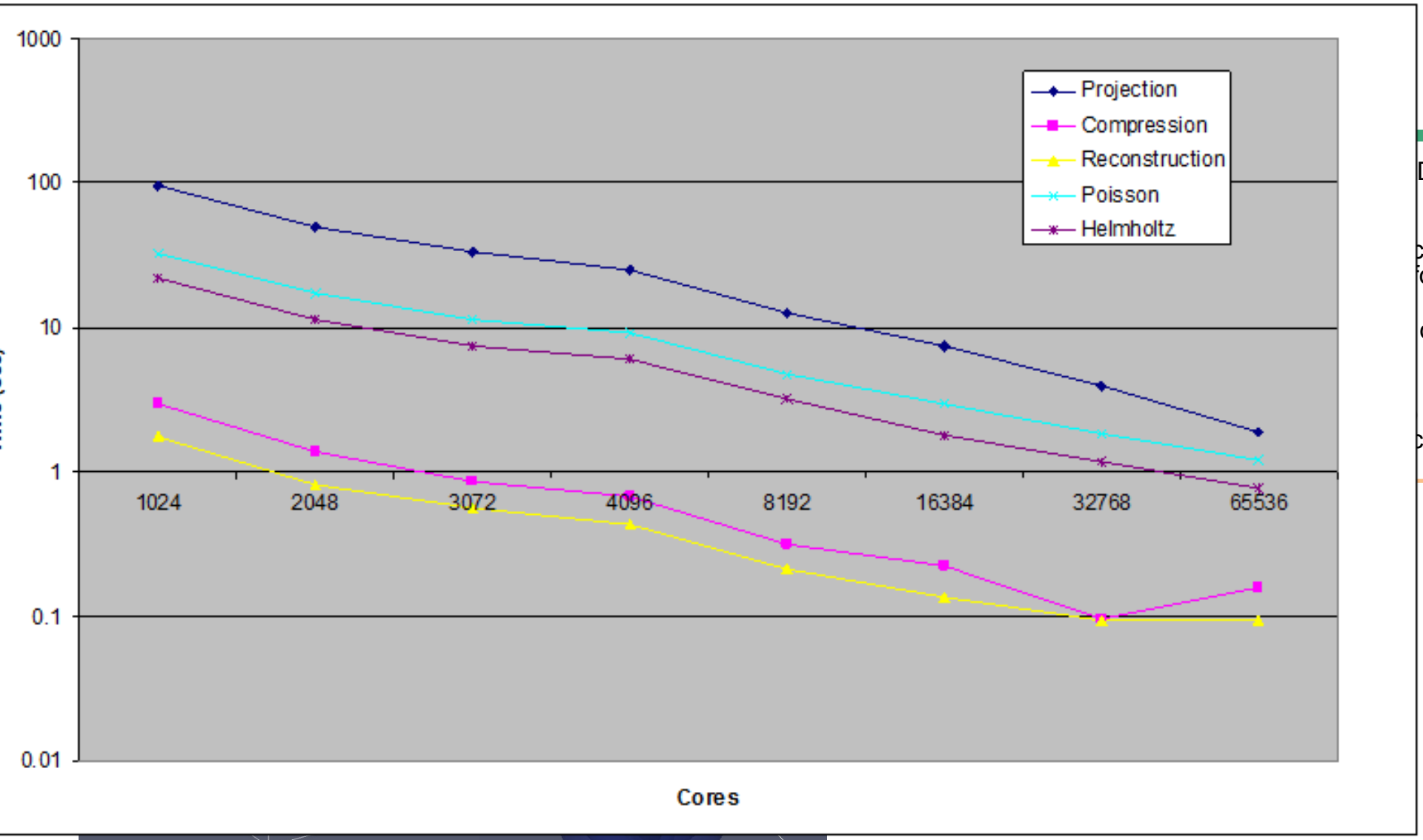
- Coding composition is close to the physics, example with h=m=1 (chemist notation)
- $$E = \left\langle \psi \left| -\frac{1}{2}\nabla^2 + V \right\rangle \psi + \int \psi^2(x) \frac{1}{|x-y|} \psi^2(y) dx dy$$

- **operatorT op = CoulombOperator(k, rlo, thresh);**
- **functionT rho = psi*psi;**
- **double twoe = inner(apply(op,rho),rho);**
- **double pe = 2.0*inner(Vnuc*psi,psi);**
- **double ke = 0.0;**
- **for (int axis=0; axis<3; axis++) {**
- **functionT dpsi = diff(psi,axis);**
- **ke += inner(dpsi,dpsi);**
- **}**
- **double energy = ke + pe + twoe;**

Adaptive Representation of Support of Wave-Functions



A 2-D slice of the 3-D support of the multiwavelet bases for the 2-cosh potential (left) and one of its wave-functions (right).



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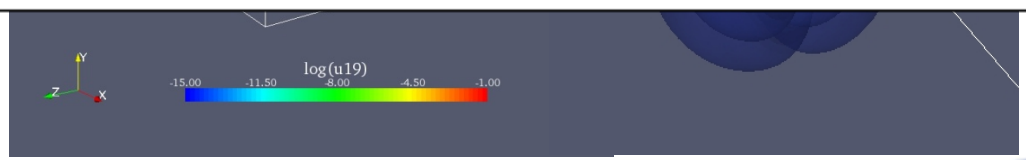
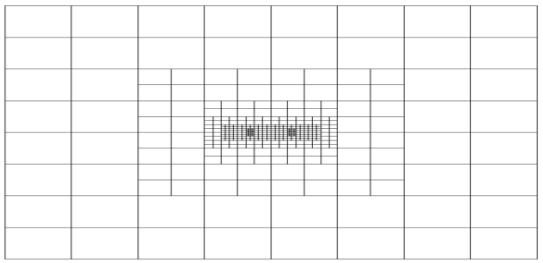




Summary

Target is to develop an accurate, scalable, portable 3D nuclear DFT solver.

What have done this year:

1) Hybrid HFB test for continuum

2) HFB solvers

   A. Reproduced SLDA/ASLDA from last year and compared well with 2-d spline (3 digits) (~2K lines)

   B. Skyrme (testing with fully 3-D, SKM* interaction) (~3K lines)

Work target:

Outlook: calculation of large deformed systems, ASLDA (20K wavefunctions), each wave function has 7+ levels of refinement (8^7 boxes), 18^3 basis functions per box, 8^7, ~12B unknowns for 1-e5 precision. For Skyrme test, 10K quasi-particle wave-functions (4 components+proton+neutron, with broken time-reversal symmetry)

Debugging problem on Jaguarpf at ORNL at 20K-120K cores

Solving nuclear problems

$$\left(-\tfrac{1}{2}\nabla^2 + V\right)\Psi = E\Psi$$

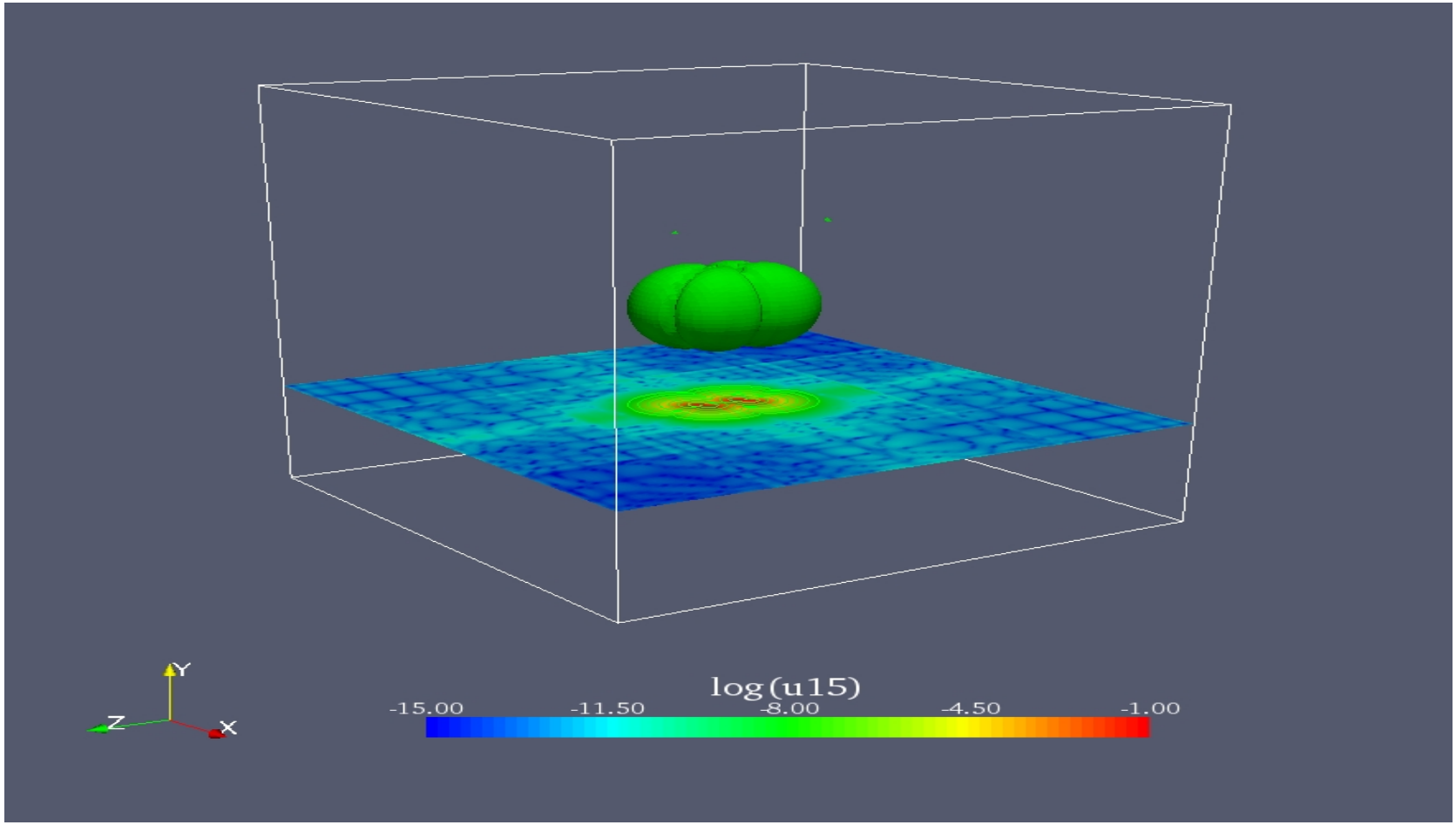
$$\Psi = -2\left(-\nabla^2 - 2E\right)^{-1} V\Psi$$

$$= -2G*\left(V\Psi\right)$$

$$\left(G*f\right)(r) = \int ds \frac{e^{-k|r-s|}}{4\pi|r-s|} f(s) \quad \text{in 3D ; } k^2 = -2E$$

- Spin-orbit coupling implemented in nuclear physics(2008)
- effective mass is density dependent (2010)
- out-going boundary condition (to do…)

Graphics Capability: generate VTK



The 15-th wave-function for the 2-cosh potential with spin-orbit

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