# *MADNESS-HFB Nuclear DFT in 3-D Toward a Multiresolution Nuclear DFT and Hartree-Fock Bogoliubov Solver*

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UNEDF 2010 Meeting, Michigan State

East Lansing, MI, June 22, 2010




# MADNESS

*Multiresolution*
*Adaptive*
*Numerical*
*Scientific*
*Simulation*

Office of Science
U.S. DEPARTMENT OF ENERGY

ASCR

SciDAC
Scientific Discovery through Advanced Computing

OAK RIDGE
National Laboratory

# The funding


- The development of MADNESS is funded by the U.S. Department of Energy, Office of Advanced Scientific Computing Research (OASCR) and the division of Basic Energy Science, Office of Science, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, by the SciDAC Base Math Program and was by SAP in computational chemistry (PI: Fann) and SciDAC BES (PI:Harrison).
- The application of MADNESS-NDFT to nuclear physics is funded through SciDAC UNEDF (PIs: R. Lusk and W. Nazarewicz, co-PI: Fann) by the DOE-OASCR.
- This research was performed in part using
  - resources of the National Energy Scientific Computing Center which is supported by the Office of Energy Research of the U.S. Department of Energy under contract DE-AC03-76SF0098,
  - the Center for Computational Sciences at Oak Ridge National Laboratory under contract DE-AC05-00OR22725 .

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

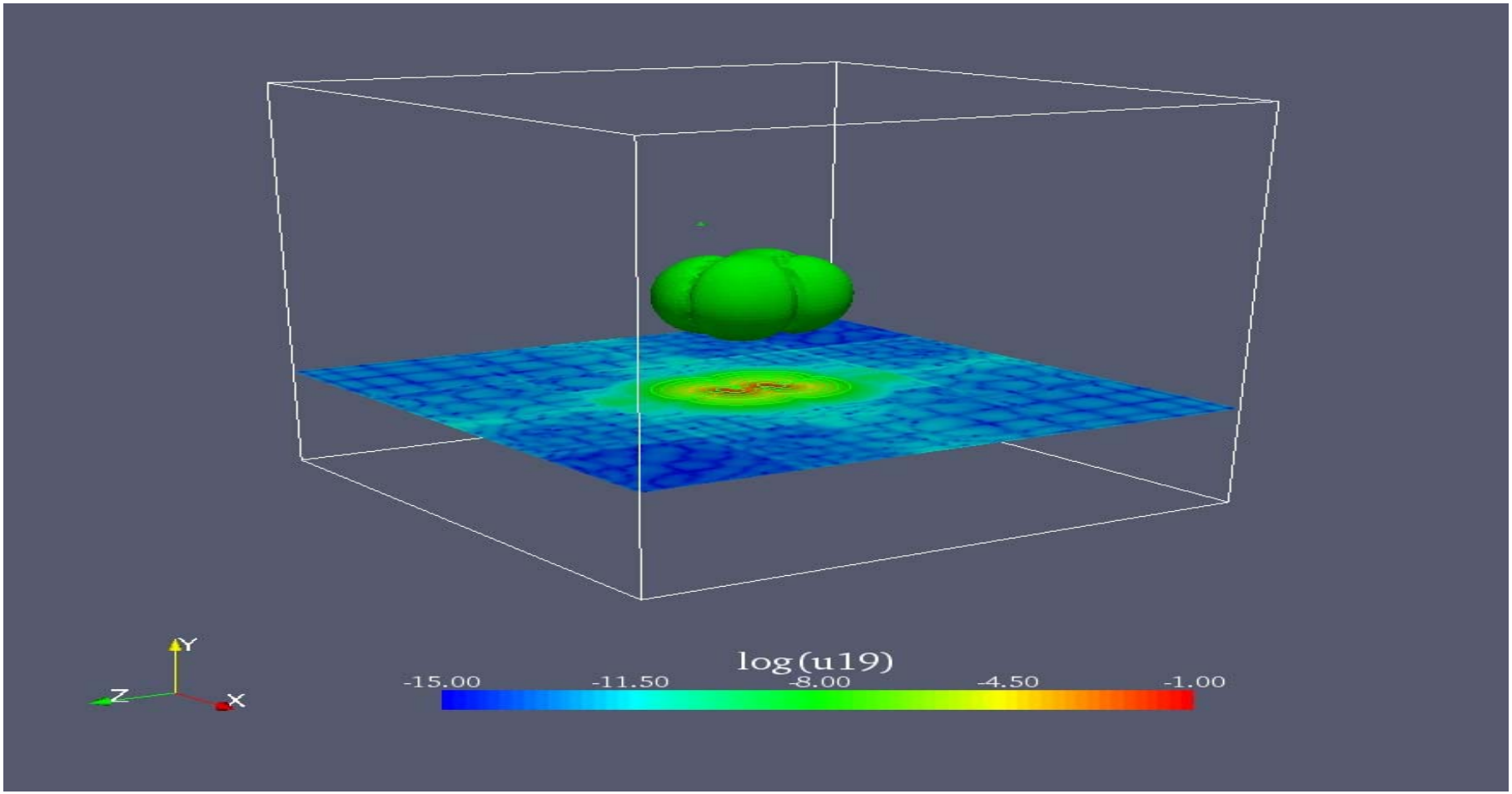

# *MADNESS release 1, Jan. 2010*

- MADNESS v. 1 released in Jan. 2010.
  - Guaranteed accuracy with controlled precision
  - With examples in nuclear DFT with two-cosh potential, 3-D
  - Non-linear Schrodinger equation (1-D version of slda)
  - Time-dependent Hartree-Fock and Density Functional Theory for molecular density functional theory, 3-D
  - Iterative solution of Lippman-Schwinger equation
  - Nano-transport with embedded ghost cells and constrained optimization
  - Integro-differential equation
  - Representation over complex and spin-coordinate
  - I/O, checkpointing of intermediate terms
  - Estimation of errors for smooth and weakly singular solutions

# *MADNESS release 1, 2010*

- CS and Math side
  - *For nuclear physics, input using HO initial guess*
  - *Representation using adaptive discontinuous pseudo-spectral*
  - *Dynamic Load Balancing*
  - *Boundary conditions*
    - Dirichlet, Neuman, Robin, Free, User-defined
    - Periodic, quasi-periodic
  - *Examples of time-stepping, explicit and implicit*
  - *Iterative solvers*
    - GMRES, BiCGStab, Conjugate Gradient, …
  - *Iterative eigensolver*
    - Davidson, …
  - *Output vtk files for graphics*

# *Example of a quasi-particle wave-functions for the 2-cosh potential with spin-orbit*

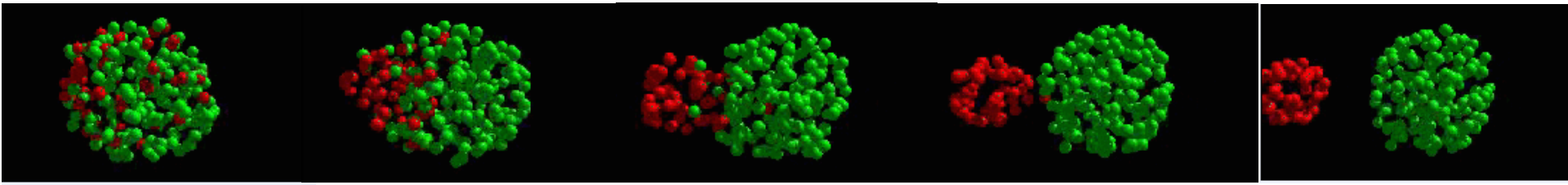


# Outline

- Motivation
- Recent SLDA and ASLDA results comparing
  - 3-D multiresolution methods with no assumption on symmetry
  - 2-D spline with assumption axial symmetry
  - Accuracy and scaling
- New solution method for non-linear self-consistent HFB equation

# Background

- *Most nuclear physics codes are based on the HO basis and spline expansion method. Precision not guaranteed in case of weakly-bound or very large deformations in 3-D.*
- *Most are not easily parallelizable nor scalable for exascale computing without significant rewrite.*
- *2-D coordinate-space Hartree-Fock-Bogoliubov code is based on B-Spline techniques:* ***HFB-AX***
- *General 3-D 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

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

- Time-reversal symmetry broken: polarized system, odd-nuclei
- 3-D: 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. (similar to the Skyrme DFT)
- We are ready to develop a Skyrme-HFB using the zero-boundary condition based on MADNESS.

# Recent Progress of MADNESS

- Solving A.Bulgac's SLDA and ASLDA equations for imbalanced Fermi condensates. [A. Bugac. PRA 76:040502, PRL 101:215301]

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

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

- Pairing regularization to avoid cutoff divergent (Bulgac)

$$\mathcal{E} = \alpha_a(x)\frac{\tau_a}{2} + \alpha_b(x)\frac{\tau_b}{2} + \frac{(3\pi^2(\rho_a+\rho_b))^{5/3}}{10\pi^2}\beta(x) - \Delta\kappa$$

$$\frac{1}{g_{eff}(\mathbf{r})} = \frac{n^{1/3}(\mathbf{r})}{\gamma} + \Lambda_c(\mathbf{r}),$$

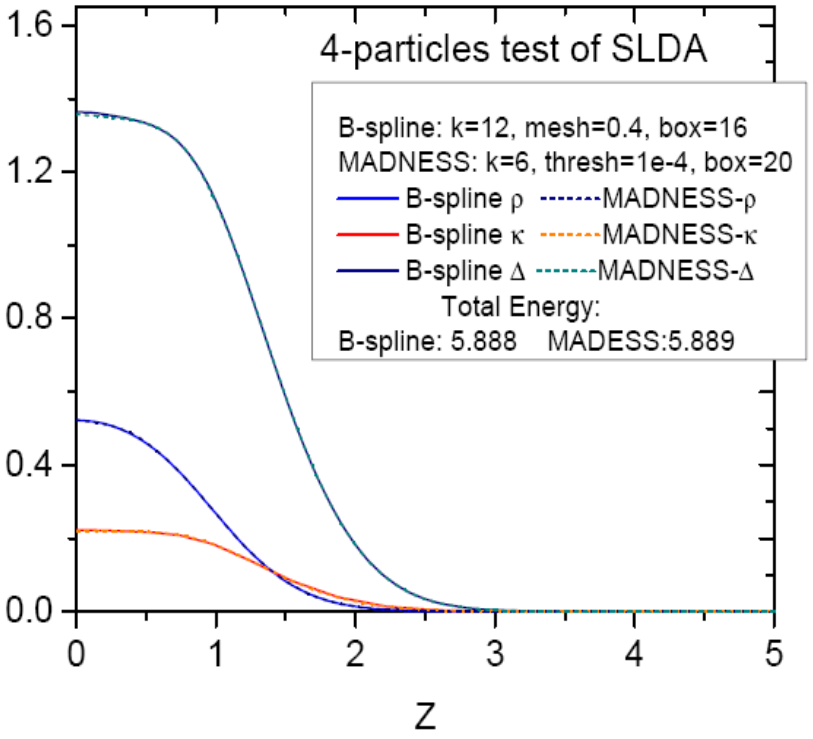
$$\Lambda_c(\mathbf{r}) = -\frac{k_c(\mathbf{r})}{2\pi^2\alpha}\left\{1 - \frac{k_0(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r})+k_0(\mathbf{r})}{k_c(\mathbf{r})-k_0(\mathbf{r})}\right\}$$

# *Recent Progress of MADNESS*

Exterior potential, a deformed

$$V_{ext}(\mathbf{r}) = V_{shift}(1 - \exp(-\frac{(\omega_r^2(x^2+y^2)+\omega_z^2 z^2)}{2 \times V_{shift}}))$$

- Benchmarking is done: densities, eigenvalues, occupation numbers (MADNESS and B-spline methods)
- SLDA-MADNESS has been benchmarked (Feb. 2010)
- ASLDA-MADNESS has been benchmarked (Mar.2010)
- Can treat 100 particles in a deformed trap
- need improved parallel diagonalization for $10^4$ particles (in development now)
- need continous spectra for nuclear HFB in 2010

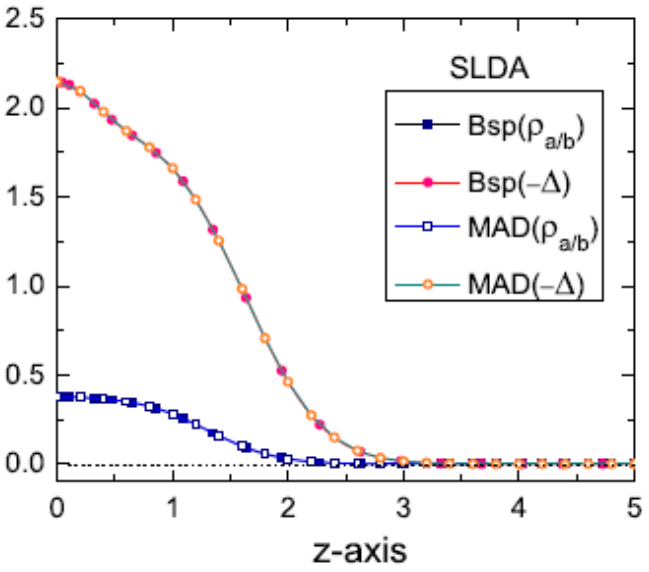


# Self-consistent HFB, SLDA, 10 Particles

- Quasiparticle energies and occupation numbers of 10 particles, to 1.e-4 precision
- ~50 minutes using 400 cores (about 40 iterations), involving 296 eigen-values, on Cray XT-5, 12 cores/node (March 2010)

| | MADNESS-HFB | | HFB-AX | |
|---|---|---|---|---|
| $E_t$ | 18.269 | | 18.268 | |
| $\lambda$ | 2.1997 | | 2.1999 | |
| states | $E_i$ | $v_i^2$ | $E_i$ | $v_i^2$ |
| 1 | 0.9070 | 0.2325 | 0.9064 | 0.2325 |
| 2 | 1.0645 | 0.1777 | 1.0638 | 0.1777 |
| 3 | 1.1158 | 0.4719 | 1.1154 | 0.4720 |
| 4 | 1.9004 | 2.335e-2 | 1.8999 | 2.333e-2 |
| 5 | 1.9897 | 0.2801 | 1.9892 | 0.2802 |
| 6 | 2.5044 | 0.3363 | 2.5041 | 0.3355 |
| 7 | 2.6665 | 3.451e-2 | 2.6661 | 3.449e-2 |
| 8 | 2.7797 | 0.5722 | 2.7795 | 0.5729 |
| 9 | 2.8756 | 4.112e-3 | 2.8752 | 4.110e-3 |
| 10 | 3.4063 | 2.356e-2 | 3.4059 | 2.355e-2 |
| 23 | 5.6835 | 1.894e-3 | 5.6832 | 1.890e-3 |
| 24 | 5.9359 | 2.581e-4 | 5.9356 | 2.563e-4 |

- Densities comparison

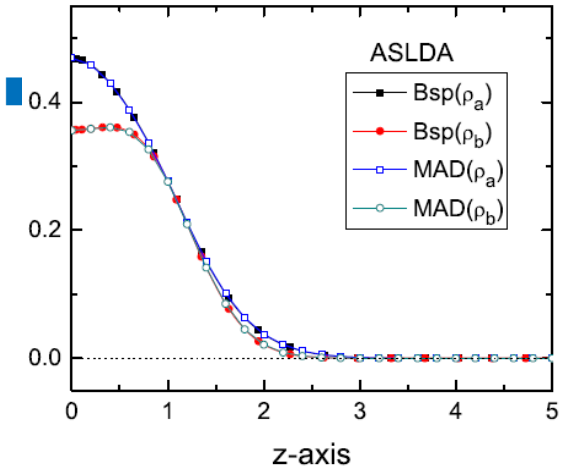


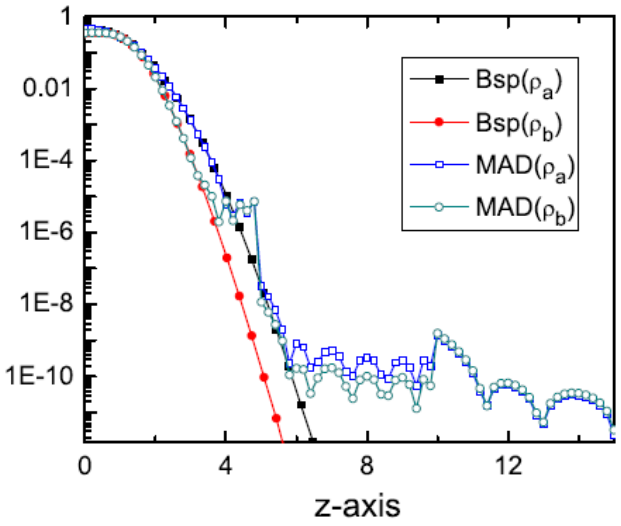
# Self-consistent HFB and nuclear structures

- Precision control ↔ Computing in multiwavelets, if smooth function, can truncate expansion to desired precision
- Benchmarking  total energy, Fermi energy, quasiparticle energy, occupation numbers

| | E | $E_{Fermi}$ | $E_{low}$ | $E_{high}$ | walltime (s) (40 iterations) |
|---|---|---|---|---|---|
| K=7, thresh=1e-3 | 6.230 | 1.8801 | 0.24760<br>0.32322 | 5.12213<br>0.00000131 | 834.9 |
| K=8, thresh=1e-4 | 6.230 | 1.8801 | 0.24765<br>0.32321 | 5.12215<br>0.00000145 | 1590.7 |
| K=9, thresh=1e-5 | 6.230 | 1.8801 | 0.24765<br>0.32321 | 5.12215<br>0.00000149 | 2818.5 |
| B-splines | 6.229 | 1.8801 | 0.24781<br>0.32373 | 5.12210<br>0.00000149 | 2-hours (1 core) |

# ASLDA multiwavelets and splines, 10 particles

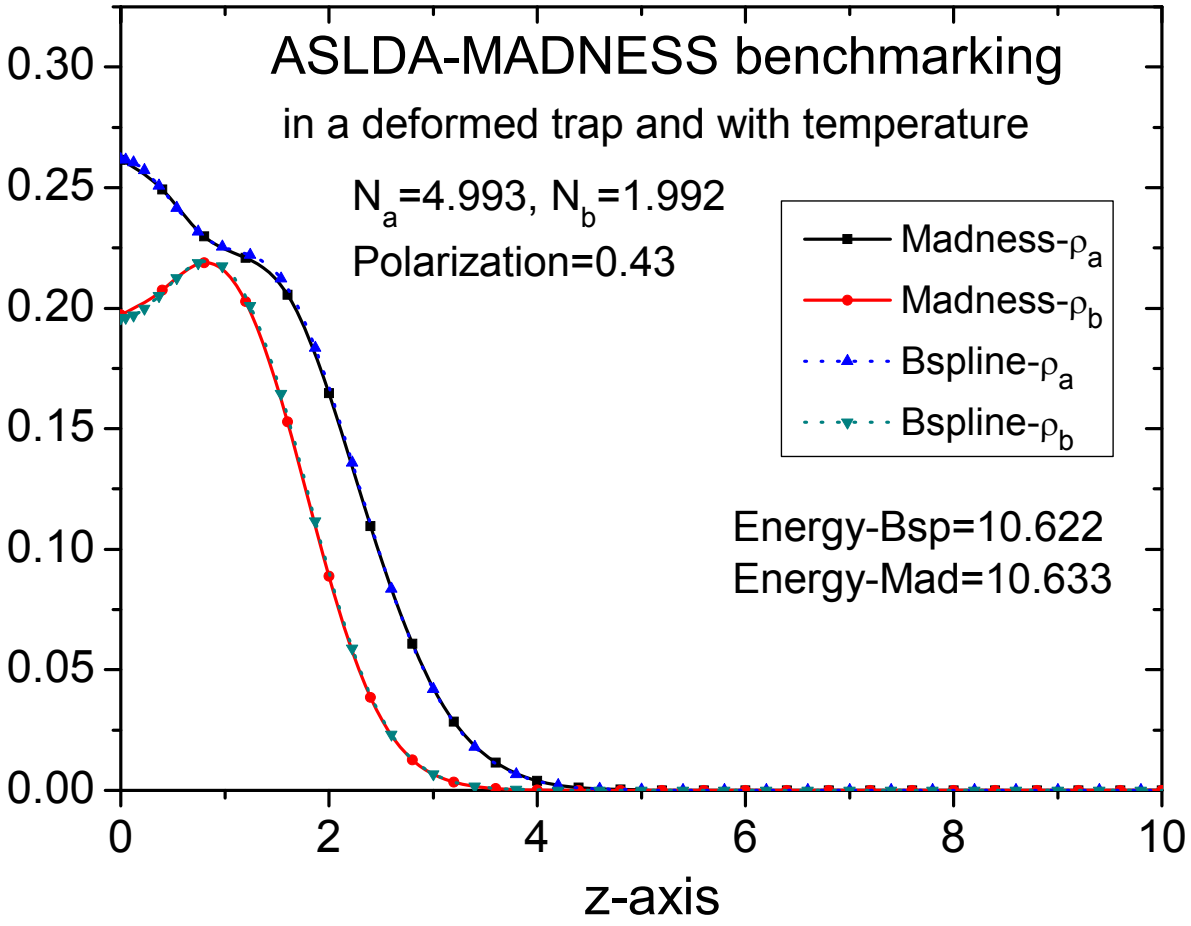



| | MADNESS-HFB | | HFB-AX | |
|---|---|---|---|---|
| $E_t$ | 19.044 | | 19.044 | |
| $\lambda$ | 2.1687 | | 2.1683 | |
| states | $E_i$ | $v_i^2$ | $E_i$ | $v_i^2$ |
| 1 | -0.1341 | 0.2090 | -0.1330 | 0.2091 |
| 2 | 0.0453 | 0.14931 | 0.0468 | 0.14939 |
| 3 | 0.0783 | 0.4694 | 0.0787 | 0.4682 |
| 4 | 0.8833 | 0.01737 | 0.8838 | 0.01742 |
| 5 | 1.0142 | 0.2746 | 1.0161 | 0.2750 |
| 6 | 1.5424 | 0.2941 | 1.5425 | 0.29274 |
| 7 | 1.6940 | 0.0321 | 1.6943 | 0.03225 |
| 8 | 1.8326 | 0.6154 | 1.8348 | 0.6161 |
| 23 | 4.6415 | 0.00155 | 4.6416 | 0.00156 |
| 24 | 4.8158 | 1.677E-4 | 4.8157 | 1.692E-4 |

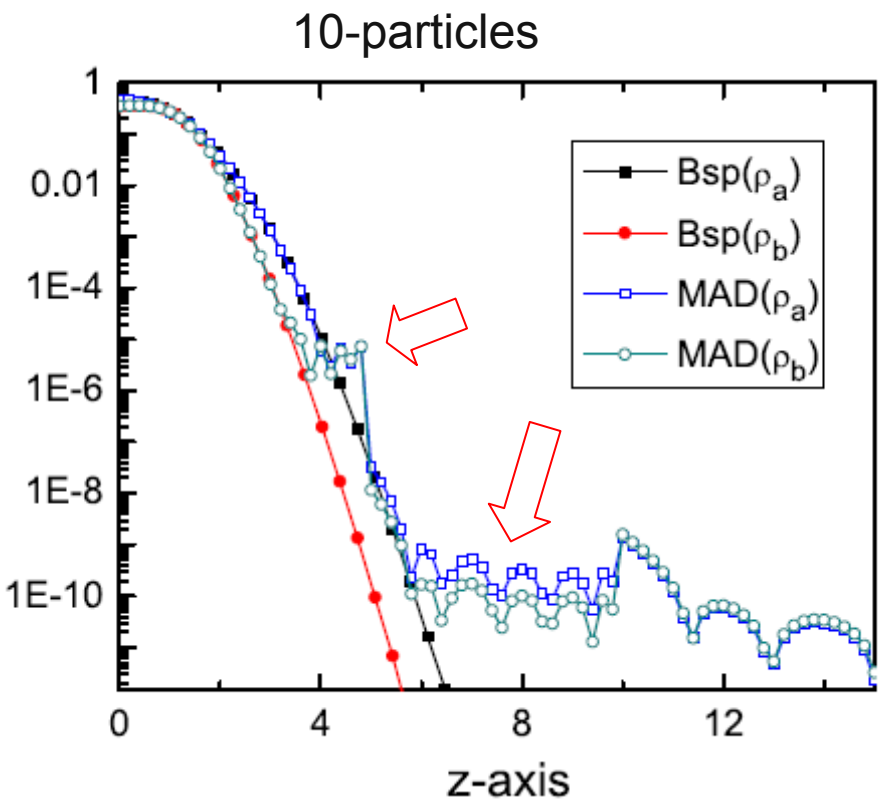
# Recent Progress of MADNESS

- ASLDA-MADNESS benchmarking:



# ASLDA Tests

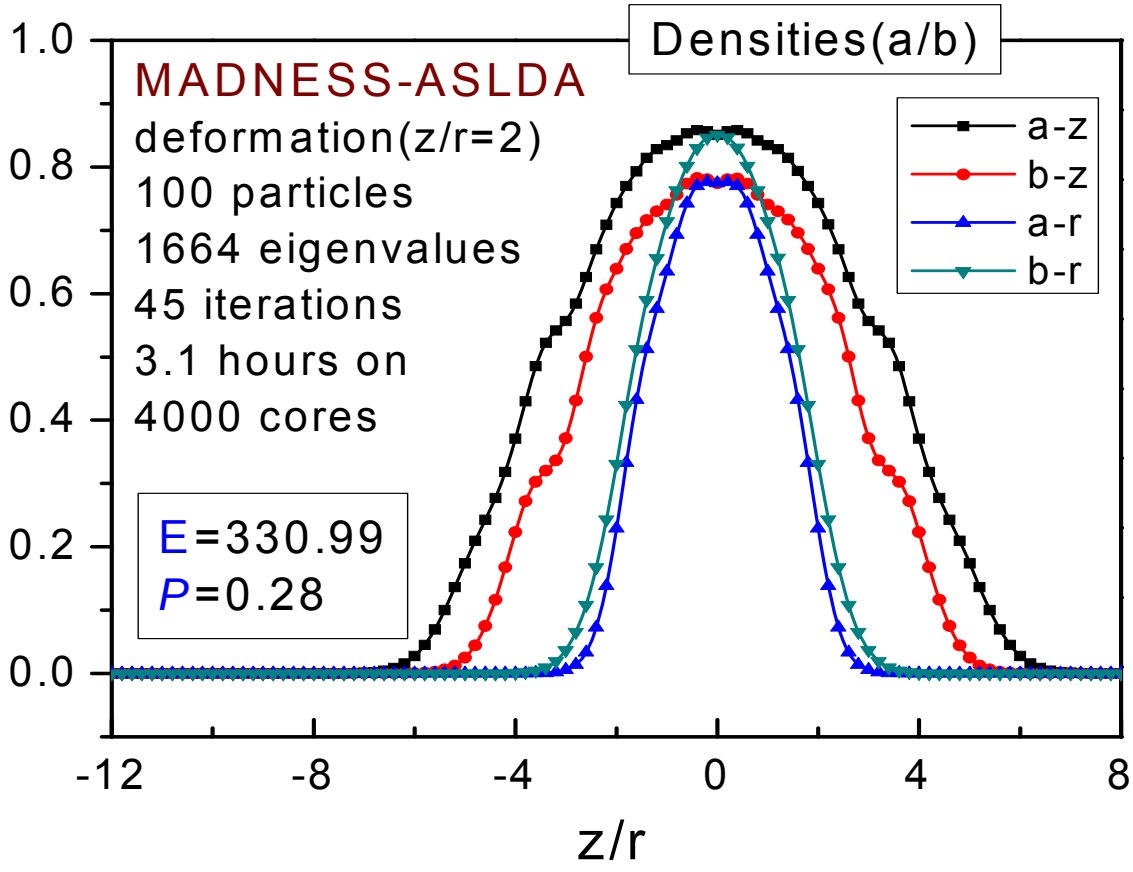
- More complicated and time-consuming than SLDA
  in the calculation of local polarization ($\rho_a/\rho_b$) with guess thresh=1.e-4



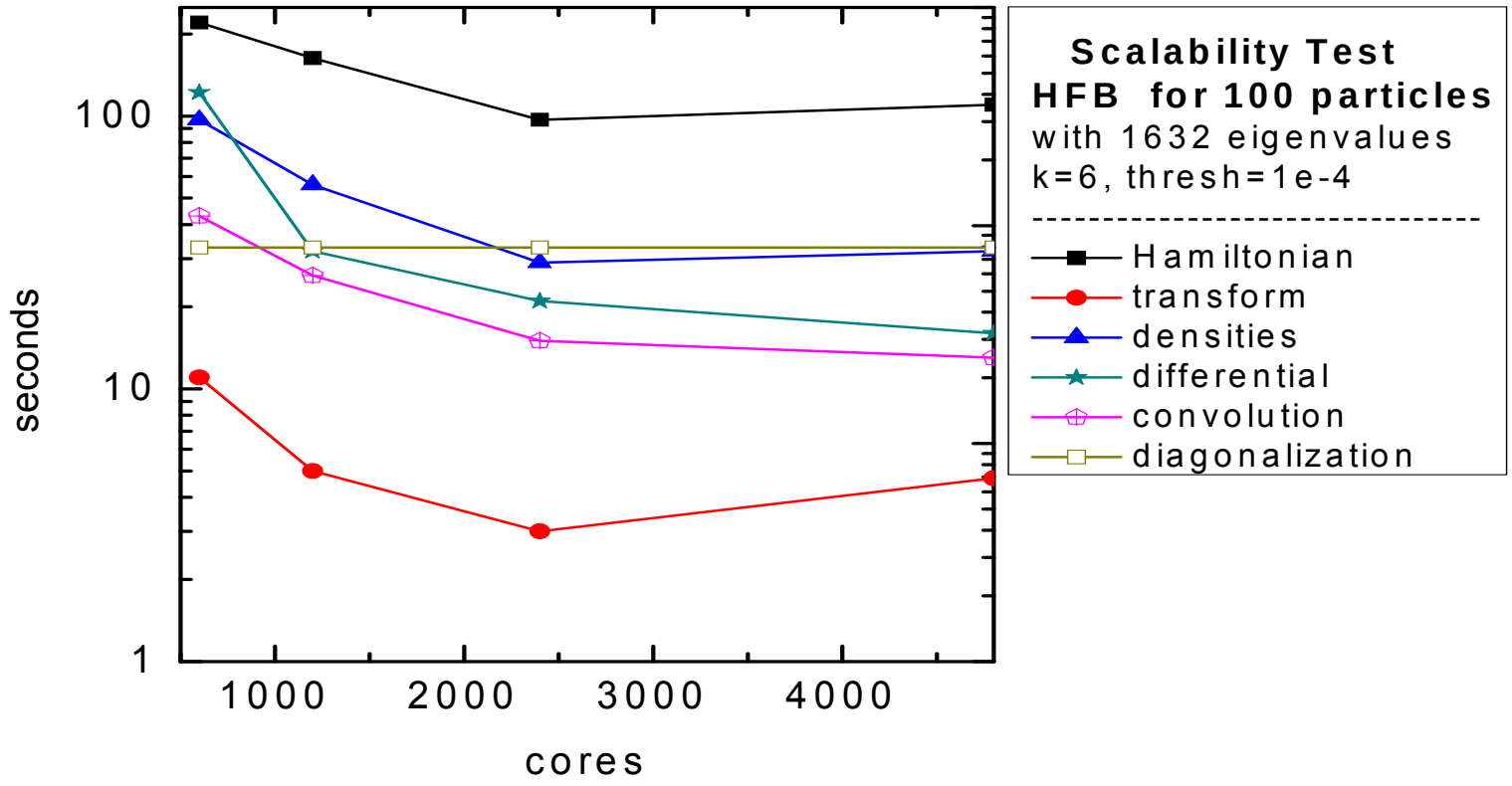

Total energy: E(bsp)=19.044
E(mad)=19.042

- Arrows point to regions which
  - may not have converged sufficiently
  - effects of possible due to spurious oscillation (Gibbs phenomena) resulting from sharp cut-offs
  - new code should resolve these issues

# ASLDA 100 particles In a Deformed Trap



# ASLDA scaling for 100 particles, June 2010

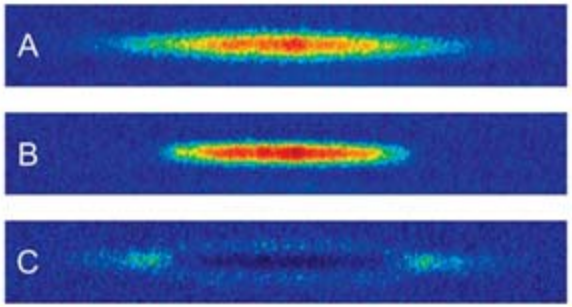



- Scales to about 2400 cores (just beyond size of eigensystem), prelim
- About 17K coefficients per wave-function with 7-8 levels of refinement
- Parallel eigensolver interfaces are being developed.

# Extreme Deformations, 100 particles

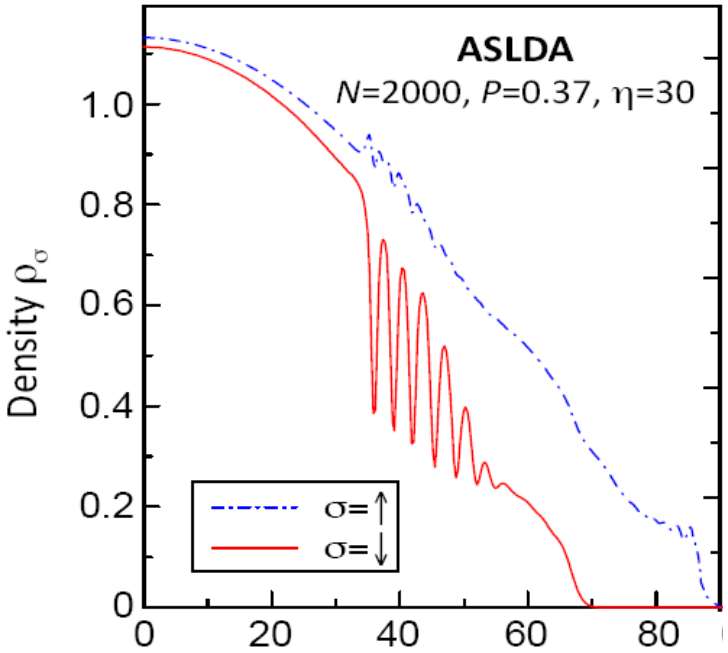
Finite-size effects indicated by experiments!

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




Motivation: Science 311(2006)503

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




- MADNESS takes 3～4 hours for 100 particles on 2400 cores in an elongated trap to convergence (prelim)
- Involving 2000+ eigen-solutions, preliminary implementation

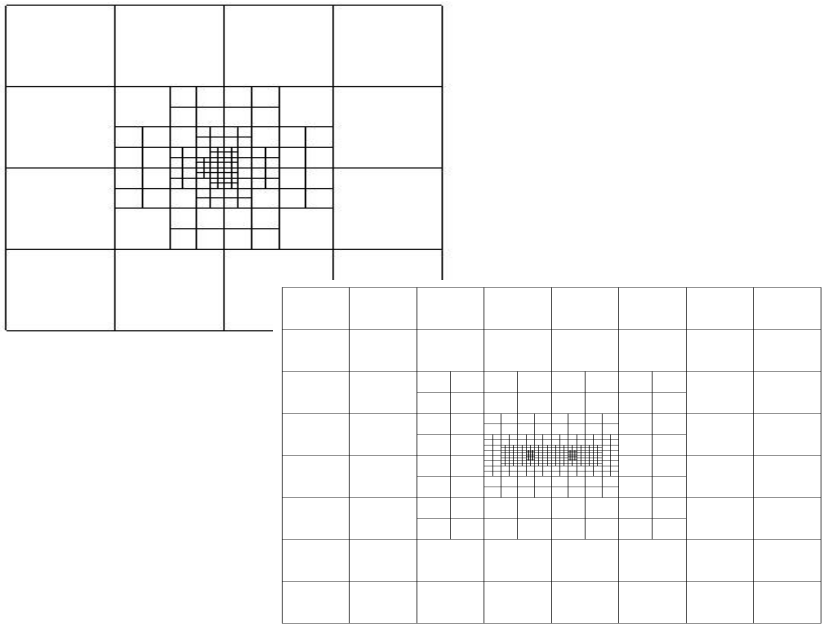
# Multiwavelets and Fast Methods

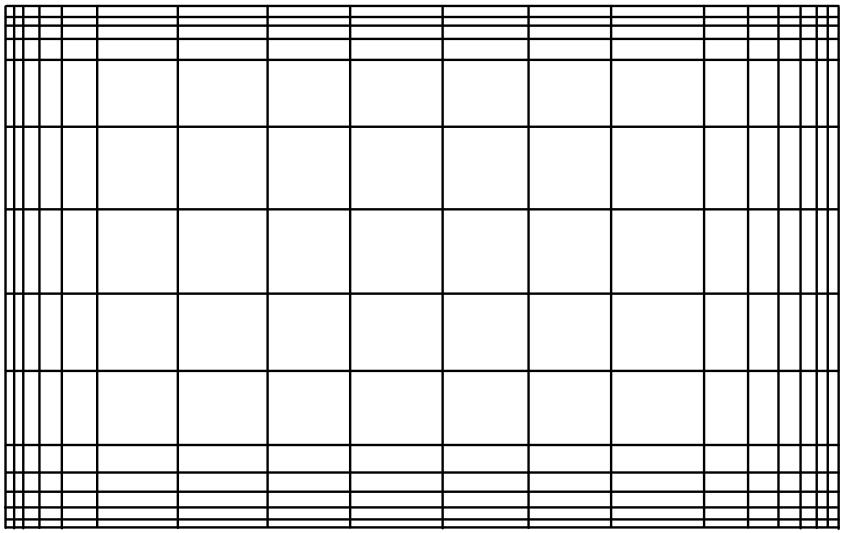
- Automatic adaptivity for discretization and order of accuracy ("h and p"-adaptivity)
  - the expansion is adaptively increased where precision is requires (basis is expanded, grouped by different support)
    - *In comparison with adapting a mesh and then increasing polynomial basis in the mesh*
  - Integral and differential operators via multiresolution and multiscale
  - Functions, projections between different level of expansions
  - Compatible between function and operator calculus
- Accurate treatment of singularities
- Accurate treatment of higher order derivatives
  - Improved adaptive treatment of Gibbs type phenomena
- Green's function (Poisson, Helmholtz, etc.)
  - Fast real analysis based O(N log $\varepsilon$), low-separation rank, method
  - Accuracy is proportional to
    - *Degrees of freedom*
    - *Work (flops)*

# *Representation of Wave-Functions*

**MADNESS** (each functions has its own adaptive pseudo-spectral expansion representation)

**B-spline Mesh** (fixed mesh, focus on boundary condition; rectangle box for deformation)





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).

# New algorithm for solving non-linear self-consistent HFB I

1. Given Hamiltonian H, and guess wavefunctions $\{\phi_i\}$ form matrix $(H_{i,j}) = <\phi_i, H\phi_j>$
   - With regularization, guess for densities, …
2. Diagonalize to obtain updated and orthogonal wave-functions
3. Update potentials, anomaly density, boundary conditions, correlations…using new eigenvalues and eigenfunctions
4. Form and solve the Lippman-Schwinger integral equation by scattering methods (approximation expansion in u,a, and G's)
   1. Construction of scattering kernel for each eigenvalue for u's via non-linear optimization
   2. Solve for u's
   3. Update potential, densities, BC, correlations, fitting which are functions of u's
   4. Construction of scattering kernel for each eigenvalue for a, via non-linear optimization
   5. Solve for a's
5. Check error estimates

# *New algorithm for solving non-linear self-consistent HFB II*

- Error estimates
  - If converged within tolerance, exit
  - If not converged go to step 1.
  - If further refinement required and not converged within a certain number of iterations
    - *Set new number of multiwavelets, precision, truncation errors, iteration count, …*
    - *Project all variables to new level of subspace*
    - *Goto step 1 on last slide*

# Solving Nuclear Problems

**Example:** Solving Schrödinger Equation via Green's function (integral form, Kalos):

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

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

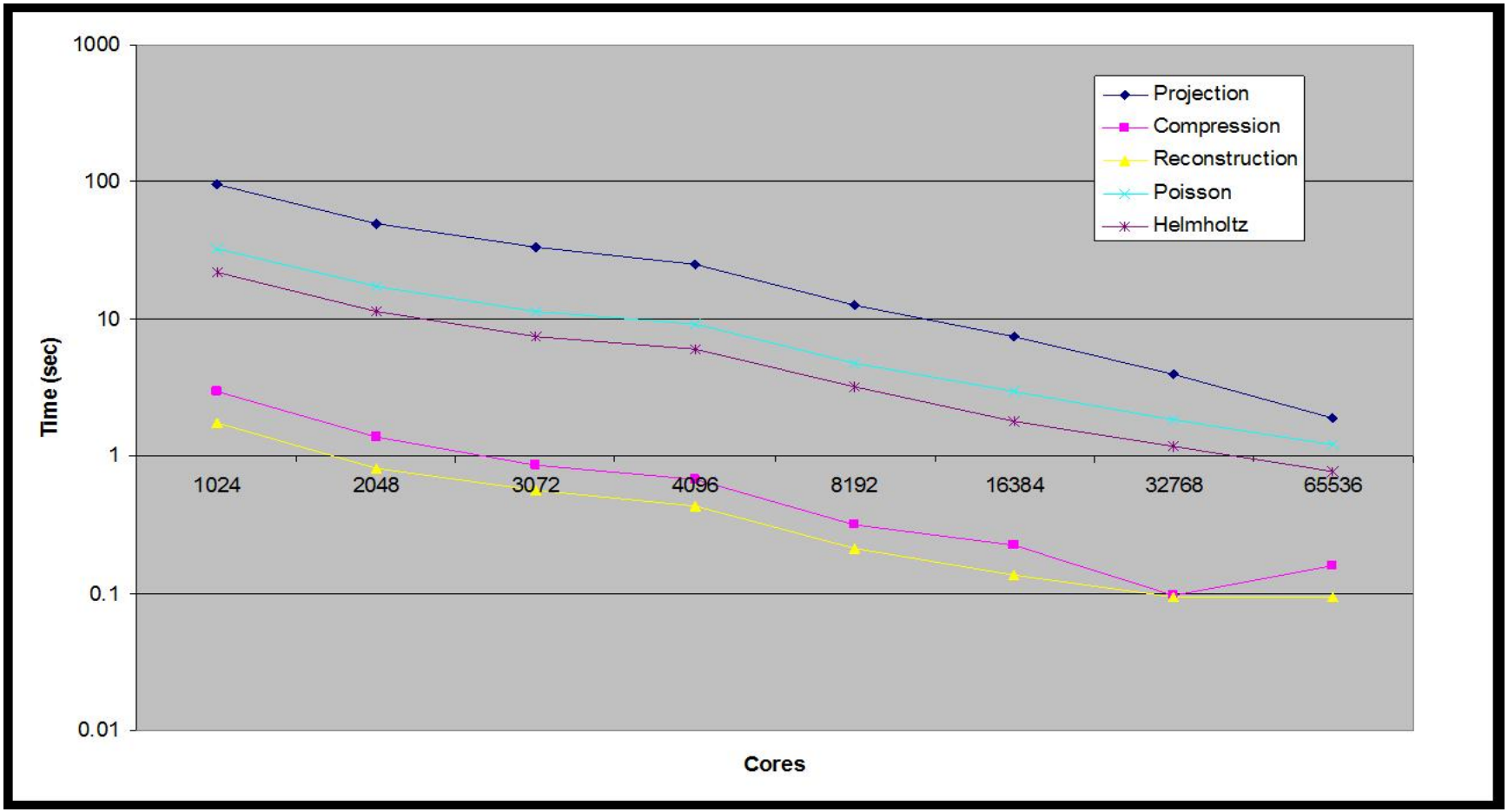
$$= -2G*(V\Psi)$$

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

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

# Solving Poisson and Helmholtz Equation Cray XT-5

## 1.91B eqns, 10 levels of refinement, accuracy 1.e-10 (8/2009)



# High Level Composition in 3-D

- Close to the physics

$$E = \langle \psi | -\frac{1}{2}\nabla^2 + V | \psi \rangle + \int \psi^2(x) \frac{1}{|x-y|} \psi^2(y)\, dx\, dy$$

```
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;
```

# Summary

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

What have done last year:

SLDA and ASLDA benchmark have been done. Tests have been run up to 100 particles in deformed trap. Improved parallel scaling.

Work target of this year:

Ready to develop a Skyrme-HFB with zero boundary condition, for a system with a few hundreds of nucleons.

For 1K+ particles, the bottle-neck is the diagonalization step. Interface to PeIGS has been done, SCALAPACK to be worked out (integer*8 interface issue)

Outlook: calculation of extremely large systems; implement of out-going boundary condition, size and domain extensivity