Multiresolution and Low-Separation Rank Methods for Nuclear DFT

George Fann, and William A. Shelton

Oak Ridge National Laboratory

Witek Nazarewicz, Nicolas Schunk and Junchen Pei

University of Tennessee/ORNL

Robert Harrison

ORNL/UTK

UNEDF Workshop, Park Forrest, WA

June 23-26, 2008

MADNESS

Multiresolution
Adaptive
Numerical
Scientific
Simulation

Office of Science
U.S. DEPARTMENT OF ENERGY

Office of Nuclear Physics
Exploring Nuclear Matter - Quarks to Stars

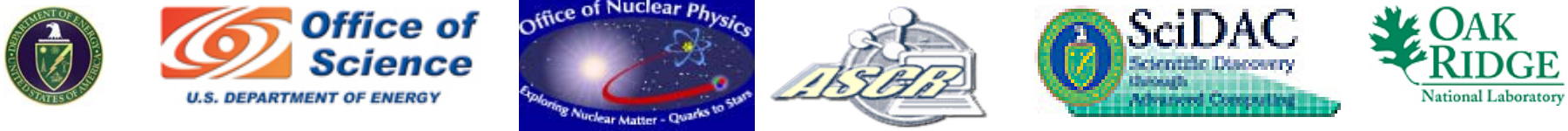
ASCR

SciDAC
Scientific Discovery through Advanced Computing

OAK RIDGE
National Laboratory

The funding

- The application of MADNESS(++) to nuclear physics is funded through SciDAC UNEDF (PI:Bertsch) by the Office of Advanced Scientific Computing Research
- The development of MADNESS and MAD++ is funded by the U.S. Department of Energy, Office of Advanced Scientific Computing Research and the division of Basic Energy Science, Office of Science, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, by the SciDAC SAP in computational chemistry (PI: Fann) and SciDAC BES (PI:Harrison).
- 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,
  - and the Center for Computational Sciences at Oak Ridge National Laboratory under contract DE-AC05-00OR22725 .

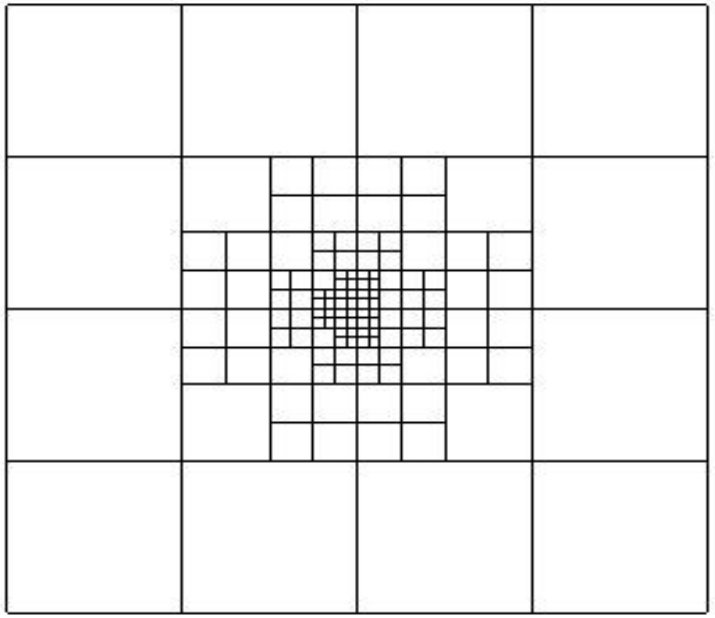


Multiwavelets and Fast Methods

- Automatic adaptivity for discretization and order of accuracy (h and p)
  - Integral and differential operators
  - Functions
  - 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) method
  - Accuracy is proportional to
    - *Degrees of freedom*
    - *Work (flops)*
- DFT, Lippmann-Schwinger, Hartree-Fock, …
- Constructive low separation rank approximation for fast and scalable (log d) methods for high dimensional and non-convolution type kernels

Multiresolution Methods for DFT

- Adaptive 3-D multiresolution pseudo-spectral methods for nuclei
  - User defined accuracy gives universal reference and good scalability
  - Consistent description of bound and resonant states
    - *Consistent accuracy in neutron-rich or super-heavy nuclei*
    - *Bridge to reaction theory*
- No assumption on symmetry
- Can handle nearly singular or discontinuous functions, and high gradients
- Work is proportional to spectral accuracy
- Controllable and guaranteed precision



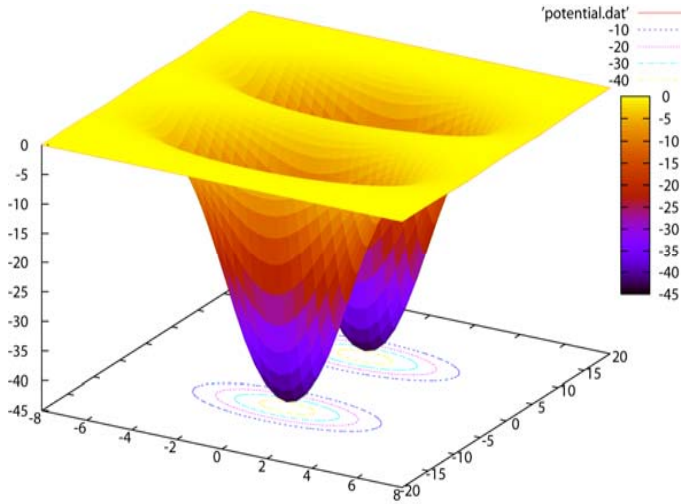
Adaptive support of basis functions. A 2-D slice of a 3-D wavefunction from the inverted two-cosh spin-orbit (SO) case

Contributions: Multiresolution Methods for DFT

- Two-cosh, and PTG are examples of non-localized potentials
- "MADNESS applied to density functional theory in chemistry and nuclear physics," J. of Physics (2007)
- Benchmarking solvers for nuclear DFT, in progress, preprint (2008), 2 papers in progress
- High accuracy calculations when compared with splines, harmonic oscillators,…(table of comparison, HO, spline, wavelets for 2-cosh, PTG) with and without spin-orbit (C++ version)
- Merging of HO with wavelets for improved starting wavefunctions.
- Parallel C++ code under development, non-spin and spin orbit working…table and preliminary scaling here.

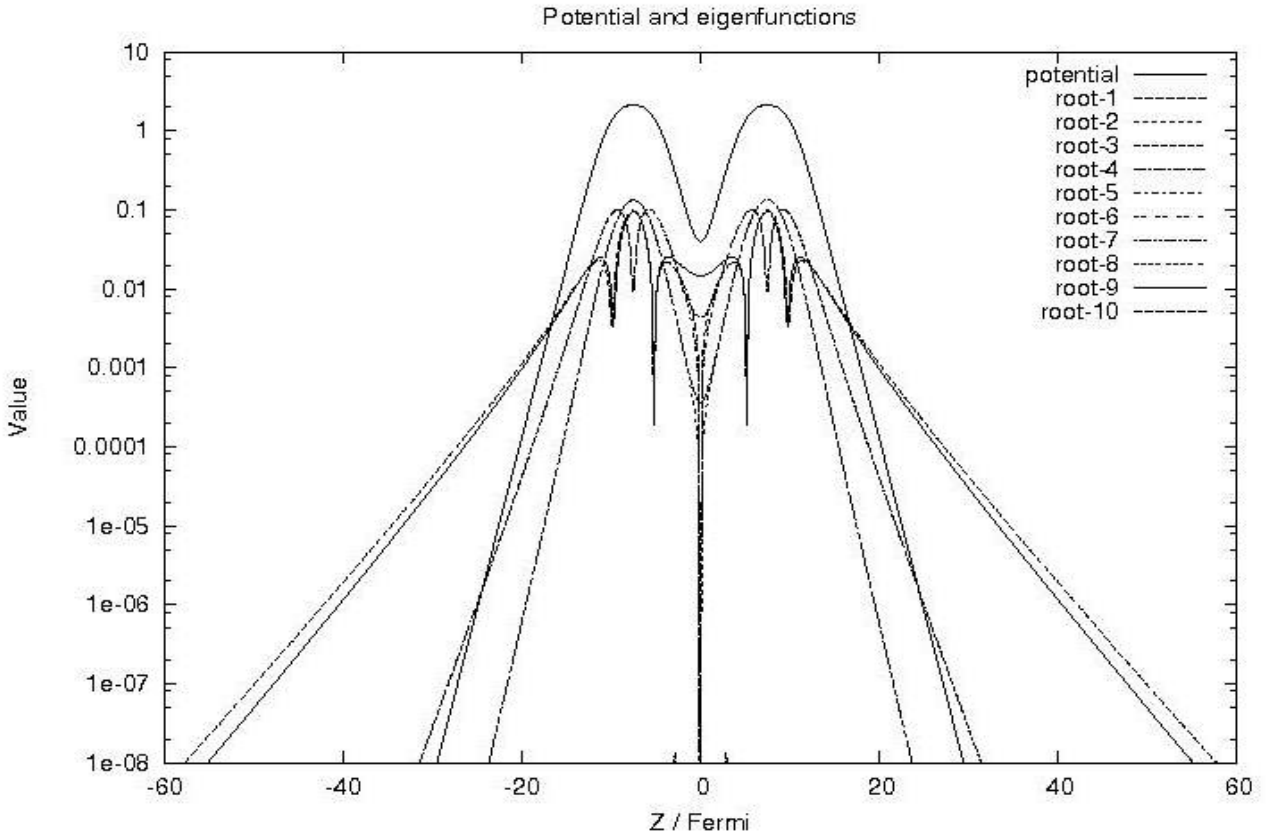
Eigenvalue (exact)	HO Expansion	Multiwavelets 10^{-3}
-39.7400, ½+	-39.7400	-39.7399
-18.8977, ½+	-18.8977	-18.8976
-0.3205, ½+	-0.1748	-0.3205

Poschl-Teller-Ginocchio Potential



Inverted 2-cosh (no SO)

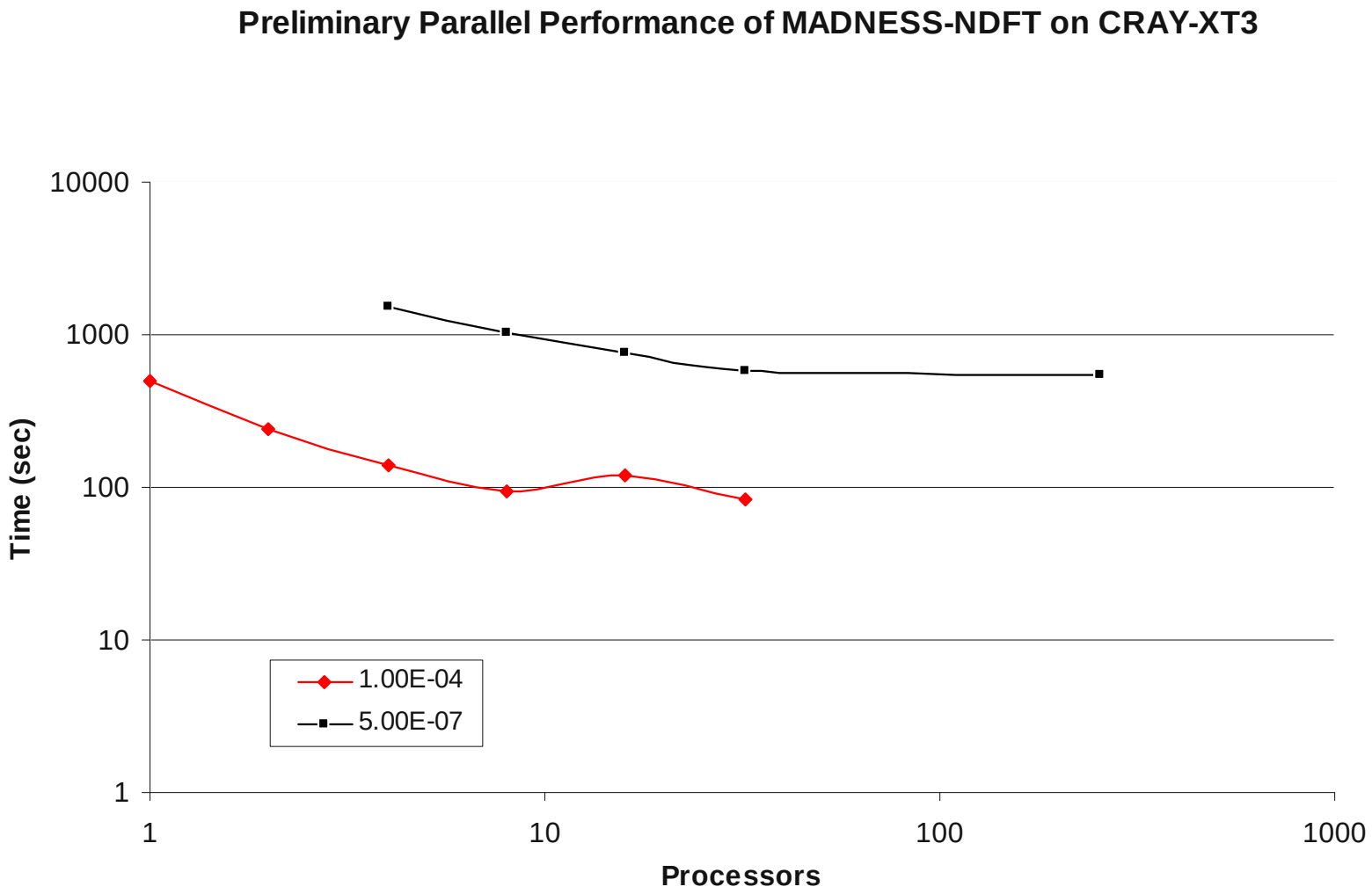
Plot of Potential and Absolute Value of Wave Functions for the 2-cosh Potential



Results from Harmonic Oscillator, Spline, Multiwavelets and 3D-lattice

Eigenvalue			Inverted 2-cosh potential without spin-orbit				Inverted 2-cosh potential with spin-orbit			
#	Spin	π	HO, N=22	Spline	Wavelets, 5e-7	3D-lattice	HO, N=22	Spline	Wavelets, 3.e-5	3D-lattice
1	1/2	+	-22.23984	-22.24011	-22.24010725	-22.24020	-22.23984	-22.2400	-22.240107	-22.2402
2	1/2	-	-22.23949	-22.23998	-22.23998058	-22.24010	-22.23949	-22.2399	-22.239980	-22.2401
3	1/2	+	-9.21869	-9.22050	-9.22050134	-9.22062	-9.43509	-9.4365	-9.43662	-9.43674
4	3/2	+	-9.20945	-9.21260	-9.21260181	-9.21271	-9.42925	-9.4319	-9.43202	-9.43214
5	1/2	+	-9.20945	-9.21247	-9.21260181	-9.21271	-9.42911	-9.4310	-9.43080	-9.43092
6	3/2	-	-9.20943	-9.21129	-9.21129039	-9.21140	-9.42490	-9.4278	-9.42788	-9.42799
7	1/2	-	-9.20943	-9.21116	-9.21129039	-9.21140	-8.77589	-8.7782	-8.77828	-8.77839
8	1/2	-	-9.20269	-9.20595	-9.20595248	-9.20606	-8.77013	-8.7737	-8.77383	-8.77394
9	1/2	+	-1.71590	-1.72467	-1.72514284	-1.72840	-1.71593	-1.7239	-1.72516	-1.72843
10	1/2	-	-1.51146	-1.52621	-1.52690510	-1.52276	-1.51149	-1.5251	-1.52693	-1.52279
Moment n=1			20.0	20.0	20.0	20.0	20.0	20.0	20.0	20.0
Moment n=2			0.717832	0.7196883	0.71902147	0.719124	0.7177410	0.719598	0.718931	0.719033
Moment n=3			0.043470	0.043865	0.04379460	0.043805	0.043463	0.043857	0.043786	0.043797

Parallel Scaling for Nuclear Multiwavelet Code w/o Spin Orbit



Test Problem for Pairing

$$\begin{pmatrix} h - \lambda & \delta \\ \delta & -h + \lambda \end{pmatrix} \begin{pmatrix} U_i(r) \\ V_i(r) \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix}$$

where

$$h = -\frac{\hbar^2}{2m}\nabla^2 + V_{2\cosh}(x, y, z) + V_{SO}(x, y, z)$$

and

$$\delta = 0.02 * V_{2\cosh}(x, y, z)$$

$$\lambda = -1$$

- Wavelet still in progress.
- Preliminary Results using Harmonics Oscillator Basis and Spline have been computed.
- Solving for occupation number, density and pairing-density

Deliverables

- Main Accomplishment:
  - Parallel MAD++ for Nuclear DFT code:
    - *Cray-XT4, Intel and AMD clusters, PCs, laptops*
  - Year 2 plan: On track, still testing on new spin-orbit problem.
    - *Code port to IBM BGL/P*
  - Paper: *G I Fann, R J Harrison, G Beylkin, J Jia, R Hartman-Baker, W A Shelton and S Sugiki*, **MADNESS applied to density functional theory in chemistry and nuclear physics**, J of Physics Conference Series, vol. 78, 2007.
  - Presentations:
    - *G. Fann, et al., "Solving 3-D and 6-D Schrödinger's Equations Using Multiresolution Adaptive Pseudo-spectral Methods on Leadership Class Computers," SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, GA, March 12-14, 2008.*
    - W. A. Shelton, *"Implementing Density Functional Theory based Electronic Structure Code on Advanced Computing Architectures, The 2nd LACM-EFES*-JUSTIPEN Workship, 2008, Oak Ridge, 2008.
    - G. Fann, *Multiresolution Methods for Solving Electronic Structure,* Joint-JUSTIPEN-LACM Workshop, Oak Ridge, TN 2007.

Current and Future Work

- Year 2
- Integration of HO with wavelets methods in 3-D
  - Testing with more spin-orbit and pairing
  - Conversion of Python to C++ version of the code for MADNESS Nuclear DFT code for parallel computers
  - Demonstration for leadership computing platforms
  - Solving the symmetry-free non-self-consistent DFT problem
  - alpha MADNESS core c++ code at http://code.google.com/p/m-a-d-n-e-s-s/
- Year 3
  - Development of HF method with realistic effective interactions (Skyrme DFT), Nuclear-MADNESS-HF
  - Optimization, code porting and scaling on NLCF machines: Cray and IBM
  - Boundary conditions
  - Alpha code release of Nuclear physics module using MADNESS
- Year 4-Testing and additions to Nuclear-MADNESS-HFB: Development of version 1.0
- Year 5-Testing of Nuclear-MADNESS-HFB: Application to the fission problem

Some General Issues

- Aspects of work which require HPC:
  - Modeling large molecule or many body systems with high accuracy with discrete and/or continuous spectra
  - 3N-systems, for N large
- General Problem in HPC:
  - *Accurate discretizations, good basis and boundary conditions*
    - Basic problems in solving PDEs and ODEs accurately
    - Our approach is adaptive spectral using discontinuous wavelet basis and low-separation rank representations of functions and operators, work is proportional to accuracy
  - *Scalable direct and iterative solvers, Green's function techniques*
  - *Fast O(N)-methods for time-dependent "stiff" problems*
  - *Dynamic load balancing*

MADNESS in Chemistry

- Current capabilities n-D, (tested n=1,2,3,4,5,6,20), object oriented, …
  - E.g. compressing f in multiwavelet f=Function(f, k=3), dfdz=f.diff(3),
  - Laplacian_of_f=f.laplacian(), normf=f.norm2()
- Example codes:
  - TDSE
  - Molecular DFT
  - Time dependent DFT
  - Hartree-Fock, TDHF

- AM and CS
  - Multiwavelet representation of functions and operators
  - Low separation rank representation of functions and operators
  - Asymptotic boundary condition
  - Periodic boundary condition
  - Iterative and Direct methods (and some combinations)

Chemistry Application
Integral Formulation of Bound State Schrödinger Equation

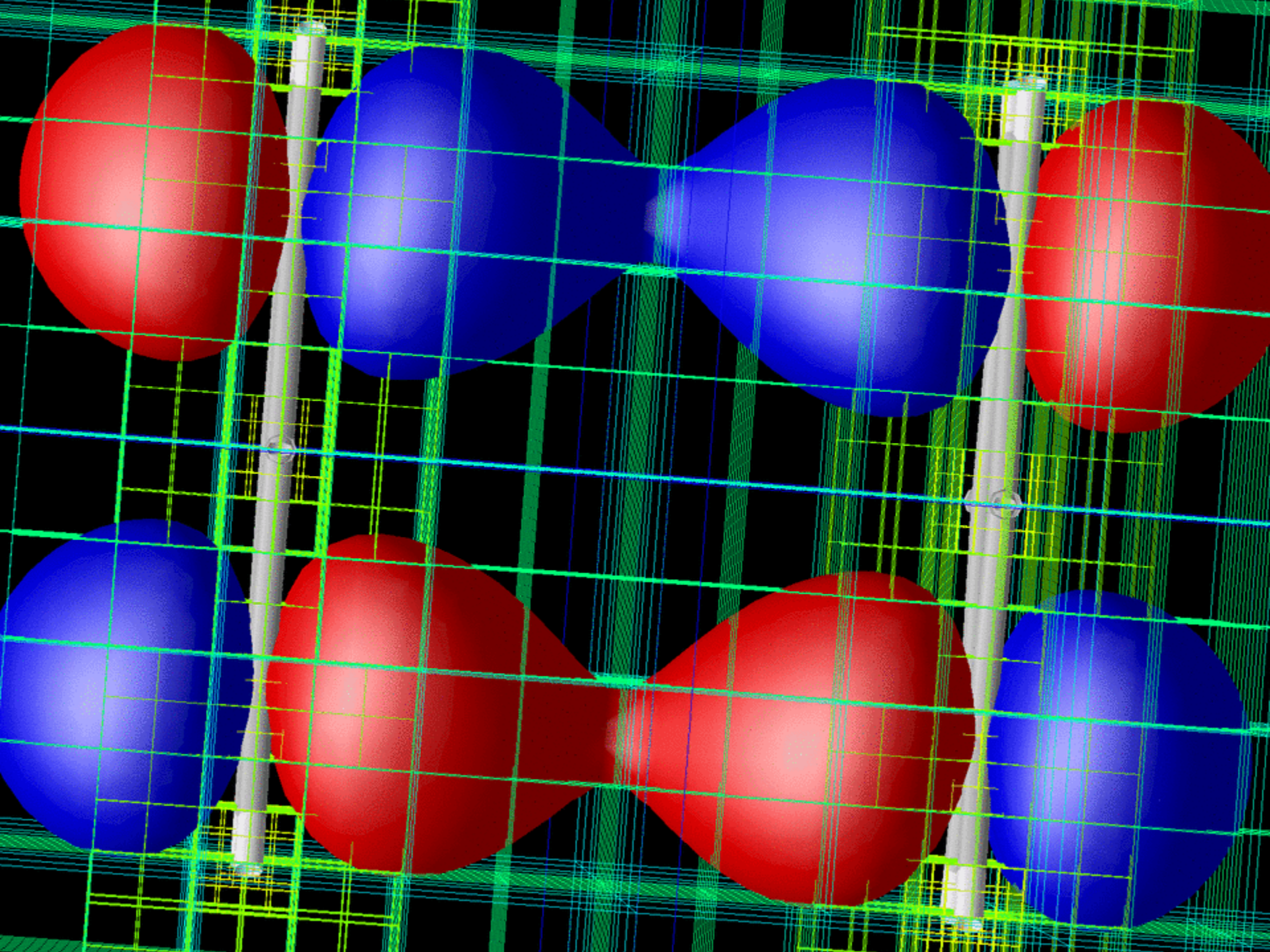
- Solving the integral equation
  - Eliminates the derivative operator and related “issues”
  - Converges as fixed point iteration *with no preconditioner*

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

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

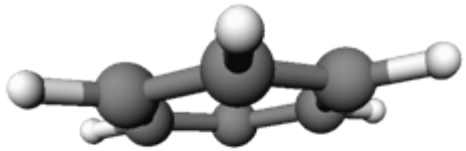
$$= -2G*\left(V\Psi\right)$$

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



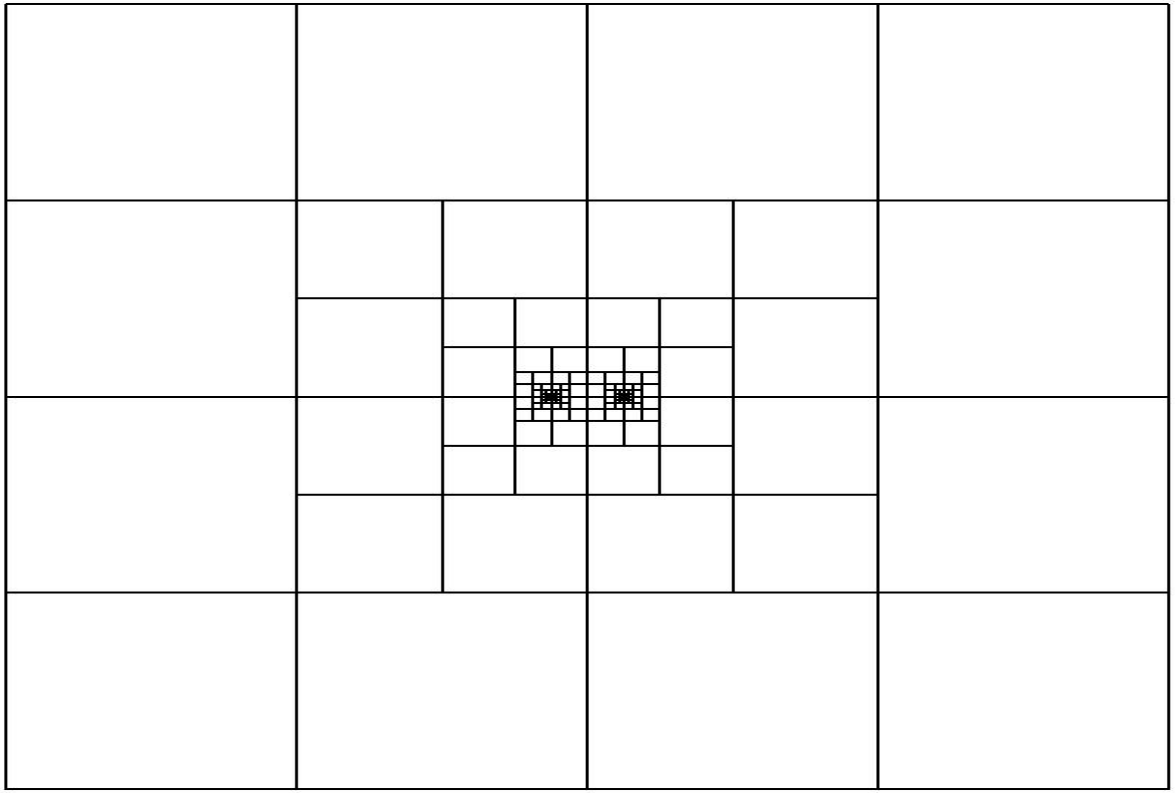
Benzene dimer LDA

aug-cc-pVDZ geometry, kcal/mol.

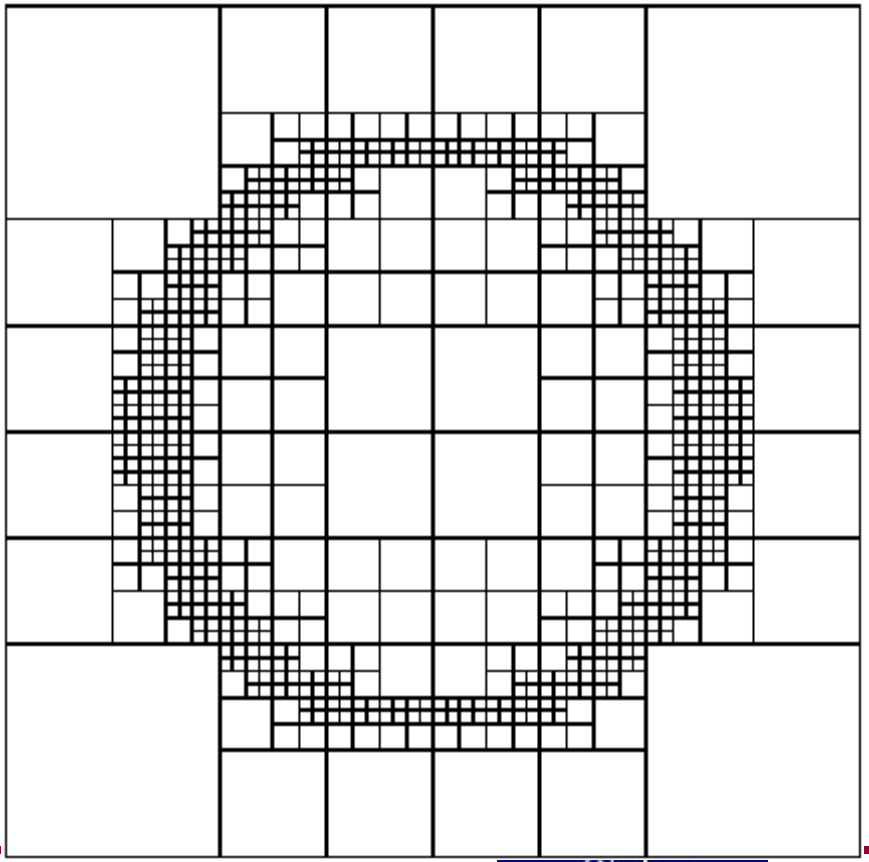


Basis	Uncorrected	BSSE	Corrected
cc-pVDZ	-1.506	-1.035	-0.471
cc-pVTZ	-1.271	-0.387	-0.884
cc-pVQZ	-1.074	-0.193	-0.881
aug-cc-pVDZ	-1.722	-0.698	-1.024
aug-cc-pVTZ	-1.159	-0.193	-0.966
$\varepsilon=10^{-5}$	-0.872		
$\varepsilon=10^{-7}$	-0.956		
$\varepsilon=10^{-9}$	-0.956		

2-D Slice of 3-D Adaptive Refinement for H_2



Approximation Near Boundary



A 2-D slice of the 3-D refinement of cubes of a k=3 multiwavelet approximation of the characteristic function for a sphere.

H_2, 2-body, 6-D Schrodinger's Equation

- Hydrogen Mol, bond length r=1.4 bohrs
- Best variational energy known to us: -1.133629571456 (Mitin)
- k=5, -1.1335567888
- k=7, -1.1336294353
- k=9, -1.1336295698
- k=11, -1.1336295713
- k=13, -1.1336295714
- Truncation 1.e(2-k), with smoothing

Scaling of MAD++ on 4096 Cu lattice (prelim) on ORNL's Cray XT-3, 2007