Multiresolution and Low-Separation Rank Methods for Nuclear DFT

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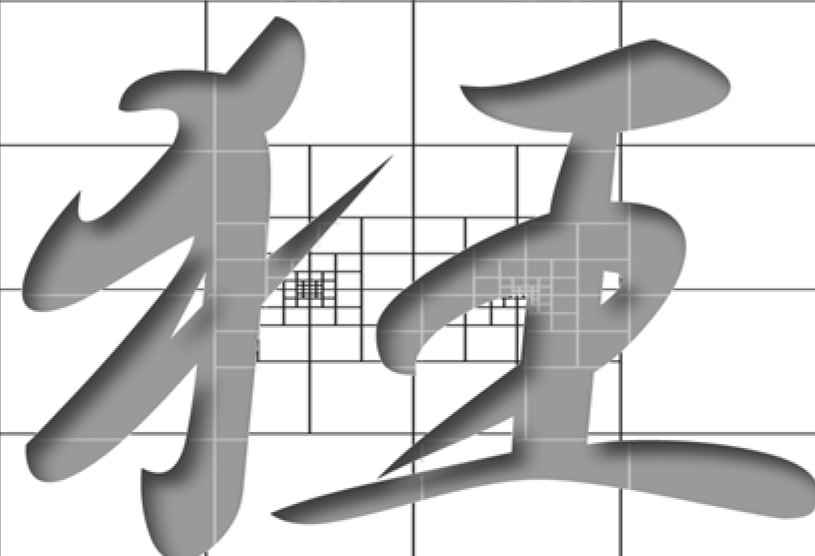
UNEDF Workshop, Park Forrest, WA

June 22-27, 2009

MADNESS



Multiresolution
Adaptive
Numerical
Scientific
Simulation

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Office of Nuclear Physics
Exploring Nuclear Matter - Quarks to Stars

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The funding

- The application of MADNESS to nuclear physics is funded through SciDAC UNEDF (PI:Lusk and Nazarewicz) by the Office of Advanced Scientific Computing Research.
- The development of MADNESS 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 .

Chemistry and Nuclear Physics Application
Integral Formulation of Bound State Schrödinger Equation

$$\left(-\nabla^2 + V + V_{SO}\right)\Psi = E\Psi,$$

$$\Psi = (u_r, u_c, v_r, v_c), 2-spinor-wavefunction,$$

$$\Psi = -G*\left(V\Psi + V_{SO}.\Psi\right)$$

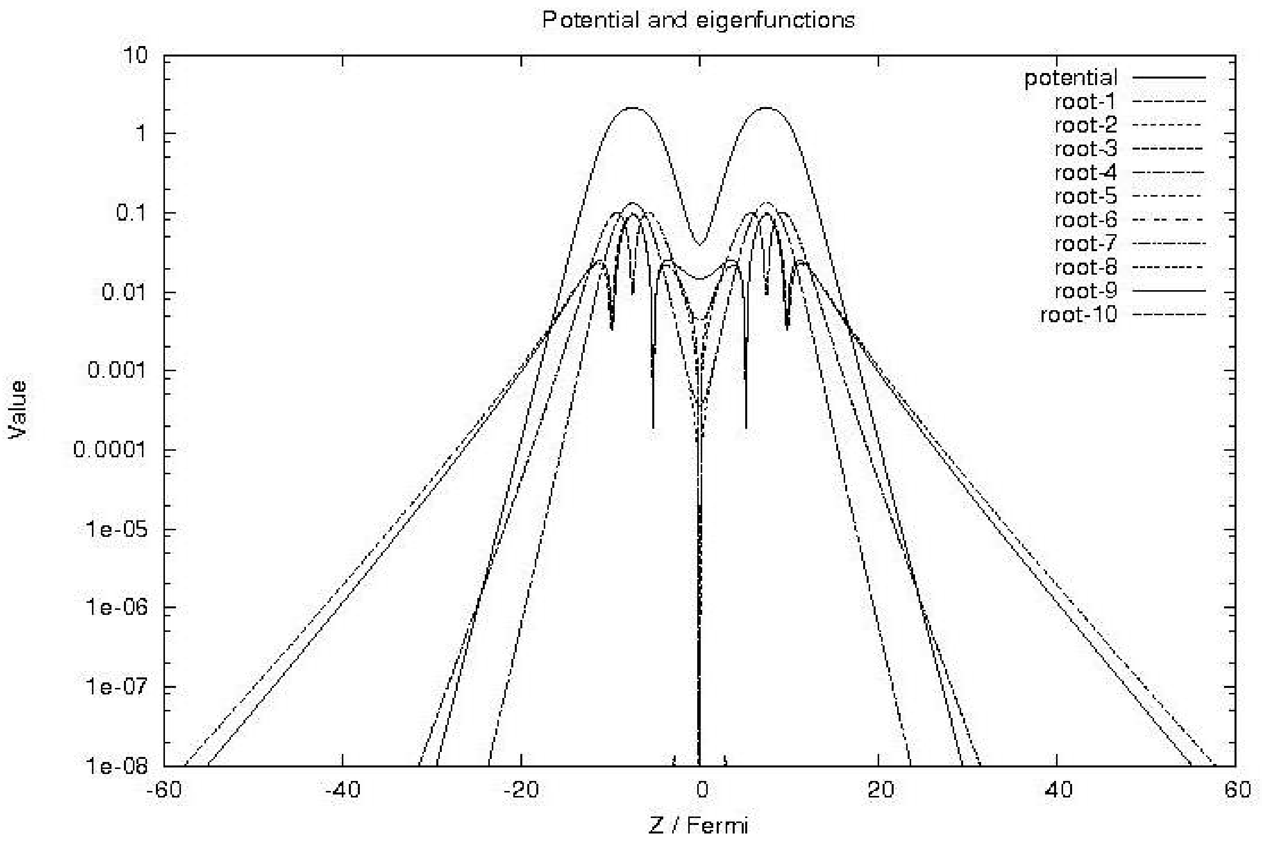
$$\left(G*f\right)(r) = \int ds \frac{e^{-k|r-s|}}{4\pi|r-s|} f(s) \ \ \text{in 3D}\,; k^2 = -E$$

$$V(x,y,z) = \frac{V_1}{1 + e^{-R_1/a_1}\cosh(r_+/a_1)} + \frac{V_2}{1 + e^{-R_2/a_2}\cosh(r_-/a_2)},$$

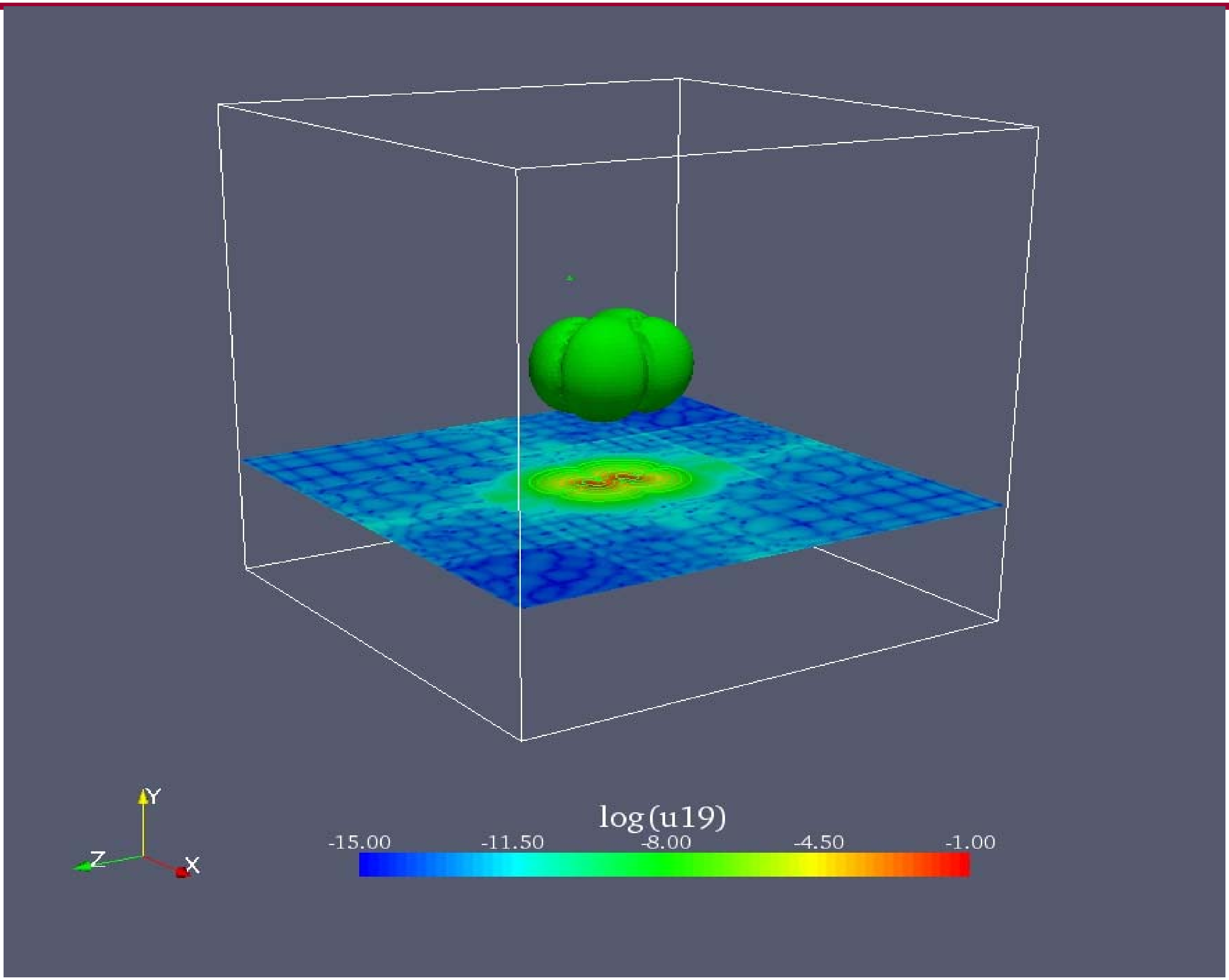
$$r_\pm = \sqrt{r^2 + (z \pm \varsigma)^2},$$

$$V_{SO} = -\sqrt{-1}\lambda_0\left(\frac{h}{2mc}\right)^2 \nabla V \bullet (\sigma \times \nabla)$$

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



Log(abs(u(x,y,z))



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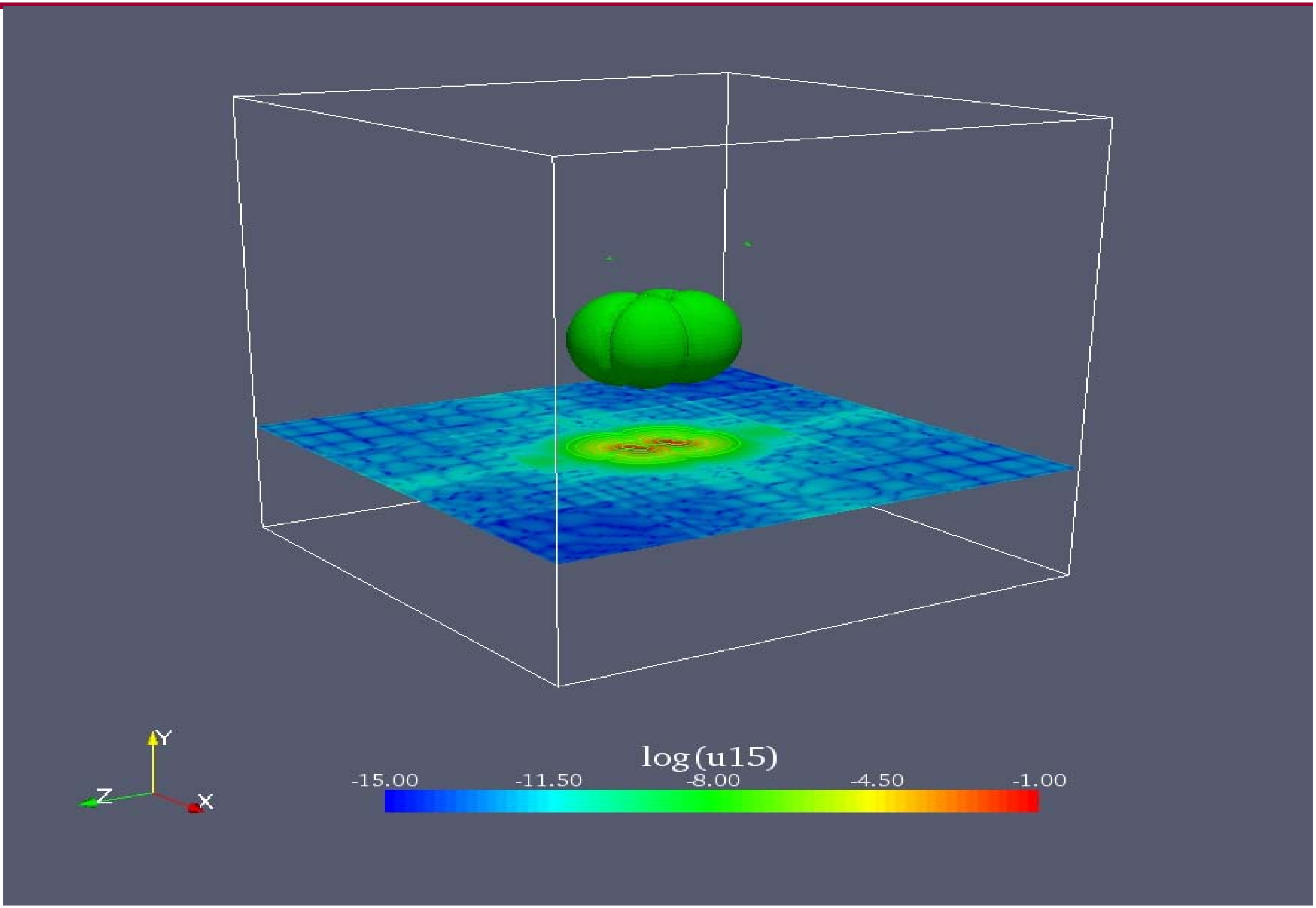

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Testing with HO, Spline, Wavelets, …

- Bound states
  - One-Cosh
  - Simple PTG
  - Two-Cosh
  - Two-Cosh with Spin-Orbit
  - HFB with two-cosh with spin-orbit

HFB with Two-Cosh Potential
Test Problem for Pairing

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

$$\text{where}$$

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

$$\text{and}$$

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

$$\lambda = -1$$

- Preliminary Results using Harmonics Oscillator Basis and Spline have been computed, and wavelets
- Solving for occupation number, density and pairing-density

Outline of Computational Setup

- Solve the Schrodinger equation for initial guess (e,u) in multiwavelet basis in the standard formulation, Hu=eSu
- Formulate using integral equation, e.g. Lippman-Schwinger Equation
- Use multiresolution analysis and low separation rank approximation
  - E.g.: representation by multiwavelets and separated representations using Gaussians
- Solve using iterative methods or combination of direct and iterative methods
- Discontinuous spectral element with multi-resolution and separated representations for fast computation with guaranteed precision.

Accomplishments 2009 (prelim)

- Solved HFB for bound states in 3-D, asymmetric potential
  - Multishift strategy for constructing scattering Green's functions
  - Same approach is being tested on continuum states
- Mixed basis for initial guess in 3-D
  - Hermite polynomials and Gaussians
- Mixed representations for computing in 3-D
  - Multiwavelets, low-separation rank and band-limited FFTs
- Threading and message passing optimization now in place
  - For many multi-cores…
- Paper (algorithms) submitted to SciDAC 2009 conference proceedings
- Two preprints for cs/math/physics journal (should submit in Sept. 2009 or place in archive)
- Ports to Linux PCs, clusters and Macs (10.4)

HFB 2-Cosh (prelim)

State No.	Ω^π	HO E_i	B-spline E_i	HO v_i^2	B-spline v_i^2	Madness E_i	Madness v_i^2
1	$1/2^+$	4.58515	4.53410	0.98377	0.96998	4.534	0.969
2	$1/2^-$	4.58131	4.53438	0.98371	0.96478	4.531	0.965
3	$3/2^+$	4.57997	4.53429	0.98369	0.96939	4.531	0.965
4	$3/2^-$	4.57769	4.53155	0.98363	0.96430	4.530	0.968
5	$1/2^-$	3.94644	3.90778	0.97854	0.96848	3.905	0.968
6	$1/2^+$	3.94287	3.90552	0.97845	0.96845	3.902	0.968
7	$1/2^+$	3.52045	3.52222	0.00579	0.00853	3.522	0.0078
8	$1/2^-$	3.31861	3.32172	0.00600	0.00789	3.321	0.0073

Deliverables 2009

- Pei is using alpha release of MADNESS on parallel machines.
- Presentations (details)
  - SIAM Computational Sciences and Engineering Conference in Miami, FL, March 5, 2009,*"Parallel Multiscale and Multiresolution Computations in Computational Chemistry and Nuclear Physics"*
  - JUSTIPEN 2009, Feb. 23-25, 2009, "Adaptive multi-resolution methods for nuclear DFT in 3D"
  - Poster at SciDAC Conference "Multiresolution DFT for Nuclear Physics," San Diego,
  - SIAM Annual Meeting 2009, July 7, 2009, Denver, "Parallel Multiscale and Multiresolution Computations in Computational Chemisty and Nuclear Physics"
- Paper
  - G. Fann, J. Pei, R. Harrison, J. Jia, J. Hill, M. Ou, W. Nazarewicz, W.A. Shelton and N. Schunck, "Fast Multiresolution Method for Density Functional Theory in Nuclear Physics," J. of Physics, Conference Series

2009: To Be Done

- In progress:
  - Boundary conditions for operators (e.g. 1st and 2nd derivatives) for Dirichlet, Neumann and Robin (mixed).
  - Boundary conditions: high order-absorbing boundary layer and layer potential for scattering operator for splitting domain into interior and exterior problems
  - Dynamic load balancing
  - More graphics
- More testing of HFB for unbounded wave-functions (e.g. Mario suggested full testing of Poschl-Teller-Ginocchio potential) and other potentials (Pei: Bulgac's SLDA)
- Submit preprints to journals
- Optimizations on Cray XT-* and finish port IBM BG/L to IBM BG-*
- If time permits: simple Skyrme functional

Applications to Other Areas

- General PDE, ODEs with complicated boundary conditions
- Direct and inverse scattering problems, interior and exterior problems
- Treatment of hypersingular integral and operators
- E.g. nuclear physics, computational chemistry, material science, fluid dynamics, electromagnetic scattering, …

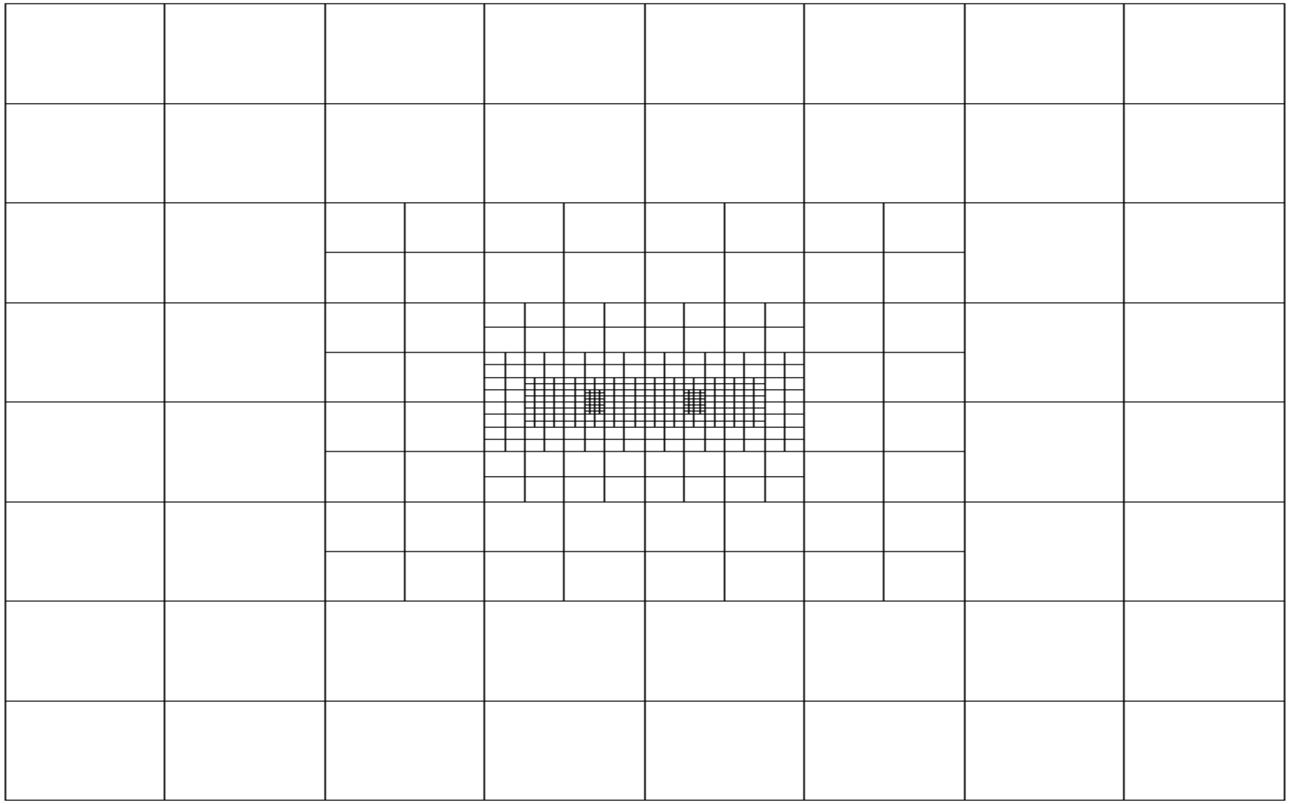
Future

- 2010
  - Testing and additions to Nuclear-MADNESS-HFB
    - *Testing with Skyrme*
    - *Extensions to continuum states*
    - *Extensions to resonant states*
  - Time-dependent problems
  - Optimization of high-order boundary conditions for interior and exterior scattering problems in 3-D
  - Optimization on petaflop boxes
- 2011
  - Testing and optimization, application to Nuclear problems

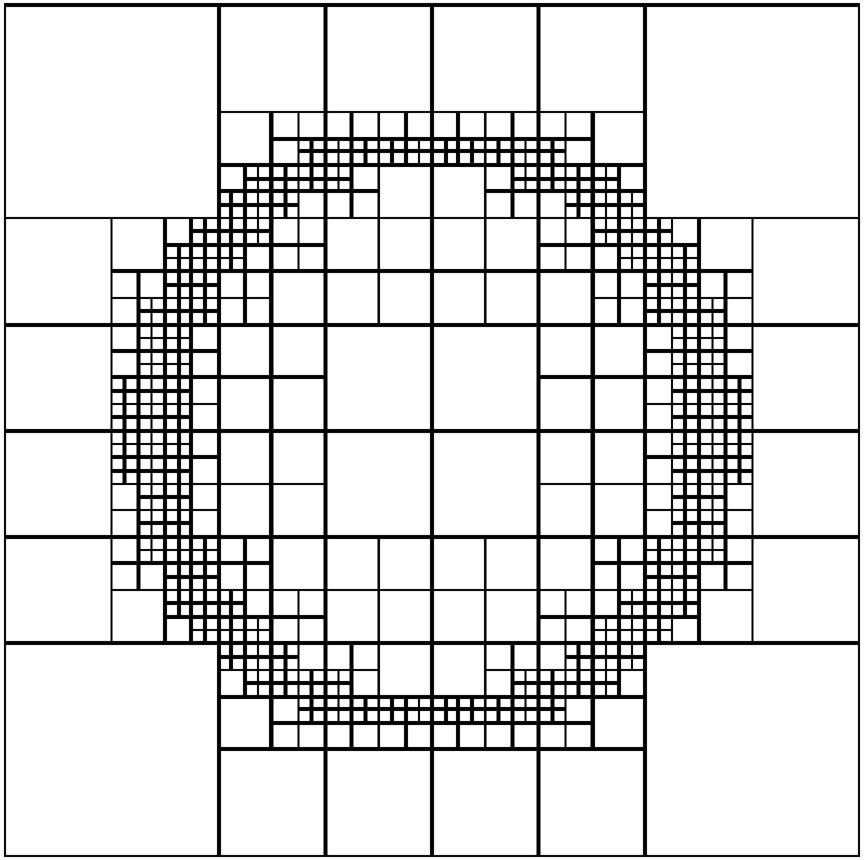
Some General Issues

- Aspects of work which require HPC:
  - Modeling many body systems with high accuracy with discrete and/or continuous spectra
  - 3N-systems, for N large
- General Scalability 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*
  - *Sync point for communication, bad for large p*
  - *Dynamic load balancing*
  - *Fast I/O*

2-D Slice of 3-D Multiresolution Support of Two-Cosh Potential

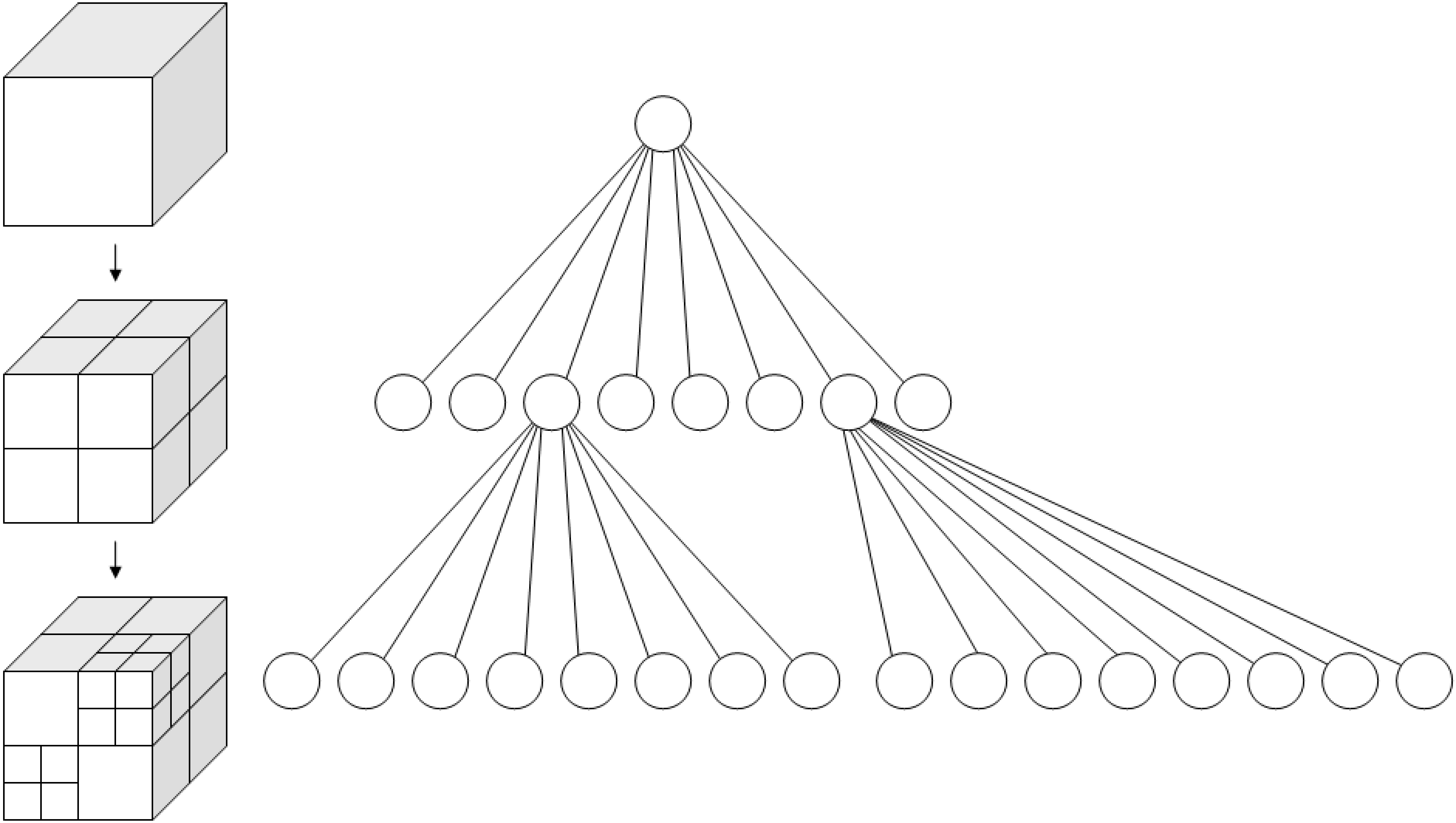


Approximation Near Boundary

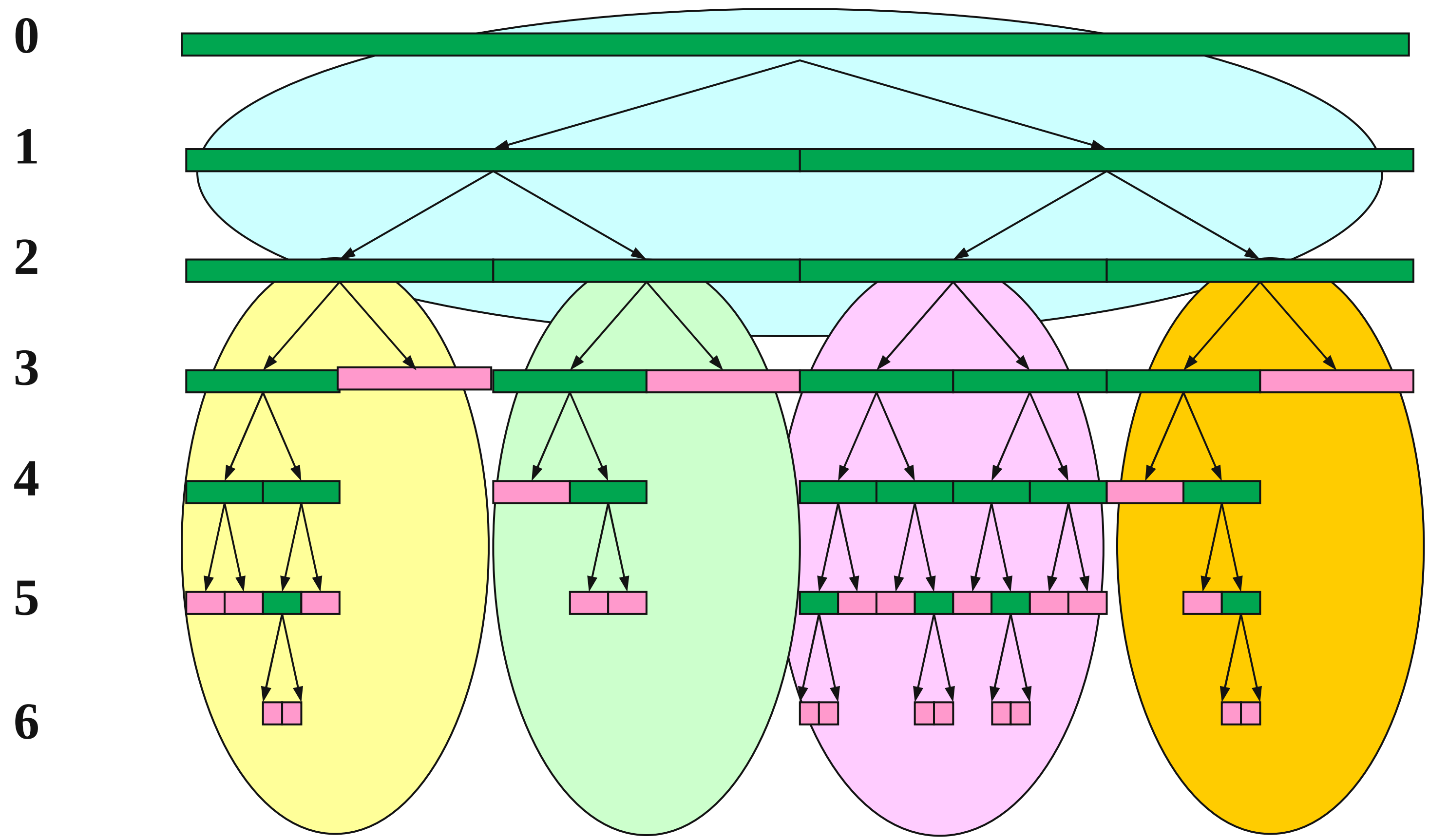


A 2-D slice of the 3-D refinement of cubes of a k=3 multiwavelet approximation of the characteristic function for a sphere.

Oct-tree Adaptivity



1-D Example Sub-Tree Parallelism



Both sub-trees can be done in parallel.
In 3-D nodes split into 8 children … in 6-D there are 64 children

Scaling of MADNESS ORNL's Cray XT-5, MPI+thread Prelim(2/23/09), 161B+ eqns, 24 levels of refinement, error 10^{-10}