The Mathematics Behind MADNESS

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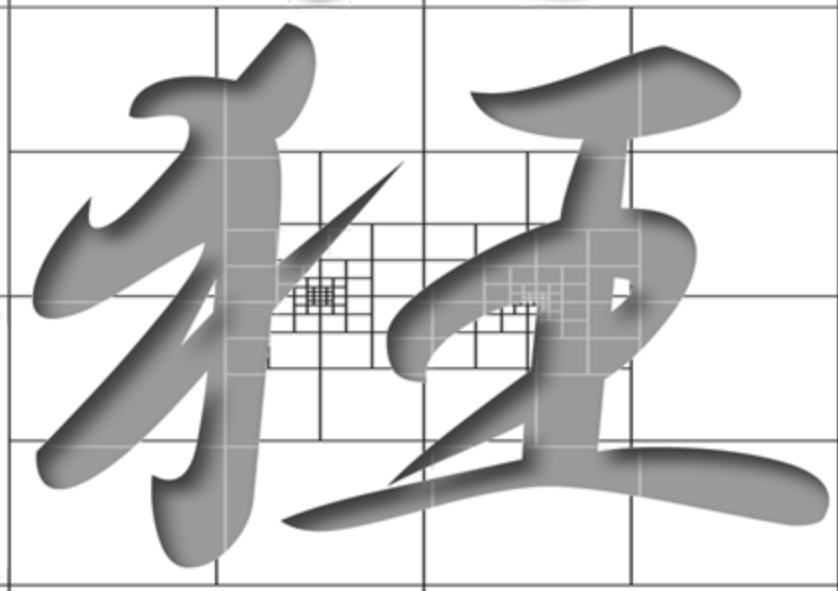
SciDAC 2010, Chattanooga, TN

MADNESS



Multiresolution
Adaptive
Numerical
Scientific
Simulation

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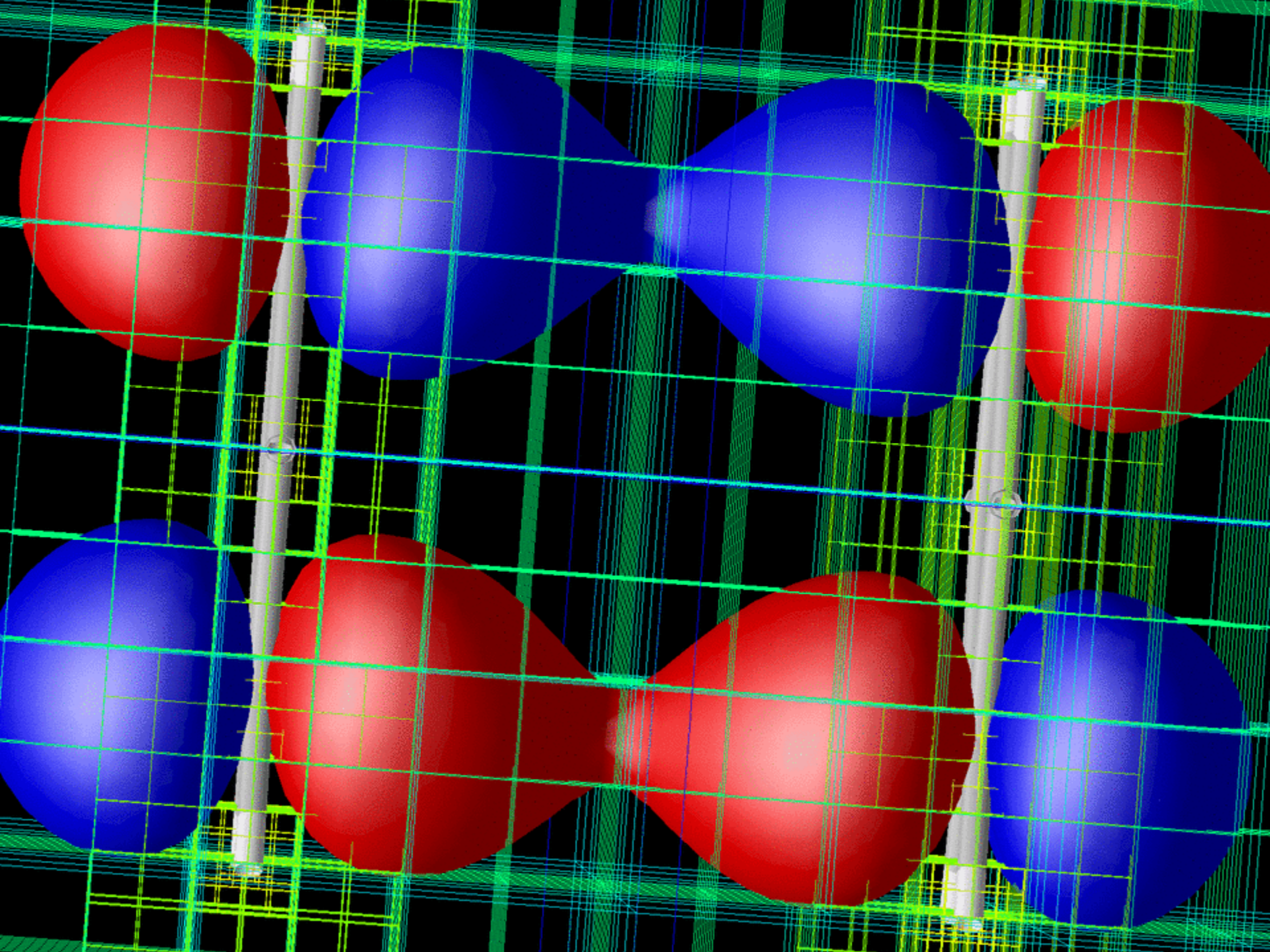


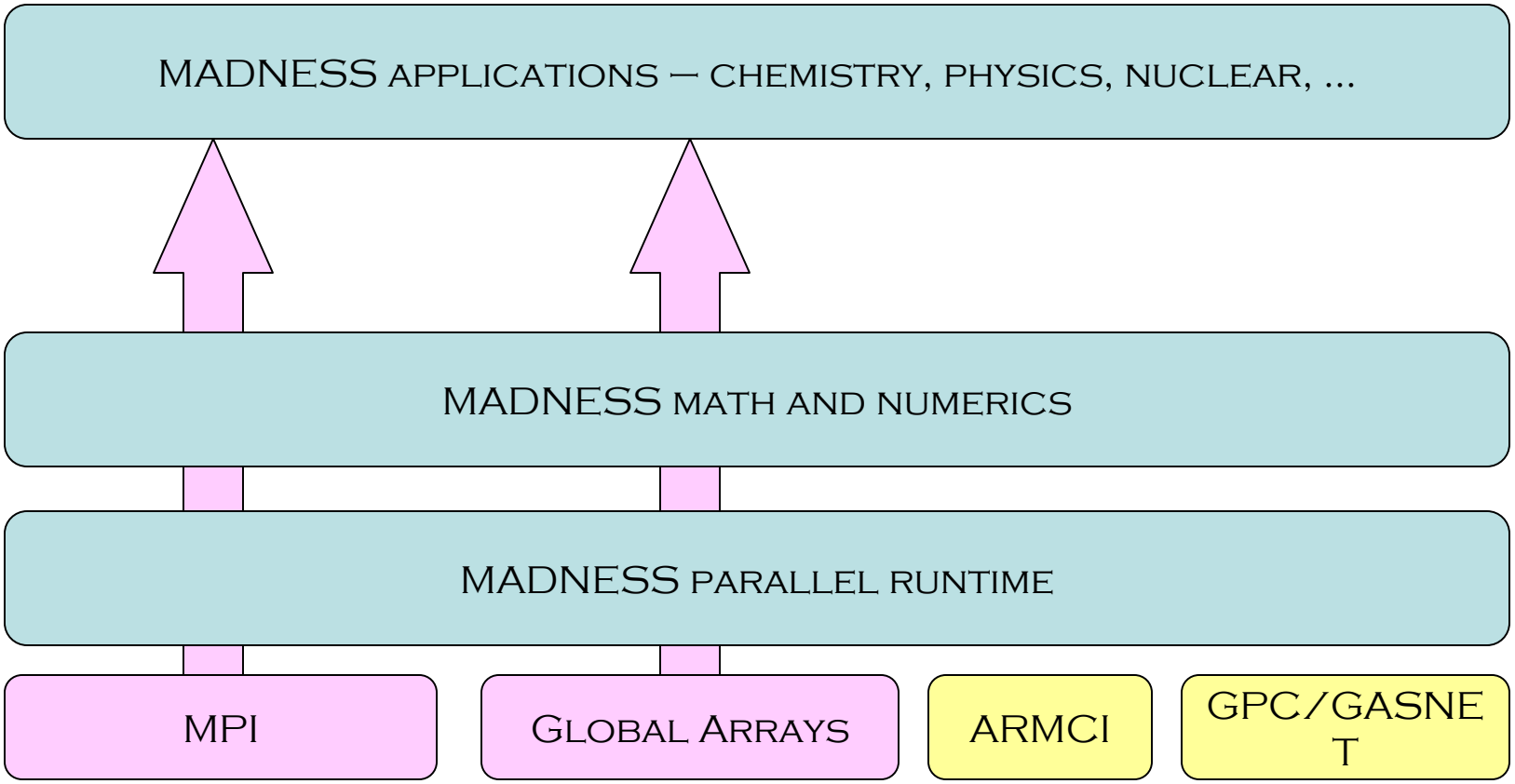
An Introduction to MADNESS

- What is it?
- Example of use
  - Computational Chemistry
  - Nuclear Density Functional Theory
  - Navier-Stokes Equation
- Multiresolution analysis and representation of functions
- Non-standard form,
- Separated representation of operators and functions
- Examples using operators

What is MADNESS?

- Multiresolution Adaptive Numerical Scientific Simulation
  - It is an environment to prototype and develop scientific applications using multiresolution methods in multiwavelet basis from 1-D to 6-D.
  - The important concepts
    - *Multiresolution, multiwavelet, low-separation rank approximation of functions and operators*
    - *Multiresolution discontinuous and singular bases*
    - *Each function and operator has its own adaptive representation*
  - It presently contains non-linear time-independent and time-dependent solvers for 3-D Density Functional Theory (DFT) code and Schrodinger equations for chemistry and nuclear physics, but others are working on nano-charge dynamics, bio-fluid, chemical reactions, …

MADNESS architecture



Intel Thread Building Blocks being considered for multicore

Example: Integral Formulation for Soln of Bound State Schrödinger Equation

- Can solve by using differential formulation and diagonalize Hamiltonian
  - Issue: high condition number resulting from adaptive representation of unbounded operators, such as Laplacian, limits accuracy and precision
  - Use as preconditioner
- We form and solving the integral equation
  - Eliminates the derivative operator and related "issues"
  - Converges as fixed point iteration *with no preconditioner*
- In dimensionless scattering formulation: with energy E and potential V

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

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

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

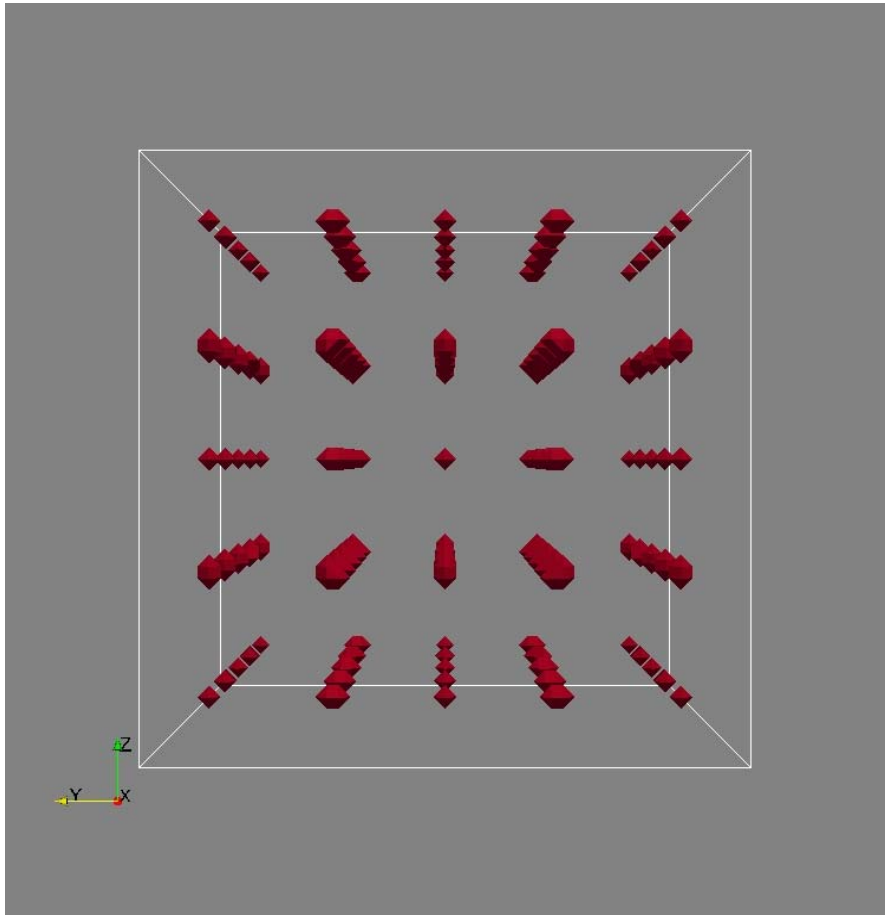
$$\left(G * f\right)(r) = \int ds\, \frac{e^{-k|r-s|}}{4\pi\,|r-s|}\, f(s) \quad \text{in 3D} \;;\; k^2 = -E$$

MADNESS: High-level composition

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

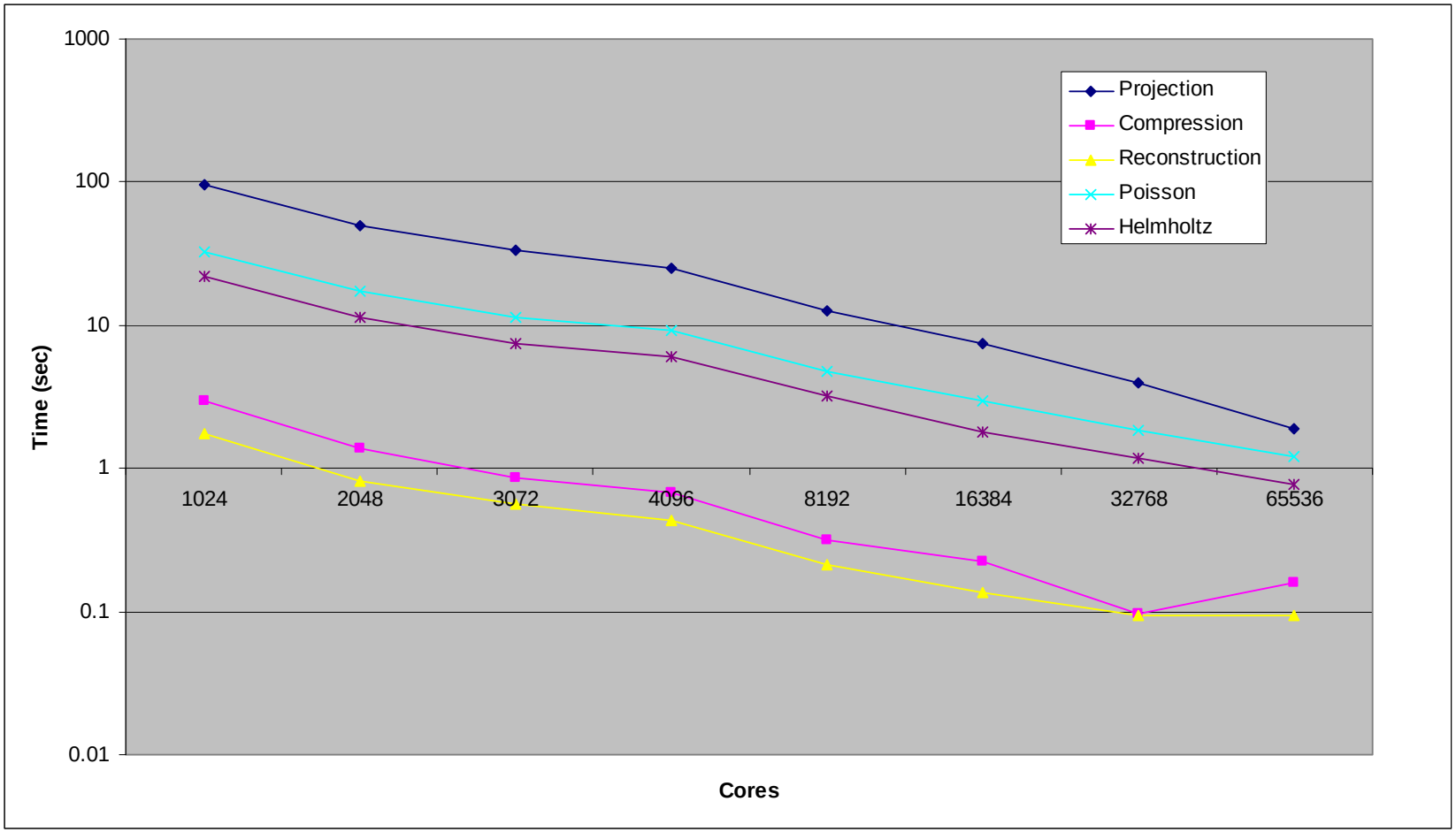
```
operatorT op = CoulombOperator(k, rlo, thresh);
functionT rho = psi*psi;
double twoe = inner(apply(op,rho),rho);
double pe = 2.0*inner(Vnuc*psi,psi);
double ke = 0.0;
for (int axis=0; axis<3; axis++) {
    functionT dpsi = diff(psi,axis);
    ke += inner(dpsi,dpsi);
}
double energy = ke + pe + twoe;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

Scaling of Poisson and Helmholtz in MADNESS with Lattice of Atom Centered Potential



- Charge density for Poisson Equation
- Scattering for Helmholtz Eqn, bound-state or Yukawa
- Lattice of 1000 atoms
- Potential centered at each atom center
- 10 levels of refinement
- 1.91B equations and variables

Scaling of MADNESS for on Cray XT-5
Poisson and Helmholtz
1.91B eqns, 10 levels of refinement, rel. accuracy 1.e-10, 12/1/2009



Chemistry and Nuclear Physics Application:No Spin-Orbit Integral Formulation of Bound State Schrödinger Equation

- Given H, in multiwavelet basis and guess wavefunctions, diagonalize
- Solving the integral equation
  - Eliminates the derivative operator and related “issues”
  - Converges as fixed point iteration *with no preconditioner*
- In dimensionless form:

$$\left(-\nabla^2 + V\right)\Psi = E\Psi$$

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

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

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

E.g., Energy of Hydrogen Atom

```
from mra import *
L = 32.0
Function.k = 7
Function.thresh = 1e-5

def psi(x,y,z):
    fac = 102.12922378276677 #sqrt(L**3/pi)
    x,y,z = (x-0.5)*L,(y-0.5)*L,(z-0.5)*L
    return fac*exp(-sqrt(x*x+y*y+z*z))

def V(x,y,z):
    x, y, z = (x-0.5)*L, (y-0.5)*L, (z-0.5)*L
    return -1.0/sqrt(x*x+y*y+z*z)

psi = Function(function=psi)
V   = Function(function=V)
px, py, pz = Del*psi
S  = psi.inner(psi)
VE = (V*psi).inner(psi)/S
TE = 0.5*(px.inner(px)+py.inner(py)+pz.inner(pz))/L**2/S
print "norm",S,"kinetic",TE,"potential",VE,"energy",TE+VE
```

$$\psi(r) = \left(\frac{L^3}{\pi}\right)^{\frac{1}{2}} e^{-r} \qquad S = \langle \psi | \psi \rangle = 1$$

$$T = \langle \psi | -\tfrac{1}{2}\nabla^2 | \psi \rangle = \tfrac{1}{2}\langle \nabla\psi | \nabla\psi \rangle$$

$$V = \langle \psi | -r^{-1} | \psi \rangle \qquad E = T + V$$

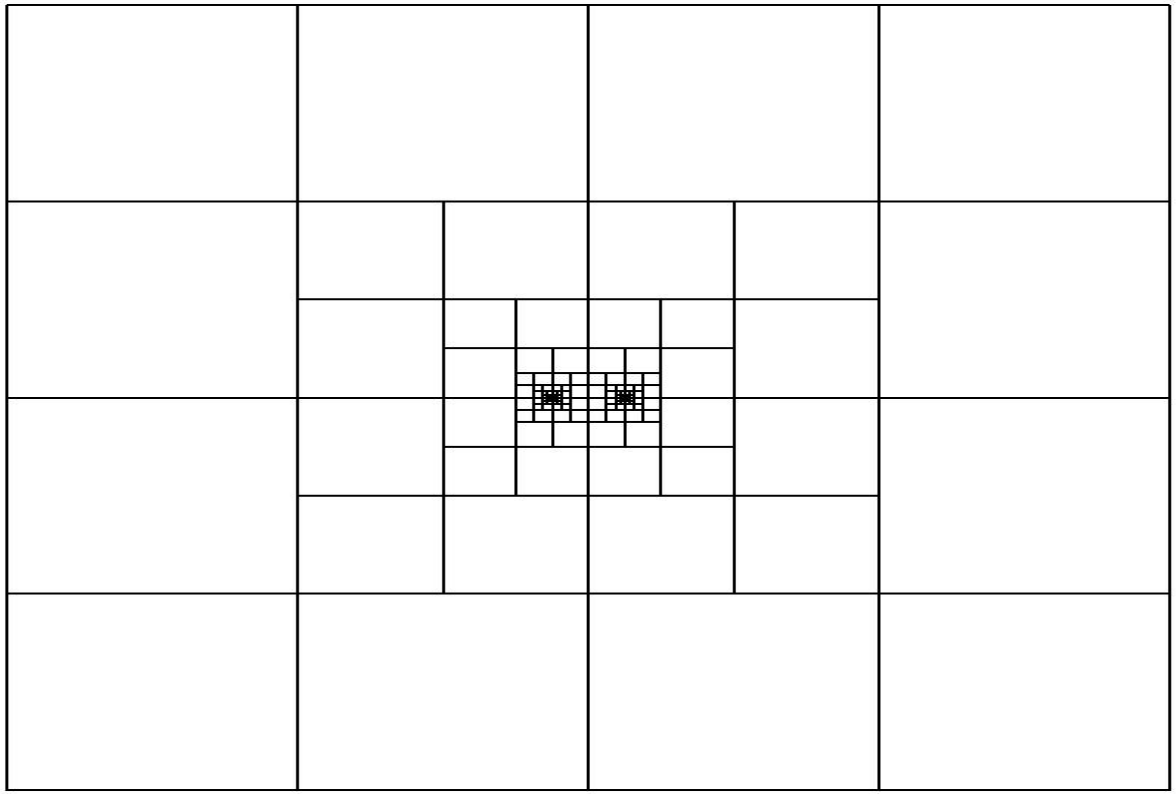
norm 1.00000000014

kinetic 0.500000335672

potential -1.00000013916

energy -0.499999803488 (exact: -0.5)

2-D Slice of the 3-D Potential for H_2



H_2, Schrodinger's Equation

- Chemists need high precision;
  - they need to compute differences of energies.
- 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

Two-Cosh Test Problem

- Potential

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

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

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

$$\varsigma = 7.5, h^2/2m = 20.721246..,$$

$$hc = 197.32696..., mc^2 = 939.56535...$$

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

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

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

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

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

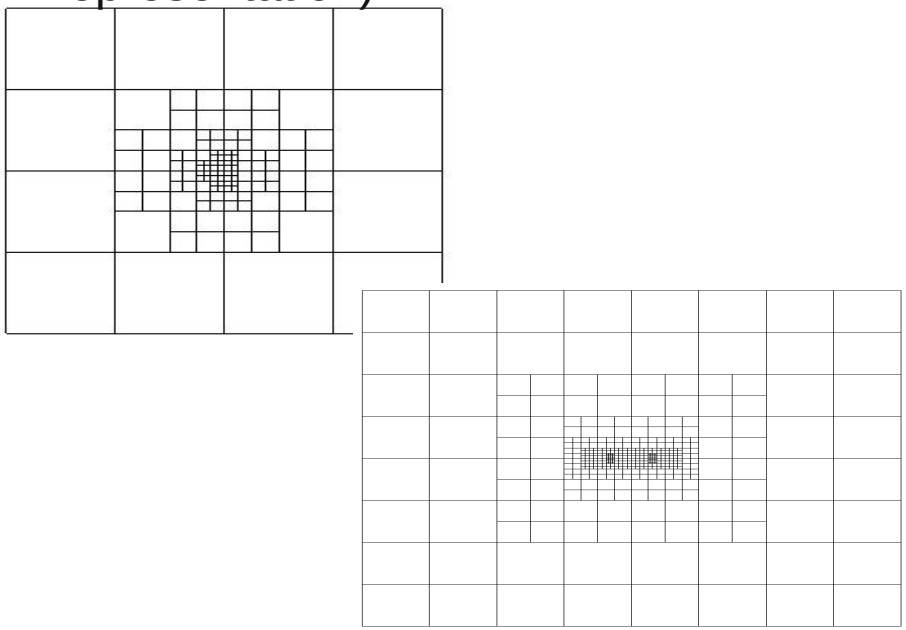
$$V(x,y,z) = \frac{V_1}{1+e^{-R_1/a_1}\cosh(r_+/a_1)} + \frac{V_2}{1+e^{-R_2/a_2}\cosh(r_-/a_2)},$$

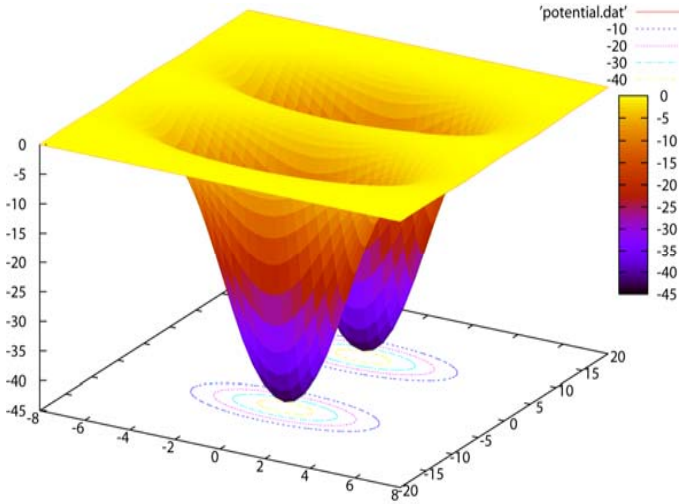
$$r_\pm = \sqrt{r^2 + (z \pm \varsigma)^2},$$

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

Representation of Wave-Functions

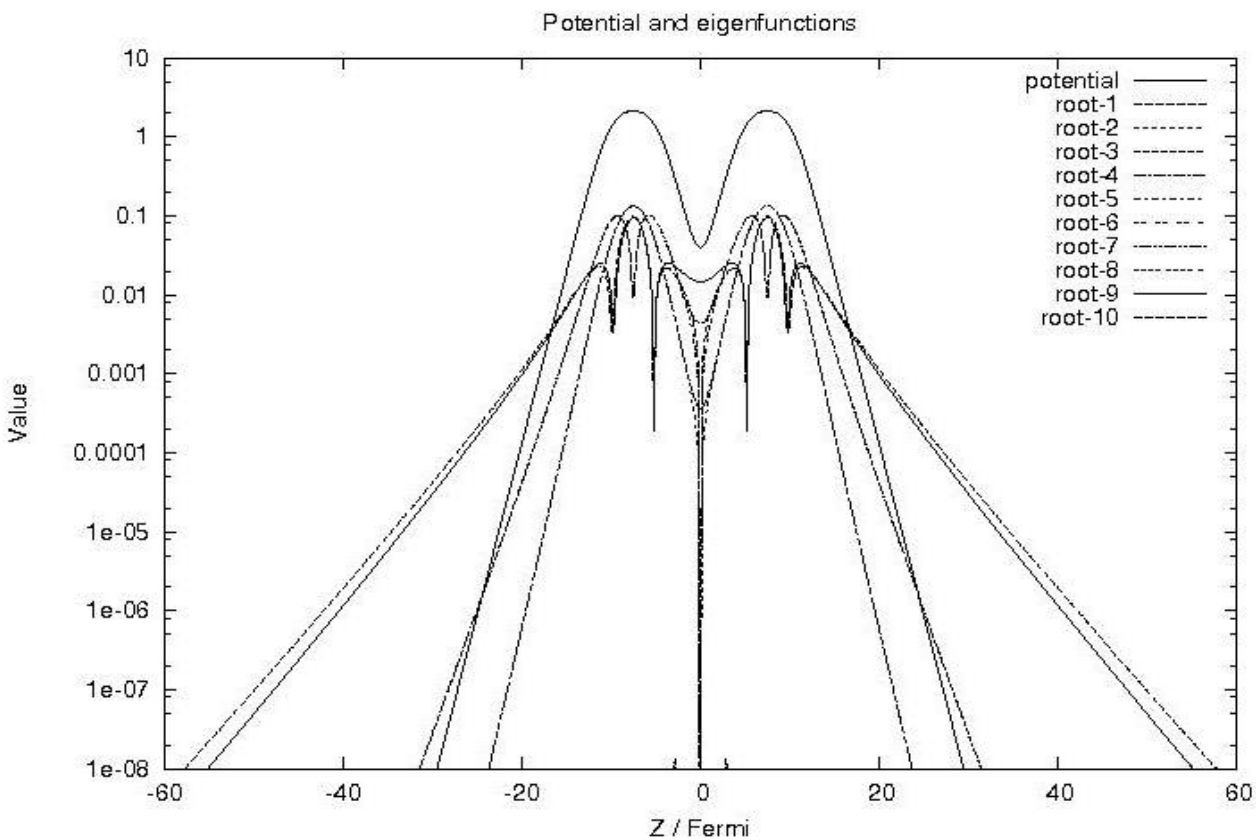
MADNESS (each function and operator has its own adaptive pseudo-spectral expansion representation)





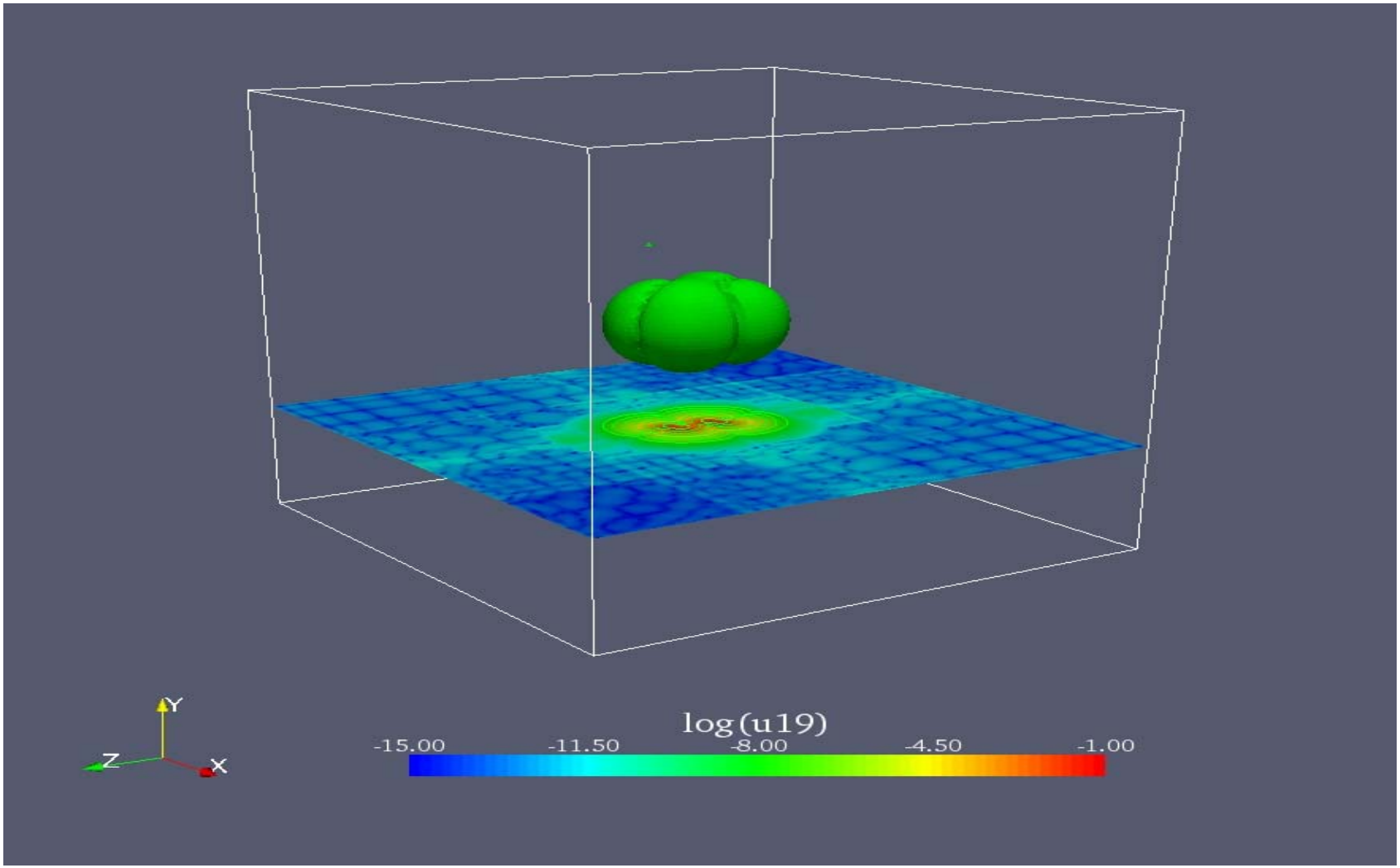
A 2-D slice of the 3-D support of the multiwavelet bases for the 2-cosh potential (left) and one of its wave-functions (right).

Plot of Potential and Absolute Value of Wave Functions for the 2-cosh Potential, domain > 120 fermi

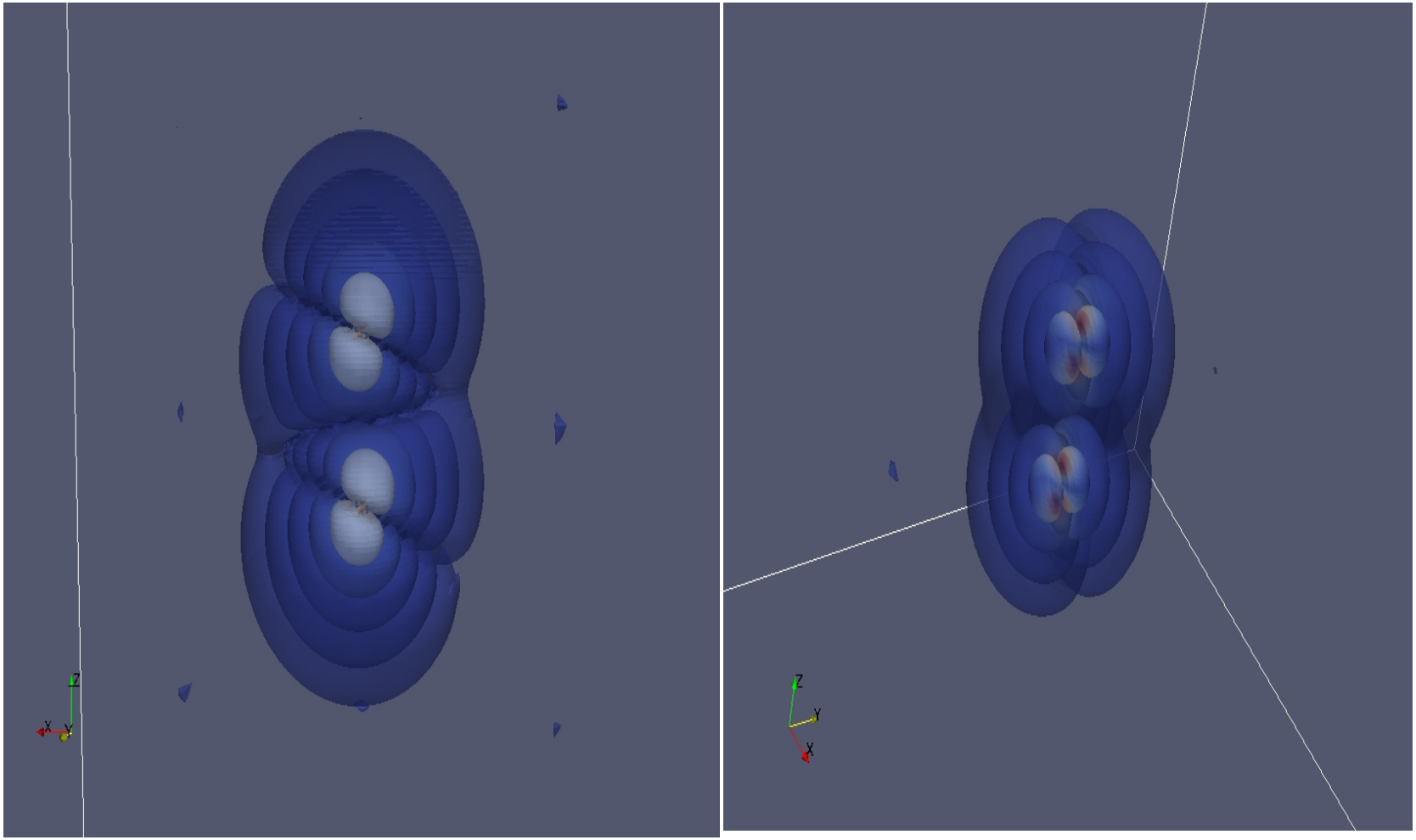


Fann, Harrison, Pei, Ou, Nazarewicz 2009

Log(abs(u_19)) for HFB 2-cosh



Nuclear structure for an anisotropic two well potential (3-D)



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)

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

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

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

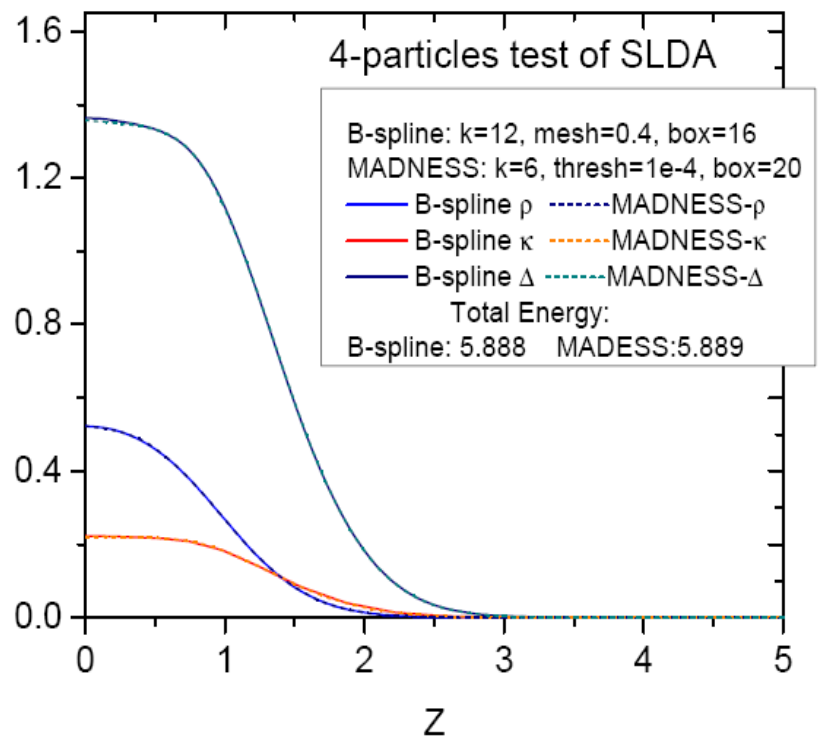
Pei, Fann, Harrison, Ou, Nazarewicz 2010

Recent Progress of MADNESS-HFB

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



Pei, Fann, Harrison, Ou, Nazarewicz 2010

Multiresolution Methods for DFT

- Adaptive 3-D multiresolution pseudo-spectral methods for nuclei using discontinuous basis
  - User defined accuracy gives universal reference and good scalability
  - Consistent description of bound and resonant states
- No assumption on symmetry
- Each wave-fn has its own adaptive structure
- Can handle nearly singular or discontinuous functions, and high gradients
- Work is proportional to spectral accuracy
- Controllable and guaranteed precision

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 Incompressible Navier-Stokes Equation

- Consider the classical incompressible Navier-Stokes equations, in a periodic domain

$$\mathbf{u}_t + \nabla p = -(\mathbf{u}\cdot\nabla)\mathbf{u} + \mathbf{Re}^{-1}\nabla^2\mathbf{u} + f \qquad \nabla\cdot\mathbf{u} = 0$$

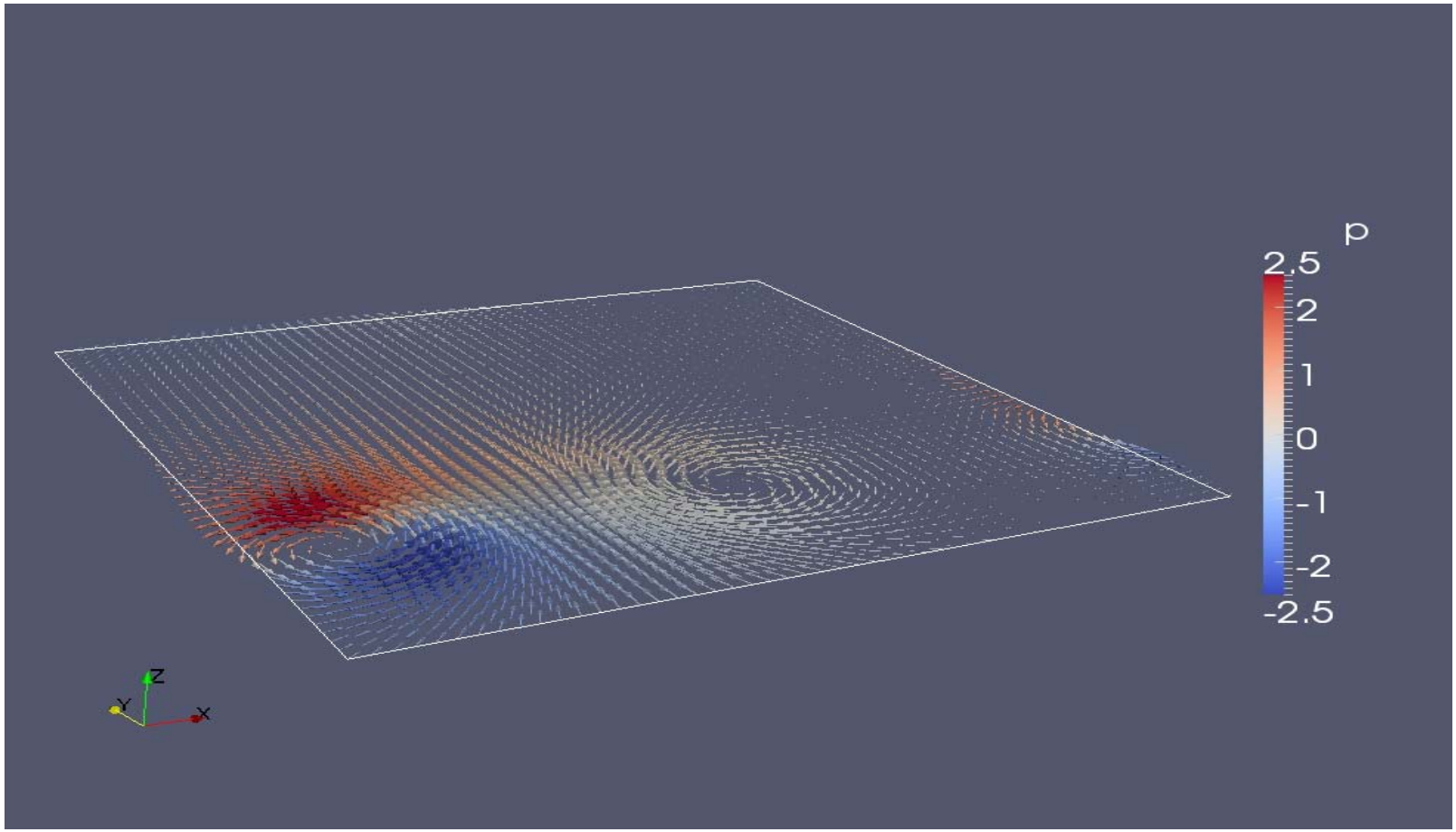
- We demonstrate a solution method using multiresolution based Poisson and Helmholtz operators
  1. Backward Euler in time, implicit (iterative solvers)
  2. Fast integral methods that decompose the system into two equations by a projection method

$$\Delta p = \nabla\cdot f - \nabla\cdot(\mathbf{u}\cdot\nabla)\mathbf{u}$$ (Poisson Problem)

$$\left(\frac{\mathbf{Re}}{\delta t} - \Delta\right)\mathbf{u}^{t+1} = \mathbf{Re}\left(f - (\mathbf{u}^t\cdot\nabla)\mathbf{u}^t - \nabla p + \frac{1}{\delta t}\mathbf{u}^t\right)$$ (Helmholtz Problem)

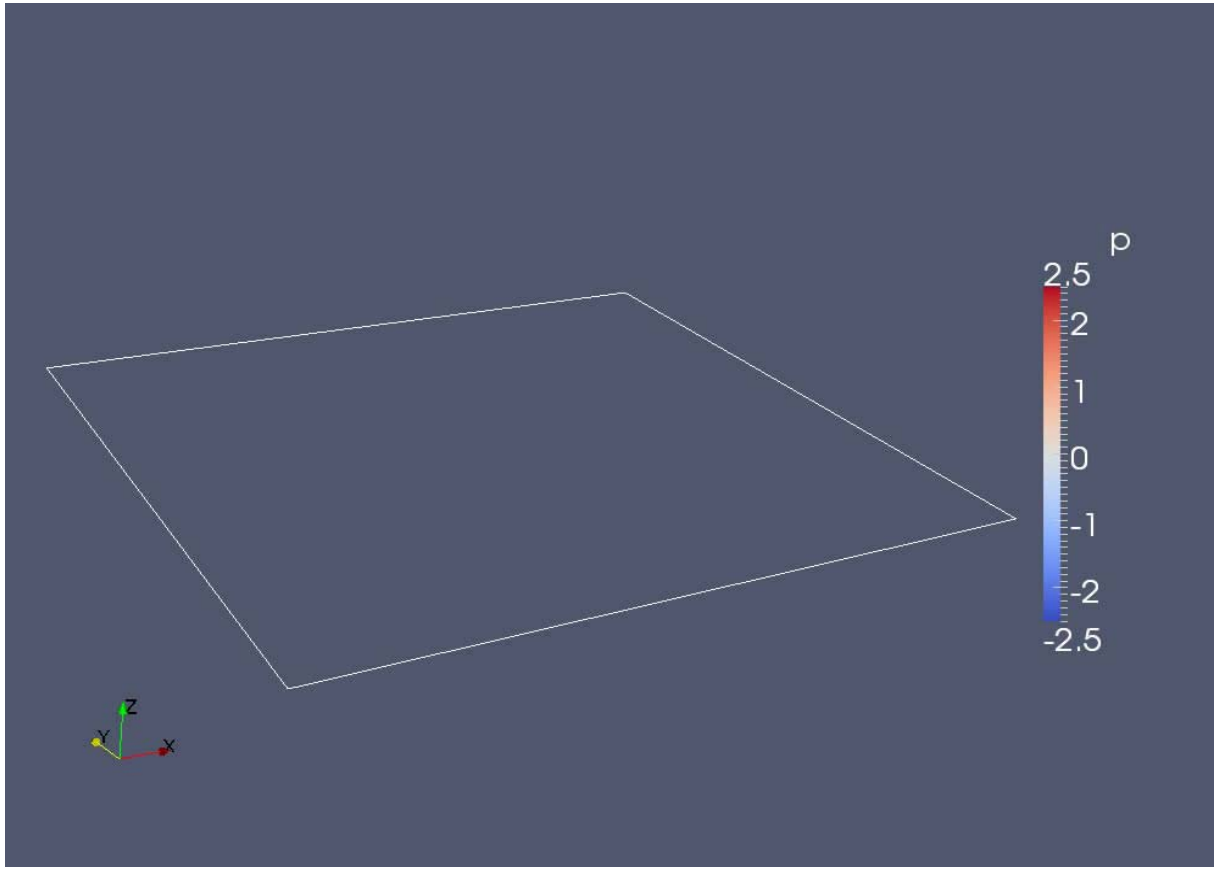
Problem from Hou's 2008 paper, (Jia, Hill, Fann, Harrison, 2009)

3-D Navier-Stokes Simulation using MADNESS periodic-domain, counter-rotating vortices



2-D slice of a 3-D simulation of two vortices rotating in opposite directions

Simulation 2-D slice



Essential techniques for fast computation

- Multiresolution Analysis

$$V_0 \subset V_1 \subset \cdots \subset V_n$$

$$V_n = V_0 + \left(V_1 - V_0\right) + \cdots + \left(V_n - V_{n-1}\right)$$

- Low-separation rank (Beylkin-Mohlenkamp)

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

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

- Low-operator rank (e.g. SVD, HOSVD)

$$A = \sum_{\mu=1}^{r} \underline{u}_\mu \sigma_\mu \underline{v}_\mu^T + O(\varepsilon)$$

$$\sigma_\mu > 0 \qquad \underline{v}_\mu^T . \underline{v}_\lambda = \underline{u}_\mu^T . \underline{u}_\lambda = \delta_{\mu\lambda}$$

Another Key Component

- Trade precision for speed –everything
  - Don't do anything exactly
  - Perform everything in $O(\varepsilon)$
  - Require
    - *Robustness*
    - *Speed*
    - *Guaranteed, arbitrary, finite precision*

Multiwavelets and Fast Methods

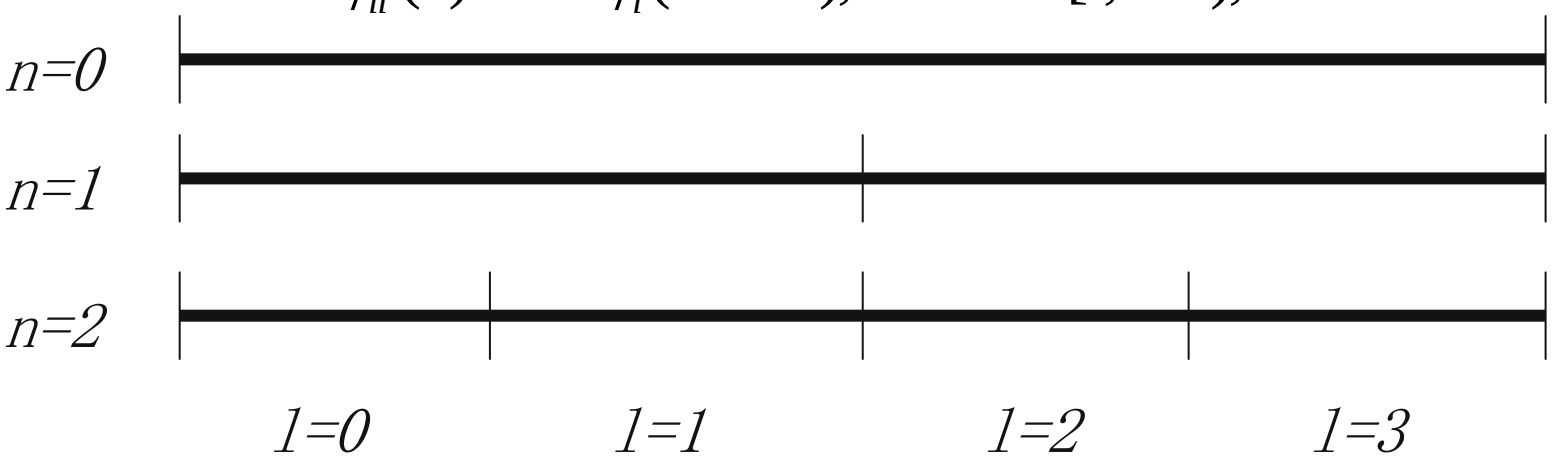
- Multiple representations permit each function and operator to have its own resolution, or representation depending on precision
- Automatic adaptivity for spectral expansion and order of accuracy (h & p)
  - Integral and differential operators (compatible)
  - Functions, projections between different level of expansions (depending on accuracy)
  - Compatible between function and operator calculus
- Accurate treatment of singularities
- Accurate treatment of higher order derivatives
  - Improved treatment of Gibbs type phenomena
- Green's function (Poisson, Helmholtz, etc.) via Low-Separation Rank
  - Fast real analysis based O(N log ε) method
  - Accuracy is proportional to
    - *Degrees of freedom*
    - *Work (flops)*
- DFT, Lippmann-Schwinger, Hartree-Fock, …
- Time-dependent DFT for molecular HF and DFT, Navier-Stokes

1-D Scaling Function Basis: Alpert's Multiwavelets

- Divide domain into 2^n pieces (level n)
  - Adaptive sub-division (local refinement)
  - l^{th} sub-interval $[l*2^{-n},(l+1)*2^{-n}]$ $l=0,\ldots,n-1$
- In each sub-interval define a polynomial basis
  - First k Legendre polynomials, P_i, rescale and normalized on [0,1)
  - Orthonormal, disjoint support

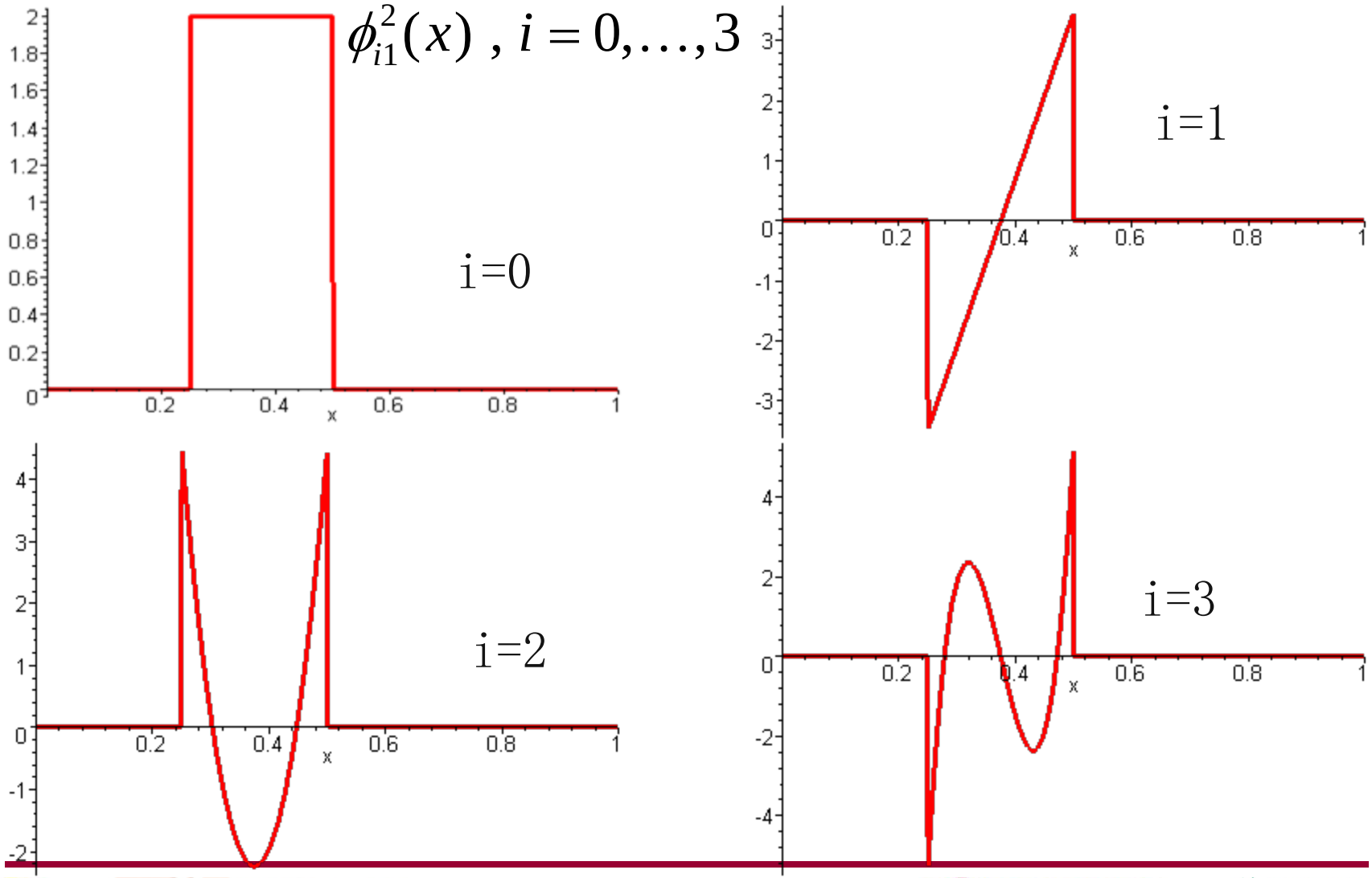
$$\phi_i(x) = \sqrt{2i+1}P_i(2x-1),\ldots x \in [0,1)$$

$$\phi_{il}^n(x) = 2^{n/2}\phi_i(2^n x - l),\ldots x \in 2^{-n}[l,l+1),\ldots 0 \le l \le n-1$$



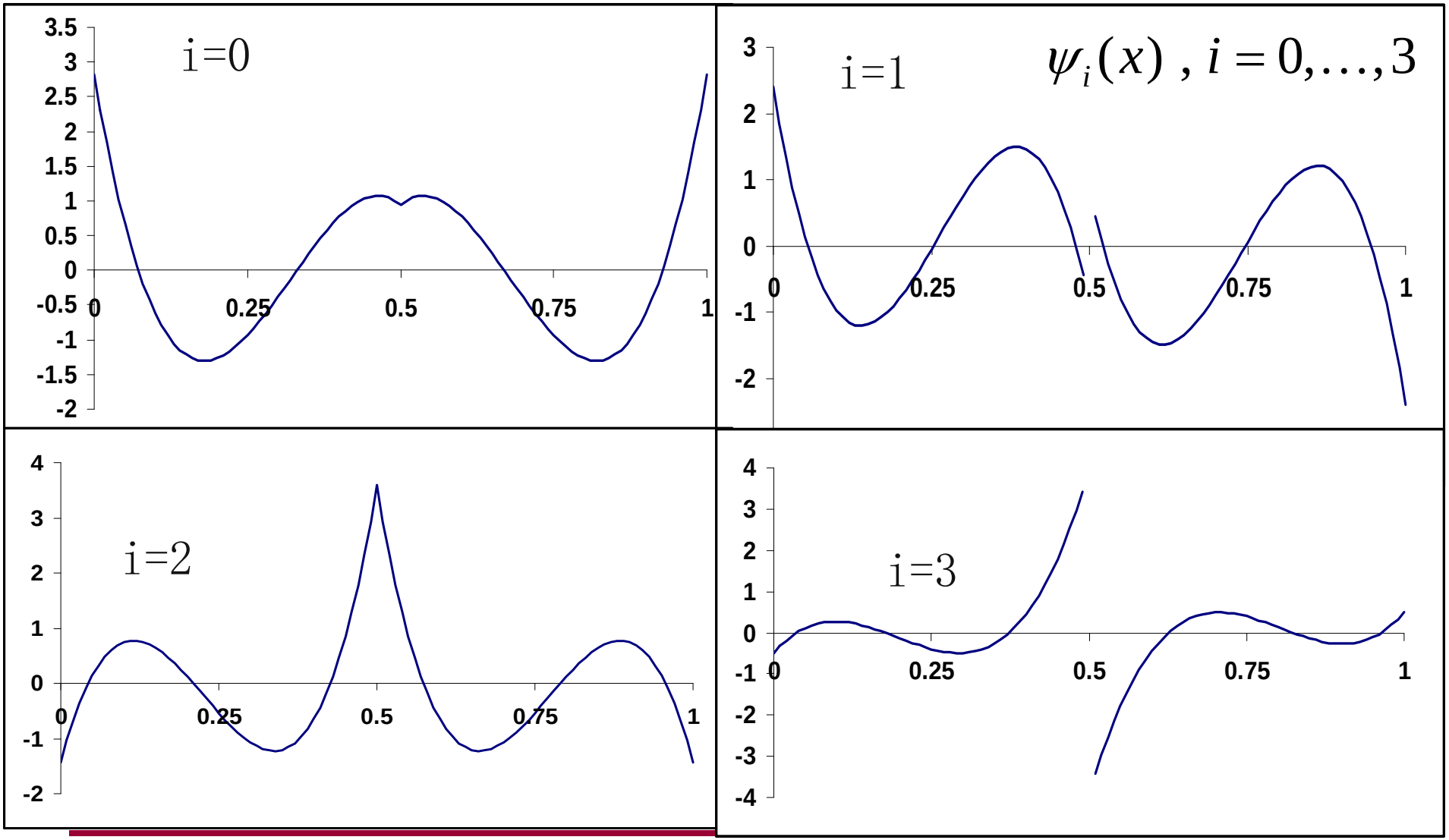
Scaling Function Basis:Alpert's, level, n=2

$$\phi_{i1}^{2}(x)\ ,\ i = 0,\ldots,3$$



Multiwavelet Basis

$k=4, \quad n=0$



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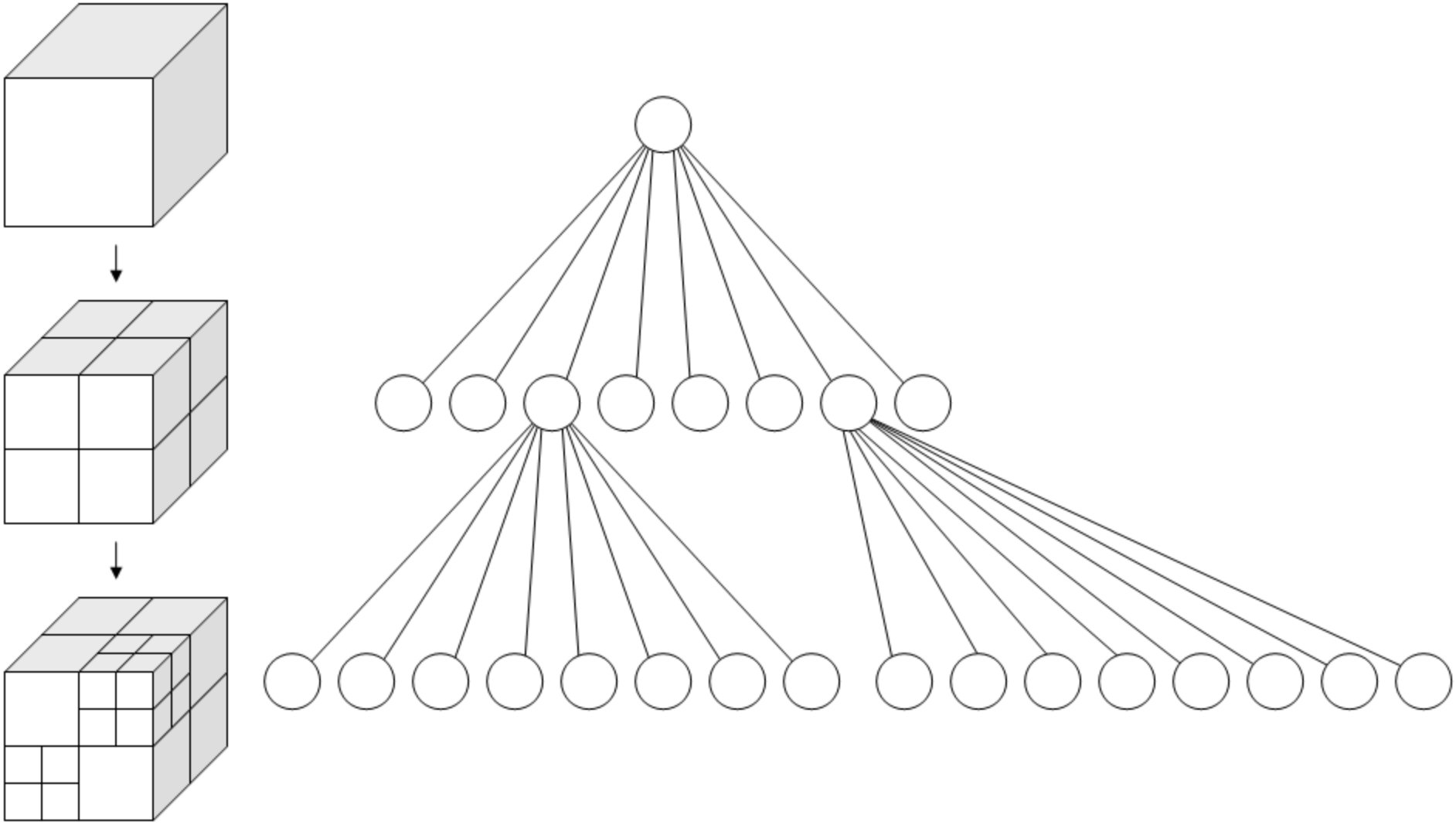
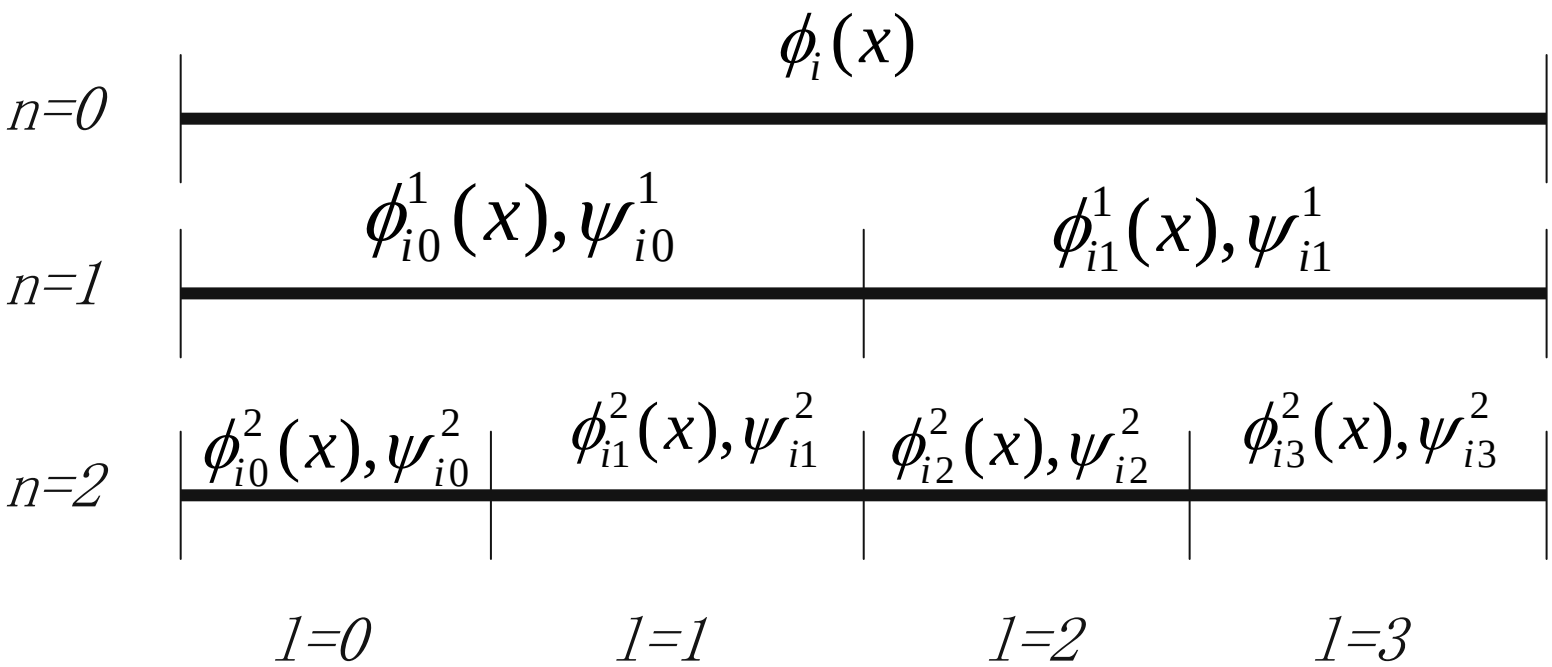
Oct-tree Adaptivity



Adaptivity by Spectral Expansion
Support of Basis Functions

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



Two-scale relationship - I

$$\begin{pmatrix} \phi(x) \\ \psi(x) \end{pmatrix} = \sqrt{2} \begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix} \begin{pmatrix} \phi(2x) \\ \phi(2x-1) \end{pmatrix}$$

Filter coefficients for k=1 (Haar)

$$\begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\begin{pmatrix} s_0^0 \\ d_0^0 \end{pmatrix} = \sqrt{2} \begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix} \begin{pmatrix} s_0^1 \\ s_1^1 \end{pmatrix} = \begin{pmatrix} s_0^1 + s_1^1 \\ s_0^1 - s_1^1 \end{pmatrix}$$

Hence, coefficients of scaling functions and wavelets are often referred to as <u>s</u>um and <u>d</u>ifference coefficients.

Compression of a function

$$V_n = V_0 \oplus W_0 \oplus W_1 \oplus \cdots \oplus W_{n-1}$$

- Recursively apply the two-scale relation
- The basis is the scaling functions at level 0 and the multiwavelets at all levels

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

- Haar basis (*k=1*) gives rise to calling coefficients of the scaling functions and wavelets as sums and differences respectively (hence notation *s* and *d*)
- Compression & reconstruction are *O(N)* operations

Two equivalent representations

- Scaling function basis (reconstructed)

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

- Multi-wavelet basis (compressed)

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

- Rapid compression/reconstruction
  - Asymptotically faster than the FFT
  - Use most appropriate basis for a given operation

A Third Equivalent Representation

- The function tabulated at the Gauss-Legendre quadrature points in each of the adaptively refined boxes
  - Enables rapid multiplication of functions and application of local functions (e.g., V_{xc})
  - Diagonal transformation from interpolating polynomials

Truncation Error

- Sparsity is from truncation.
- To satisfy the global error condition

$$\left\| f - f^{n} \right\|_2 \le \varepsilon \left\| f \right\|_2$$

- Truncate according to

- This is rather conservative – usually use

$$\left\| d_l^n \right\|_2 \le 2^{-n/2} \varepsilon \left\| f \right\|_2$$

$$\left\| d_l^n \right\|_2 \le \varepsilon$$

Summary I

- Scaling functions
  - Easy to manipulate, evaluate, integrate, …
- Multi-resolution analysis
  - Separates behavior between length scales
  - Local truncation while preserving global error bound
  - Vanishing moments
- Multi-wavelets
  - High-order convergence with adaptive representation
  - Disjoint support – efficient description of singularities if locacated at faces/edges/corners (more efficient than smooth wavelets since they do not have disjoint support)
- Fast compression and reconstruction
  - Orthogonal transformations – numerically stable

Extension to higher dimensions

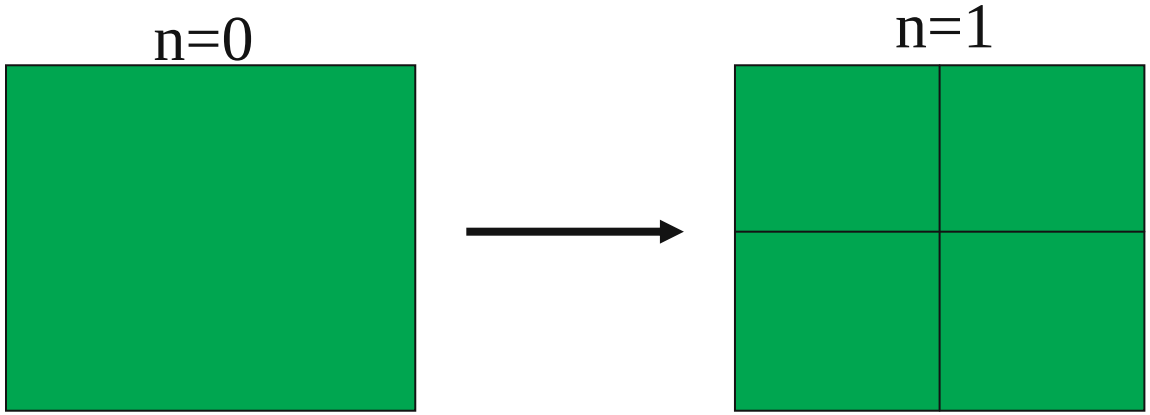
- Scaling function basis is tensor product

- Wavelet basis – tensor product is one choice
  - Standard form – compress each dimension just as for a matrix
  - But cannot refine strictly locally since length scales are mixed between dimensions
- To refine locally need the non-standard form

$$\phi^n_{ii'll'}(x,y) = \phi^n_{il}(x)\phi^n_{i'l'}(y)$$

Non-standard form of functions

- Construct local basis for $W_{n-1}=V_n - V_{n-1}$



$$V_0 = \phi(x)\phi(y)$$

$$V_1 = \sqrt{2}\left\{\begin{array}{l}\phi(2x)\phi(2y), \phi(2x)\phi(2y-1), \phi(2x-1)\phi(2y), \\ \phi(2x-1)\phi(2y-1)\end{array}\right\}$$

$$= \{\phi(x)\phi(y), \phi(x)\psi(y), \psi(x)\phi(y), \psi(x)\psi(y)\}$$

$$W_0 = V_1 - V_0 = \{\phi(x)\psi(y), \psi(x)\phi(y), \psi(x)\psi(y)\}$$

Non-standard form of operators

- Standard form
  - Matrix elements between different length scales
  - Not very efficient on modern computers with deep memory hierarchies
  - Potentially *O(Nlog N)* non-zero terms
- Non-standard form
  - No matrix elements between lengths scales
  - *O(N)* terms
  - Act on (modified) non-standard form of functions
  - Derivation is instructive

Non-standard form of operators - II

- P_n an orthogonal projection into V_n
- Q_n an orthogonal projection into $W_n = V_{n+1} - V_n$

  $P_n + Q_n = P_{n+1}$
- Consider the projection of an operator T

$$
\begin{aligned}
T_n &= P_n T P_n \\
&= \left(P_{n-1} + Q_{n-1}\right) T \left(P_{n-1} + Q_{n-1}\right) \\
&= P_{n-1} T P_{n-1} + Q_{n-1} T Q_{n-1} + Q_{n-1} T P_{n-1} + P_{n-1} T Q_{n-1} \\
&= T_{n-1} + A_{n-1} + B_{n-1} + C_{n-1} \\
&= T_0 + \sum_{\eta=0}^{n-1} A_\eta + B_\eta + C_\eta
\end{aligned}
$$

NS Form of Operators III

- Matrix elements in the scaling function basis

- Matrix elements of the NS form

$$\left[r_{lm}^{n} \right]_{ij} = \int \phi_{il}^{n}(x) \left(T \phi_{jm}^{n}(x) \right) dx$$

$$\begin{pmatrix} r_{l,m}^{n-1} & \gamma_{l,m}^{n-1} \\ \beta_{l,m}^{n-1} & \alpha_{l,m}^{n-1} \end{pmatrix} = \begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix} \begin{pmatrix} r_{2l,2m}^{n} & r_{2l,2m+1}^{n} \\ r_{2l+1,2m}^{n} & r_{2l+1,2m+1}^{n} \end{pmatrix} \begin{pmatrix} H^{(0)} & H^{(1)} \\ G^{(0)} & G^{(1)} \end{pmatrix}^{T}$$

Integral operators - I

- Consider

$$Tf(x) = \mathrm{pv}\int dy K(x-y) f(y)$$

$$\left[r_{lm}^{n}\right]_{ij} = \int dx \int dy K(x-y)\phi_{il}^{n}(x)\phi_{jm}^{n}(y)$$

$$= 2^{-n}\int dx \int dy K(2^{-n}\left(x-y+l-m\right))\phi_i(x)\phi_j(y)$$

$$= 2^{-n}\int dz K(2^{-n}\left(z+l-m\right))\Phi_{ij}(z)$$

$$\Phi_{ij}(z) = \int dx \phi_i(x)\phi_j(x-z)$$

$$= \sum_{p=0}^{2k-1}\left(c_{ijp}^{(-)}\phi_p(z+1) + c_{ijp}^{(+)}\phi_p(z)\right)$$

$$\left[r_{l}^{n}\right]_{p} = 2^{-n}\int dz K(2^{-n}\left(z+l\right))\phi_p(z)$$

Integral operators - II

- The autocorrelation and cross-correlation functions also have a 3 term 2-scale relations.
- Matrix elements easy to evaluate from compressed form of kernel *K(x)*
- Application in 1-d is fairly efficient
  - $O(k^2)$ operations
- In 3-d seems to need $O(N_{box}k^6)$ operations
  - Prohibitively expensive
  - Cross-correlations reduces to $O(8N_{box}k^4)$
  - LSR does more
- More intelligent approach
  - $O(N_{box}k^4)$ operations for many "physical" kernels
  - Even better is known to be possible

Example: Poisson Kernel

- Example: Poisson Kernel

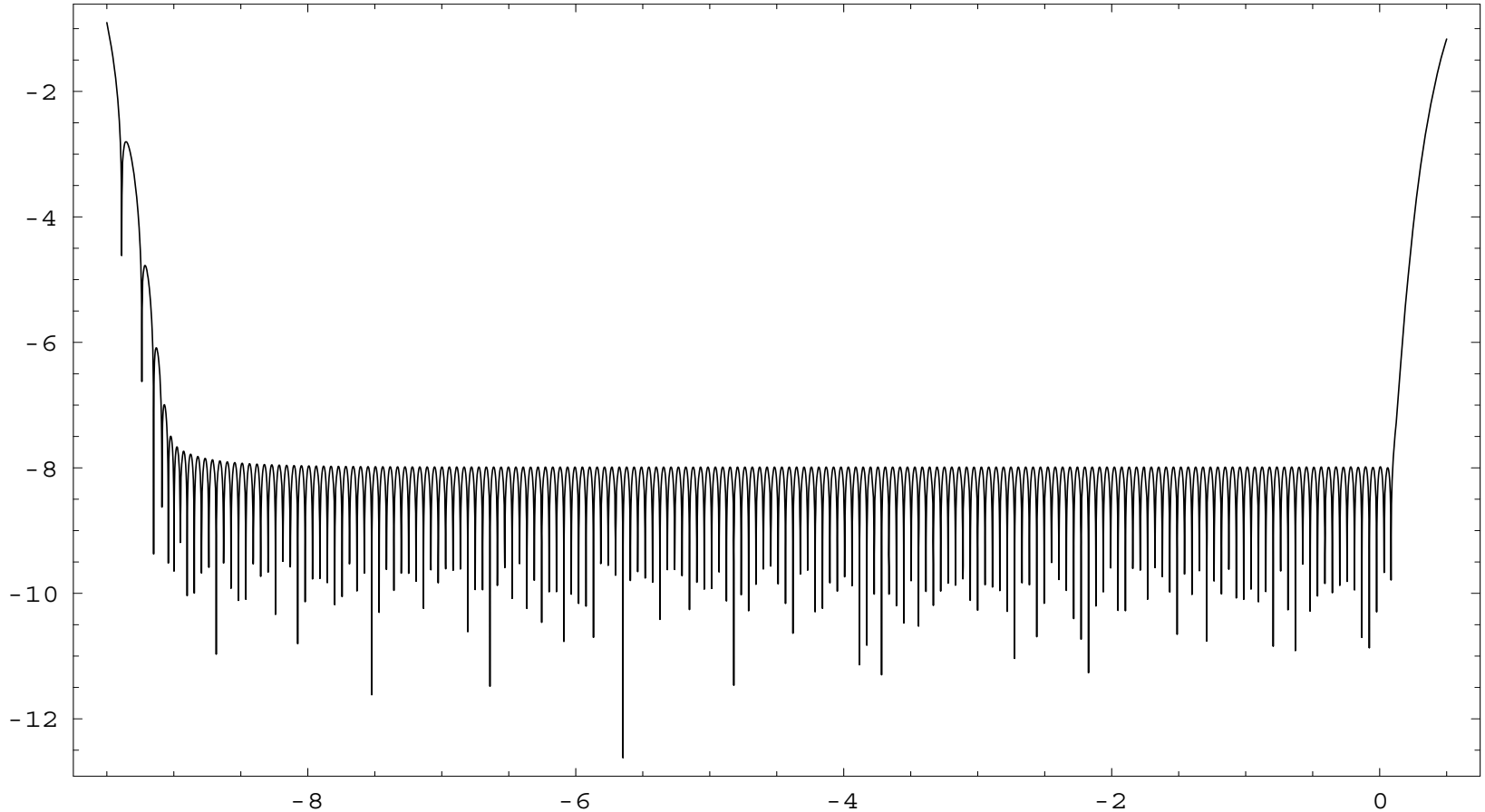
$$\left| \frac{1}{r} - \sum_{m=1}^{M} w_m e^{-p_m r^2} \right| \le \frac{\varepsilon}{r}$$

$$\delta \le r \le 1,$$

$$0 < p_m, w_m$$

$$M = O(-\log \delta)$$

Approximation of Poisson Kernel



Error ($\log_{10}$-scale) of approximating the Poisson kernel from [1e-9, 1] with M=89 terms.

Low Separation Rank Approximation, Poisson Example

Proposition 2. *For any $\alpha > 0$, $0 < \delta \leqslant 1$, and $0 < \epsilon \leqslant \min\{\frac{1}{2}, \frac{8}{\alpha}\}$, there exist positive numbers p_m and w_m such that*

$$\left| r^{-\alpha} - \sum_{m=1}^{M} w_m e^{-p_m r^2} \right| \leqslant \epsilon_0 r^{-2} \quad \text{for all } \delta \leqslant r \leqslant 1, \tag{3}$$

where

$$M = \log \epsilon^{-1} \left[c_0 + c_1 \log \epsilon^{-1} + c_2 \log \delta^{-1} \right]. \tag{4}$$

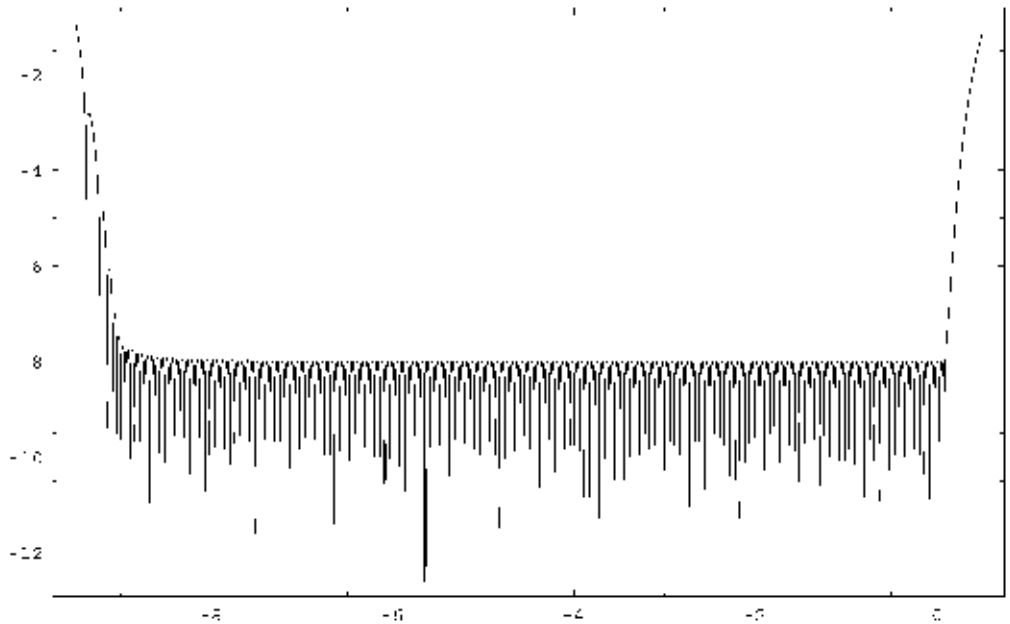
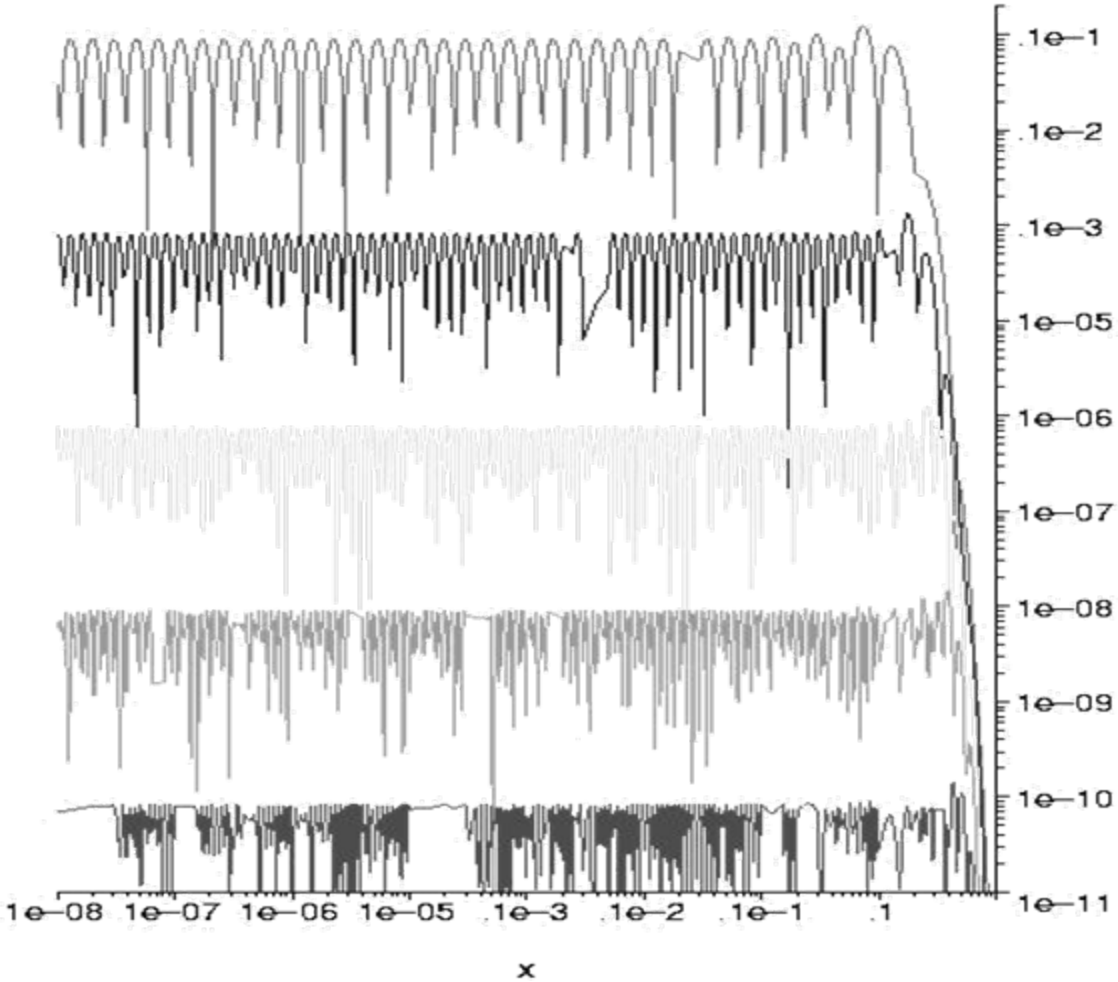


Fig. 1. Error ($\log_{10}$) of approximating the Poisson kernel using Proposition 1 with consequent optimization, where $\epsilon \approx 10^{-8}$, $10^{-9} \leqslant \|\mathbf{x}\| \leqslant 1$ and $M = 89$.

B-C-F-H, Achä, 2007



Automatically generated representations of *exp(-30r)/r* accurate to 1e-10, 1e-8, 1e-6, 1e-4, 1e-2 (relative error) for *r* in [1e-8,1] (92, 74, 57, 39 and 21 terms, respectively).

Low-energy *scattering* states also possible (but stronger dependence on range)

Summary of Computational Setup

- 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
- Now relax the tree structure—map tree to hash table

- *Download, FAQ and wiki*

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

--will require mpicc, mpicxx, mpif90,.., lapack, blas, gfortran

Example code in m-a-d-n-e-s-s/src/apps/examples

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