Adaptive Pseudo-spectral Method in 6-D

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MADNESS

Multiresolution Adaptive Numerical Scientific Simulation

MADNESS is a framework for fast computation with guaranteed precision using adaptive pseudo-spectral methods and discontinuous bases on high performance computers. Initial application is to determine the electronic structures of molecules, and nuclear structures. The methods are widely applicable. We compute in 1-6 D and higher dimensions using combinations of multi-resolution and separated representations of functions and operators.

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Objectives

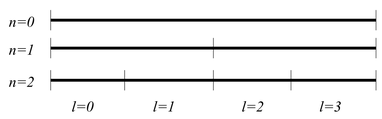
- Fast and Adaptive Solvers
  - Computational Chemistry (e.g. Hartree-Fock, Density Functional Theory, Schrodinger's eqn)
  - Materials, fluids, electricity and magnetism
- Scaling of computational cost with size
- General approach
  - Readily accessible by students in sciences and mathematics
  - More accessible than current computational chemistry code
  - Focus on integro-differential equations

Distinguishing Features

- Multiwavelet bases
  - Disjoint support and discontinuous basis maintains high-order convergence up to singularities and complex boundary conditions
- Non-standard form of operators and functions
  - Fully adaptive local representation
  - Operators are easy to compute and fast to apply
- Integral operator formulation
  - Operators are bounded
  - *O(N log ε)* and with rapid convergence
- Separated form of operators
  - Adaptive representation for each function and operator

Scaling Function Basis

- 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 $\phi_i(x) = \sqrt{2i+1}P_i(2x-1)$
  - Orthonormal, disjoint support $\phi_{il}^n(x) = 2^{n/2}\phi_i(2^n x - l)$



Multiwavelet Basis

A discontinuous orthonormal basis to span wavelets

$$W_n = V_{n+1} - V_n$$

Using Alpert's and interpolating basis

Vanishing moments

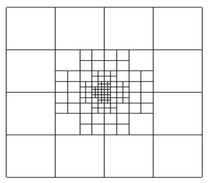
- Since W_n is orthogonal to V_n the first k moments of functions in W_n vanish, i.e.,

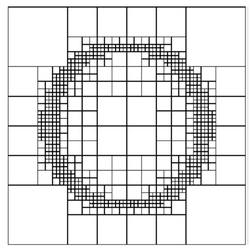
$$\int x^j \psi_i(x)dx = 0,\ j = 0,\ldots,k-1$$

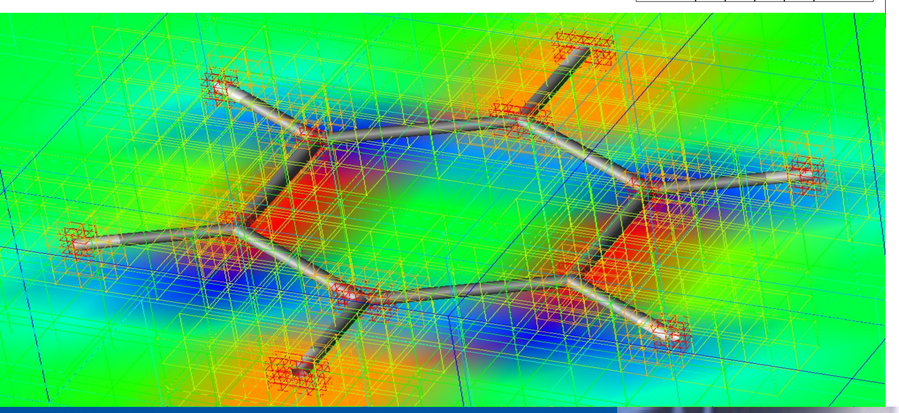
Sparse representations of many physically important kernels (e.g. Poisson, Hilbert, Helmholtz, …)

Adaptive Refinement

- Adaptive truncation of multiwavelet coefficients to satisfy accuracy condition
- Refinement is given by scaling relationships of scaling functions and multiwavelets
- Unequally spaced dyadic subdivision also developed
- Interoperability with low-separation rank approximation
- On the right, 2-D slice of a 3-D potential function and a 3-D sign-function with spherical support







Separated Representations

- The separated representation of a function or operator of many variables is an approximation

$$|\varphi(x_1,x_2,\ldots,x_N) - \sum_{l=1}^{r}\prod_{i=1}^{N}\varphi_i^l(x_i)| \le \varepsilon$$

- Functions φ_i^l are determined adaptively to achieve error bound and minimizing r, the number of terms in the sum
- A general method with controlled numerical approximation, not a reduced model

Application to Fast Computations

- Representation by Gaussians works for convolution kernels
- Poisson
- Helmholtz
- Square root of Laplacian
- Projector on divergence-free functions
- …

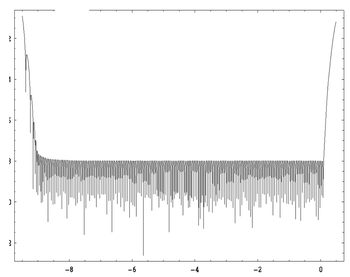
Example: Poisson Kernel

- For a given accuracy, ε, we can compute

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

- with

$$\delta \le r \le 1,$$
$$0 < p_m, w_m$$
$$M = O(-\log\delta)$$



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

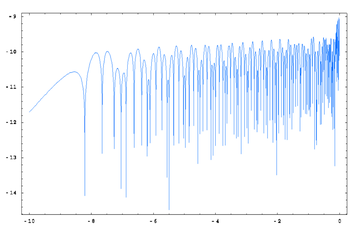
Helmholtz Green Function

- Approximate

$$\frac{\exp(ikr)}{r}$$

- For K~100

$$\frac{e^{iKr}}{r} \approx \sum_m w_m e^{\tau_m r^2}$$



Relative error ($\log_{10}$-scale) of approximating the real part of the Helmholtz Green function, M_{real}=52, k=50, from [1e-10,1].

Examples of Separated Representations of Non-Convolutional Operators

Dirichlet problem in a d-dimensional box. The Green's function G^μ for the d-dimensional Dirichlet problem,

$$(-\Delta_x + \mu^2)\,G^\mu(x,y) = \delta(x-y)$$
$$G^\mu(x,y) = 0 \text{ for } x \in \partial[-1/2,1/2]^d,$$

has a separated representation (ϵ-accurate in the operator norm),

$$\tilde{G}^\mu(x,y) = \sum_{m=1}^{M} w_m \prod_{j=1}^{d}\sum_{n_j\in\mathbb{Z}}\left(e^{-\tau_m(x_j-y_j+n_j)^2} - e^{-\tau_m(x_j+y_j+n_j+1)^2}\right),$$

where $\tau_m > 0$, $w_m > 0$, and $M = \mathcal{O}\left((\log\epsilon^{-1})^2\right)$.

Details in G. Beylkin, G. Fann, R. J. Harrison, C. Kurcz, L.Monzón, "Multiresolution Representation of Operators with Boundary Conditions on Simple Domains", to appear in ACHA

Green's function for confining harmonic potential. The multiparticle Green's function

$$\mathcal{G}_N(\mu) = (\mathcal{H}_N + \mu^2)^{-1},\ \text{where}\ \mathcal{H}_N = \sum_{j=1}^{N}(-\frac{d^2}{dx_j^2} + x_j^2),$$

has a separated representation

$$(0.1)\quad \tilde{\mathcal{G}}_N(x_1,y_1,\cdots,x_N,y_N) = \sum_{m=1}^{M} w_m \prod_{j=1}^{N} e^{-\tau_m x_j^2} e^{-\sigma_m(x_j-y_j)^2} e^{-\tau_m y_j^2},$$

where $M = \mathcal{O}\left((\log\epsilon^{-1})^2\right)$ and parameters of representation are of the form

$$w_m = \frac{\alpha_m}{(2\pi\sinh(2t_m))^{N/2}},\quad \tau_m = \tanh(t_m)/2,\quad \text{and}\quad \sigma_m = \frac{1}{2\sinh(2t_m)}.$$

Application to Chemistry and Nuclear Physics

- Density Functional Theory (DFT)
  - Kohn-Sham
  - Practical approach to DFT, parametrizing the density with orbitals (easier treatment of kinetic energy)
  - Similar computationally to Hartree-Fock, but potentially exact

$$\left(-\tfrac{1}{2}\nabla^2 + V_{coul}(r;\rho) + V_{xc}(r,\rho) + V_{ext}(r)\right)\theta_i(r) = \varepsilon_i\theta_i(r)$$
$$\rho(r) = \sum_i \theta_i^2(r)$$

Integral Formulation for Schrodinger Equation

$$\left(-\tfrac{1}{2}\nabla^2 + V\right)\Psi = E\Psi$$
$$\Psi = -2\left(-\nabla^2 - 2E\right)^{-1} V\Psi$$
$$= -2G^*(V\Psi)$$
$$\left(G^* f\right)(r) = \int ds \frac{e^{-k|r-s|}}{4\pi|r-s|} f(s)\ \ in\ 3D\ ;\ k^2 = -2E$$

- Eliminate need for derivative operators and possibly high norm and conditional numbers
- Converge using nonlinear functional fixed point iteration has been developed (2011) for

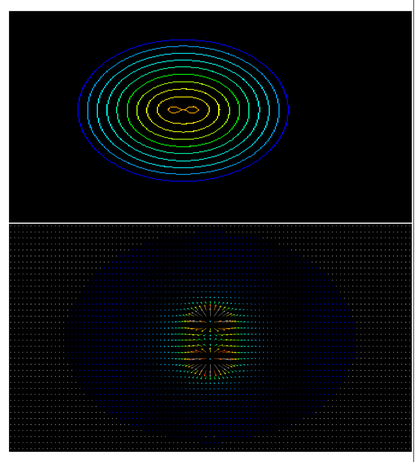
Operations in MADNESS

- Fast Direct Solvers
  - Poisson Solver
  - Bound-state Helmholtz solver
  - Linear and non-linear solvers in compressed wavelet form
  - Non-linear solvers for functions and operators in separated form
  - Application of operators on functions in multiwavelet compressed form and in separated form
  - Fix point iterations and non-linear accelerations
  - Quotient by symmetry group
  - Parallel computating using distributed memory (e.g. ORNL's Cray XT4, ANL's BG/P-port underway, Linux clusters, Apple Macs)

Dynamics of H2+ in Laser

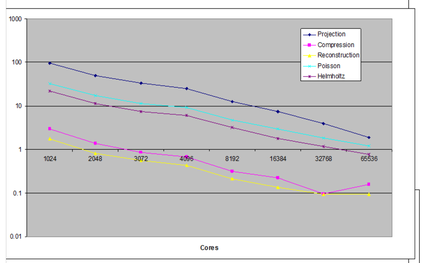
4-D, 3 electron with internuclear coordinates

First simulation with quantum nuclei and non-colinear field



The image is the flux field in a 2-D slice of a 3D simulation of the hydrogen molecular ion in an atto-second laser pulse.

Scaling with System Size Cray XT5



2-particles 6-D Schrodinger's Equation

$$(-\Delta_1 - \Delta_2 + V_1 + V_2 + V_{12})\varphi = E\varphi,$$
$$r = (x_1,\ldots,x_6),$$
$$r1 = (x_1,x_2,x_3), r2 = (x_4,x_5,x_6)$$
$$V_1(r) = 1/r_1$$
$$V_2(r) = 1/r_2$$
$$V_{12}(r) = 1/|r_1 - r_2|$$

Singularities are of hyper-plane type

$$H\Psi(r_1,r_2,\ldots,r_n) = E\Psi(r_1,r_2,\ldots,r_n)$$
$$H = -\tfrac{1}{2}\sum_{i=1,m}\nabla_i^2 - \sum_{\substack{i=1,n\\ \mu=1,N}}\frac{Z_\mu}{|r_i - r_\mu|} + \sum_{\substack{i=1,n\\ j=1,i-1}}\frac{1}{|r_i - r_j|}$$

$$\Psi(r_1,r_2) = e^{u(|r_1-r_2|)}\phi(r_1,r_2)$$

Quantum Monte Carlo calculations

Choose u to eliminate singularity at r_{12}=0

Best to eliminate all hyperplanes r_1=r_2=0 and $r_1 - r_2$=0 with a similiar tranformation.

$$e^{-u}He^{u}\phi = -\frac{1}{2}\Delta_1\phi - \frac{1}{2}\Delta_2\phi - u'\frac{r_1 - r_2}{|r_1 - r_2|}\cdot(\nabla_1\phi - \nabla_2\phi)$$
$$+\left(V - \left((u')^2 + u''\right) + \frac{1}{|r_1 - r_2|}(1 - 2u')\right)\phi$$

Fokker-Planck—Stochastic PDE describing the evolution of particle distribution. For Brownian motion without forcing, we have in 6-d, in r, u, t

$$\partial W/\partial t = \beta\, div_u(Wu) + q\nabla(u^2 W)$$

With Green's function (a la Chandrasekhar)

$$W(u,t;u_0) =$$
$$1/[2q\pi\,(q - e^{-2\beta t})/\beta\,]^{3/2}$$
$$\exp[-\beta\,|u - u_0 e^{-\beta t}|^2/2q(1 - e^{-2\beta t})]$$

Future

- Better and faster way of handling multiparticles, spin-orbit, relativistic terms, Dirac equation, time-dependent DFT and Fokker-Planck equations.
- Explore new algorithms for reducing the number of terms in the separated representation, other representations and GPUs
- Application to non-convolution based operators

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