Multiresolution and Low-Separation Rank Methods for Nuclear DFT

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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
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
- 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.

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>HO Expansion</th>
<th>Multiwavelets 10⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>(exact)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-18.8977, ½⁺</td>
<td>-18.8977</td>
<td>-18.8976</td>
</tr>
<tr>
<td>-0.3205, ½⁺</td>
<td>-0.1748</td>
<td>-0.3205</td>
</tr>
</tbody>
</table>

**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

<table>
<thead>
<tr>
<th>#</th>
<th>Spin</th>
<th>Inverted 2-cosh potential without spin-orbit</th>
<th>Inverted 2-cosh potential with spin-orbit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>HO, N=22</td>
<td>Spline</td>
</tr>
<tr>
<td>9</td>
<td>1/2 +</td>
<td>-1.71590</td>
<td>-1.72467</td>
</tr>
<tr>
<td>10</td>
<td>1/2 -</td>
<td>-1.51146</td>
<td>-1.52621</td>
</tr>
</tbody>
</table>

| Moment n=1 | 20.0 | 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

Preliminary Parallel Performance of MADNESS-NDFT on CRAY-XT3

![Graph showing parallel performance with time in seconds and processors on the x-axis.]
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

\[
\delta = 0.02 \times V_{2 \cosh}(x, y, z)
\]

\[
\lambda = -1
\]

- 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
- Presentations:
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)
Solving the integral equation

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

\[
\left(-\frac{1}{2} \nabla^2 + V\right)\Psi = E\Psi
\]

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

\[
= -2 G^* (V\Psi)
\]

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

*aug-cc-pVDZ geometry, kcal/mol.*

<table>
<thead>
<tr>
<th>Basis</th>
<th>Uncorrected</th>
<th>BSSE</th>
<th>Corrected</th>
</tr>
</thead>
<tbody>
<tr>
<td>cc-pVDZ</td>
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<td>-1.035</td>
<td>-0.471</td>
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<tr>
<td>cc-pVTZ</td>
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<td>-0.387</td>
<td>-0.884</td>
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<tr>
<td>cc-pVQZ</td>
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<td>-0.881</td>
</tr>
<tr>
<td>aug-cc-pVDZ</td>
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<td>-0.698</td>
<td>-1.024</td>
</tr>
<tr>
<td>aug-cc-pVTZ</td>
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<td>-0.193</td>
<td>-0.966</td>
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<tr>
<td>ε=10^{-5}</td>
<td>-0.872</td>
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<tr>
<td>ε=10^{-7}</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>ε=10^{-9}</td>
<td>-0.956</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2-D Slice of 3-D Adaptive Refinement for $H_2$
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 $1.\times 10^{2-k}$, with smoothing
Scaling of MAD++ on 4096 Cu lattice (prelim) on ORNL’s Cray XT-3, 2007