Computational Infrastructure for Nuclear Energy Density Functional Theory

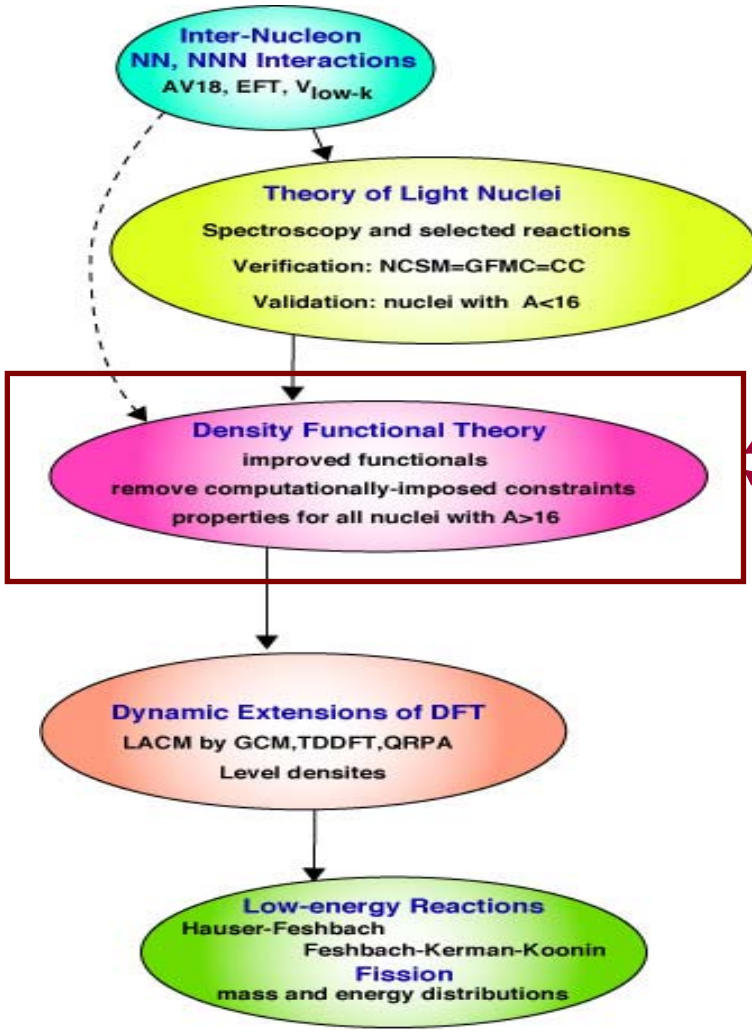
Witek Nazarewicz, Oak Ridge National Laboratory

George Fann, Oak Ridge National Laboratory

Jorge Moré, Argonne National Laboratory

April 17, 2008

The Big Picture



- Nuclear EDF
- Global Properties
- Spectroscopic Quality

- DFT Solvers
- Nonlinear Optimization
- Performance Analysis

UNEDF Researchers

Nuclear Energy
Density Functional Theory

- Witek Nazarewicz
- Mario Stoitsov
- William Shelton
- Jacek Dobaczewski (HFODD)
- Nicolas Schunk (postdoc)
- Carlos Bertulani
- Junchen Pei (postdoc)

Applied Mathematics
Computer Science

- George Fann
- Jorge Moré
- Boyana Norris
- Jason Sarich

Research Issues: Nonlinear Optimization

- What are the best techniques for nonlinear, noisy optimization problems

$$\min \{f(x) : x_L \leq x \leq x_U\}$$

when the gradient ∇f of f is not available and the evaluation of f is computationally intensive (125 CPU days)

- How can we solve systems of n nonlinear equations

$$H(x) = 0$$

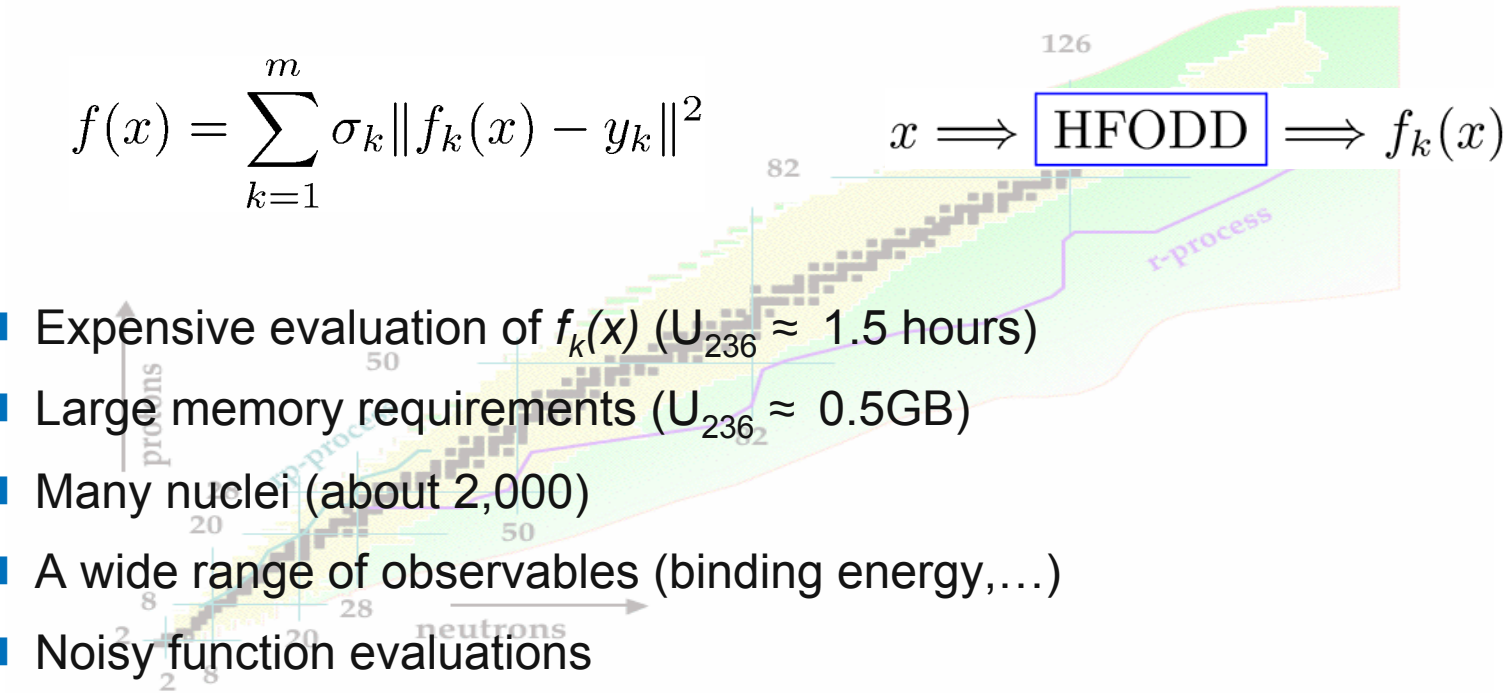
when derivatives are not available and the number of variables n is large?

Parameter Estimation in Nuclear Fission: Challenges

The least-squares approach (χ^2) requires the minimization of

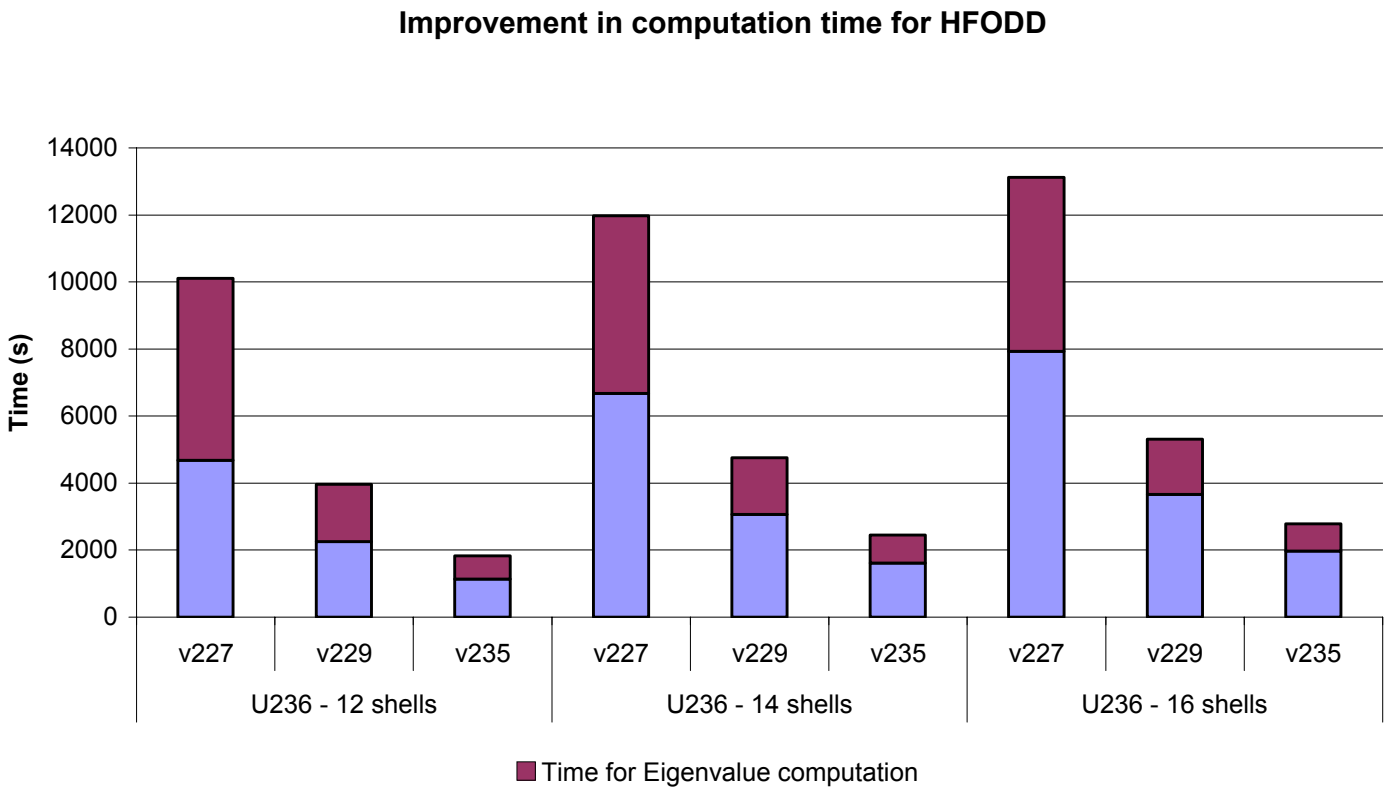
$$f(x) = \sum_{k=1}^{m} \sigma_k \| f_k(x) - y_k \|^2$$

$$x \Longrightarrow \boxed{\text{HFODD}} \Longrightarrow f_k(x)$$

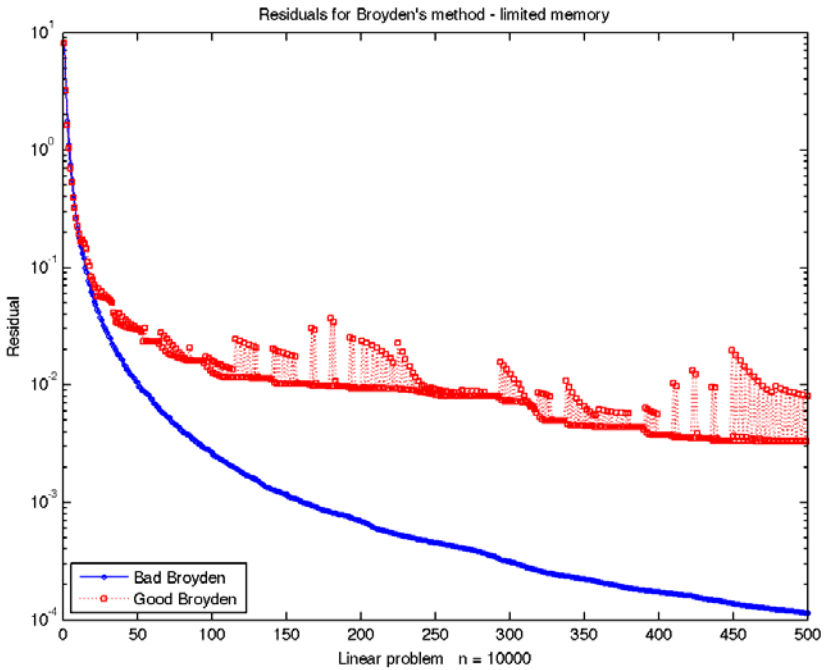


- Expensive evaluation of $f_k(x)$ ($U_{236} \approx$ 1.5 hours)
- Large memory requirements ($U_{236} \approx$ 0.5GB)
- Many nuclei (about 2,000)
- A wide range of observables (binding energy,…)
- Noisy function evaluations
- Lack of derivatives with respect to parameters
- Several minima with different predictive powers

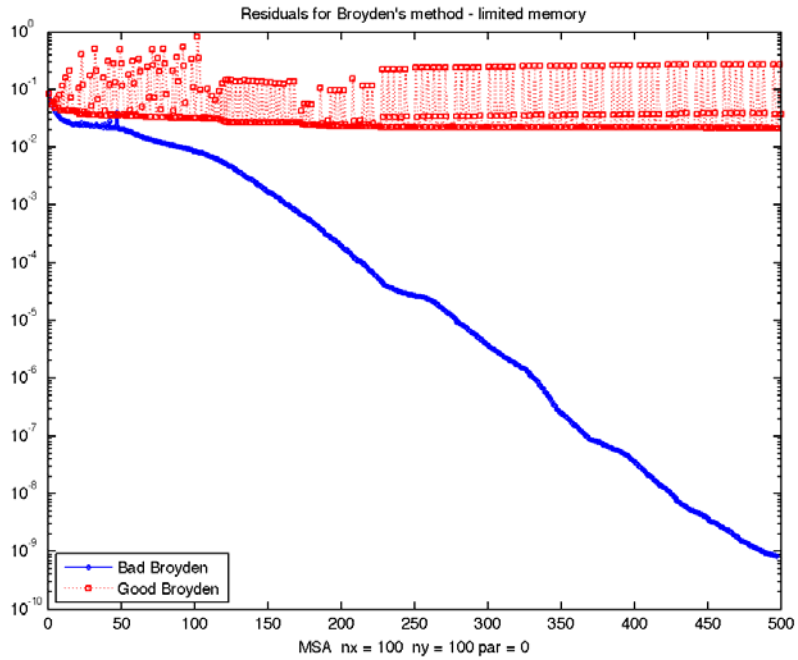
Performance of HFODD with U_{236}



Broyden's Method for Systems of Nonlinear Equations



Linear problem



Nonlinear problem

Compact storage, 10 vector pairs of memory, random starting point

Contributions: Optimization and Performance Analysis

- HFODD majordomo list (January 2007)
- Profile of HFODD using Tuning and Analysis Utilities (TAU)
- Introduction of BLAS (40% computing time reduction)
- NEDFT planning meeting (March 2007)
- Full storage eigenvalue solver (60% computing time reduction)
- NEDFT planning workshop (August 2007)
- Analysis of Broyden's method
- Determination of the Nuclear Energy Functional workshop (January 2008)
- *Optimization in SciDAC Applications*, J. of Physics (2007)
- *Benchmarking derivative-free optimization algorithms*, Preprint (2007)

Future Work

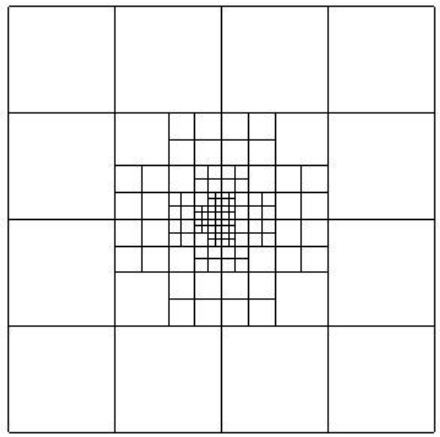
- Year 2
  - Broyden's method for large-scale systems of equations
  - Evaluation of Broyden's method in SCF calculations in HFODD
- Year 3
  - Development and performance of mass-table algorithms in BG
  - Investigation of derivative calculations/sensitivity in HFODD
  - Development of model-based derivative-free algorithms
- Year 4
  - Model-based and geometry-based optimization algorithms for DFT
  - Preliminary investigation of performance on new DFT functionals
- Year 5
  - Fission pathways
  - Performance, evaluation, and validation of new DFT functional

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*
- 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



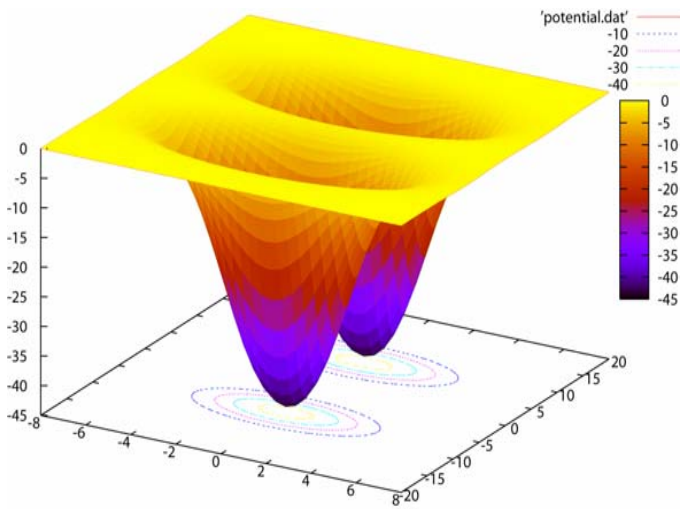
Adaptive support of basis functions. A 2-D slice of a 3-D wavefunction from the inverted two-cosh spin-orbit (SO) case

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.

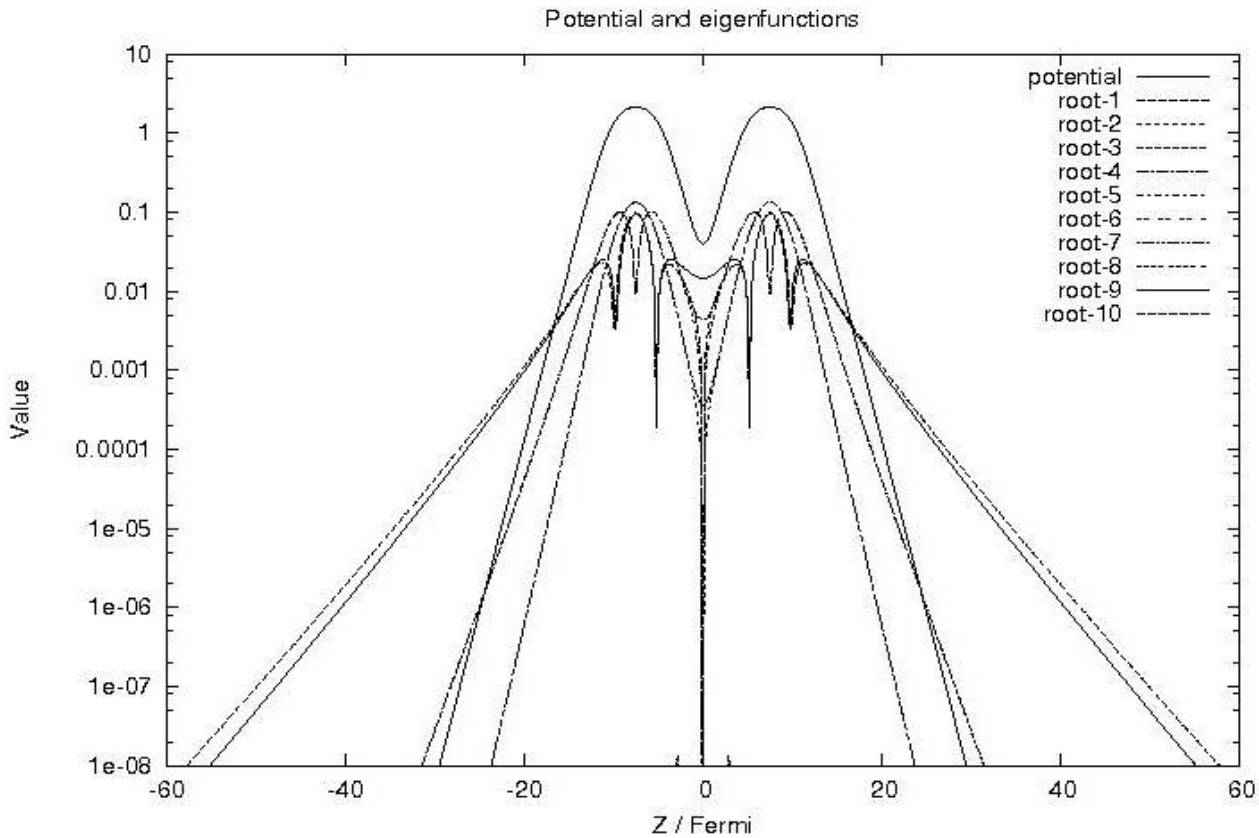
Eigenvalue (exact)	HO Expansion	Multiwavelets 10^{-3}
-39.7400, ½+	-39.7400	-39.7399
-18.8977, ½+	-18.8977	-18.8976
-0.3205, ½+	-0.1748	-0.3205

Poschl-Teller-Ginocchio Potential



Inverted 2-cosh (no SO)

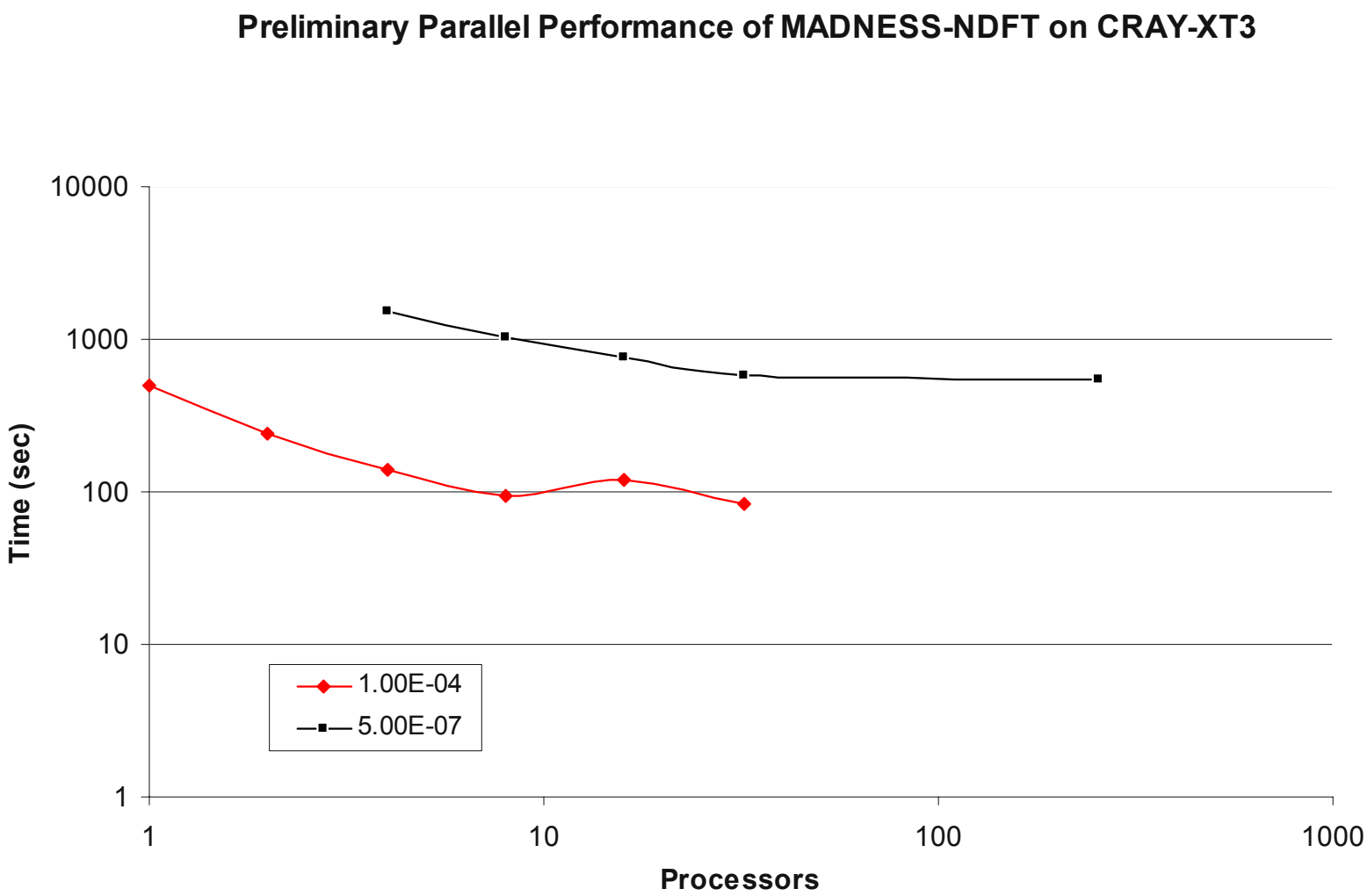
Plot of Potential and Absolute Value of Wave Functions for the 2-cosh Potential



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



Future Work

- Year 2
  - Integration of HO with wavelets methods in 3-D
  - Testing with other examples
  - Conversion 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