UNEDF Workshop
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Broyden's Method for Large Systems of Nonlinear Equations

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Optimization Applications in SciDAC

- Quantum Chemistry
  - Energy minimization
  - Transition states
- Nuclear Physics
  - Nonlinear eigenvalues
  - Parameter estimation
  - Least action pathways
- Accelerator Design
  - Shape optimization
  - Nonlinear eigenvalues
- Groundwater Flow
  - Parameter estimation

TOPS

Towards Optimal Terascale Simulations

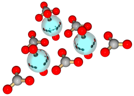
Have optimization technology,
will tackle applications

Toolkit for Advanced Optimization (TAO)

An optimization toolkit for solving large-scale optimization problems on advanced (massively parallel) architectures.

- ◇ Portability, performance, scalability
- ◇ An interface independent of architecture
- ◇ Leverage existing parallel computing infrastructure (PETSc)

TAO (www.mcs.anl.gov/tao)



NWChem, MPQC

- ◇ Source code and documentation
- ◇ Installation instructions, example problems, . . .

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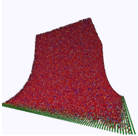
TAO Impact

Selected applications

- Semiconductor modelling
- Magnetic nanostructures
- Subsurface remediation
- Variational surfaces

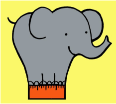


P. Bauman

P. Joshi

Toolkits

- `TADM` - Parameter estimation
- `BUSTER` - Protein structures
- `ELEFANT` - Statistical machine learning



UNEDF: Parameter Estimation in Nuclear Fission

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

- Expensive evaluation of $f_k(x)$ ($U_{236} \approx$ 12 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

UNEDF Research Issues: Nonlinear Optimization

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

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

when the gradient ∇f of f is not available and the evaluation of f is computationally intensive (1,000 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?

Broyden's Method: A Biased Bibliography

- Broyden (1965). Introduced two methods. *...since Method 2 apears to be unsatisfactory in practice ...*
- Gay and Schnabel (1977). Projected updates.
- Gay (1979). Broyden's method for linear systems. Refers to the second method as Broyden's **bad** method.
- Srivasta (1984). Modified Broyden's second method so that only a few vectors of storage of order n are needed.
- Johnson (1988). Modified Srivasta's approach to incorporate additional information from previous iterates.
- Byrd, Nocedal, Schnabel (1994). Compact form.
- Baran, Bulgac, Forbes, Hagen, Nazarewicz, Schunk, Stoitsov (2008). Improvement of Johnson's approach

Systems of Nonlinear Equations

Given a function $f : \mathbb{R}^n \to \mathbb{R}^n$, find a vector x^* that solves the system of nonlinear equations

$$f(x) = 0$$

Notation

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \qquad f(x) = \begin{pmatrix} f_1(x) \\ \vdots \\ f_n(x) \end{pmatrix}$$

The Jacobian matrix is

$$f'(x) = (\partial_1 f(x), \ldots, \partial_n f(x))$$

Broyden's Method 1

Given a sequence of iterates $x_0, x_1, \ldots$, Broyden's method generates approximation to the Jacobian matrix $f'(x_k)$ via

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) s_k^T}{\|s_k\|^2},$$

where the vectors y_k and s_k are defined by

$$y_k = f(x_k + s_k) - f(x_k), \qquad s_k = x_{k+1} - x_k$$

Note that B_{k+1} satisfies the secant equations

$$B_{k+1} s_k = y_k$$

Broyden's Method 2

$$H_{k+1} = H_k + \frac{(s_k - H_k y_k) y_k^T}{\|y_k\|^2}$$

Compact Form

$$H_{k+1} = H_0 + (S_k - H_0 Y_k) N_k^{-1} Y_k^T$$

where

$$[N_k]_{i,j} = \begin{cases} y_i^T y_j & \text{if } i \le j \\ 0 & \text{otherwise} \end{cases}$$

$$S_k = [s_1, ..., s_k], \qquad Y = [y_1, ..., y_k]$$

Broyden's Method 2: Projected Updates

$$H_{k+1} = H_0 + (S_k - H_0 Y_k)\left(Y_k^T Y_k\right)^{-1} Y_k^T$$

where

$$S_k = [s_1, ..., s_k], \qquad Y = [y_1, ..., y_k]$$

Remarks The projection into the space spanned by Y_k is

$$P_k = \left(Y_k^T Y_k\right)^{-1} Y_k^T$$

Note that

$$H_{k+1} Y_k = S_k$$

and thus secant equations from previous iterations are satisfied.

Johnson (1988) method

In our notation, Johnson's method is of the form

$$x_{k+1} = x_k - J_k f(x_k),$$

where J_k depends on constants α, w_0, and w_j for $j = 1, \ldots m$.

Theorem. If $H_0 = -\alpha I$, $w_0 = 0$, and $w_j \equiv 1$, then Johnson's method is the projected Broyden method, that is,

$$J_k = H_0 + (S_k - H_0 Y_k)\left(Y_k^T Y_k\right)^{-1} Y_k^T$$

Implementation for Large Problems: The Main Issues

- Broyden's method 1 or Broyden's method 2?
- How do we globalize Broyden? A line search method

$$x_{k+1} = x_k - \alpha_k H_k f(x_k)?$$

  But the search direction $-H_k f(x_k)$ may not be downhill.
- At each iteration we keep the last $s_1, \ldots, s_m$ and $y_1, \ldots, y_m$. How many vectors of storage should we keep?
- Do we need to re-start? At some point it may be better to throw away all previous information and re-start with the current best iterate x_k and some inverse Hessian H_k.

Computational Experiments: Benchmark Problems

Eight nonlinear variational problems of the form

$$\min \{ V(x) : x \in \mathbb{R}^n \}$$

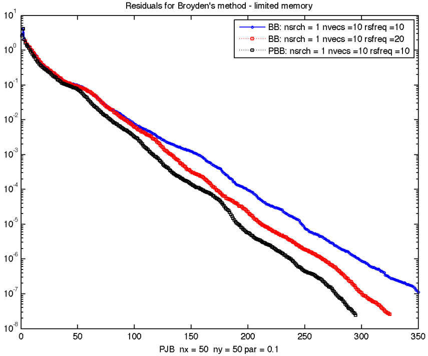
The nonlinear systems are the gradient equations

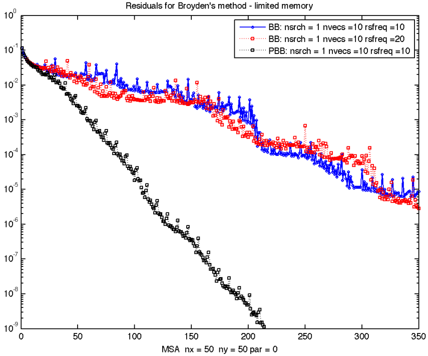
$$f(x) = \nabla V(x)$$

We show results for 4 problems with $n = 2500$ variables.

- PJB. Pressure in a journal bearing. Convex, ill-conditioned
- MSA. Minimal surface area. Convex, ill-conditioned
- ODC. Optimal design. Convex, discontinuos Jacobian $\nabla^2 f$
- GL2. Ginzburg-Landau conductor. Non-convex, ill-conditioned

Computational Experiments: BB or PBB





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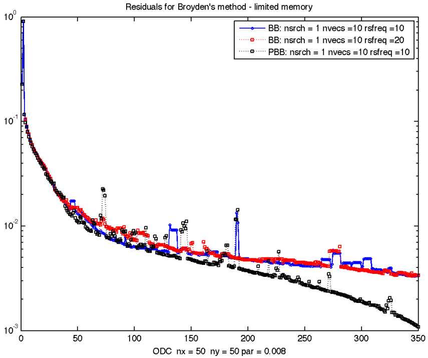

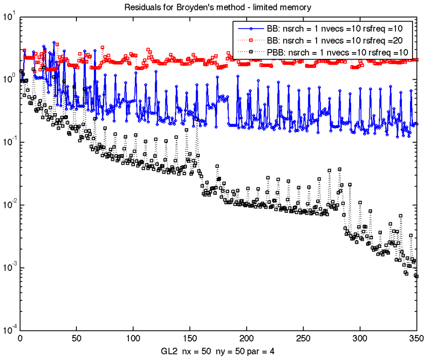

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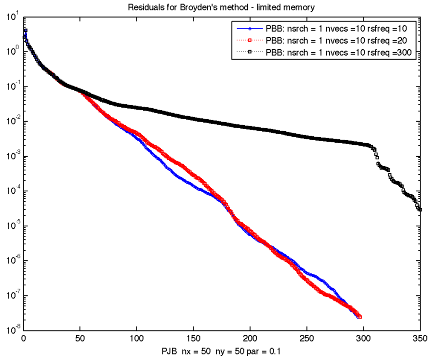
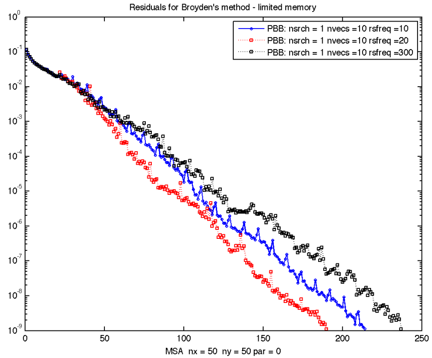
Computational Experiments: Restart Frequency





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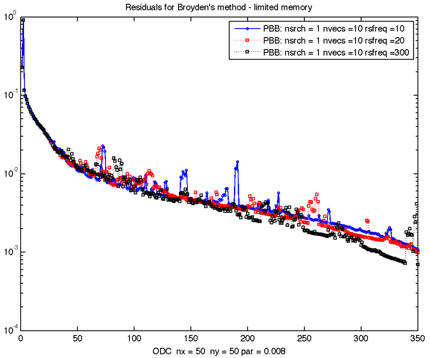

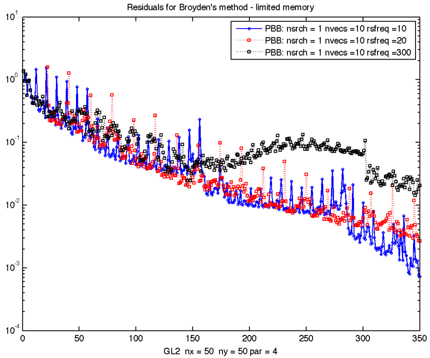

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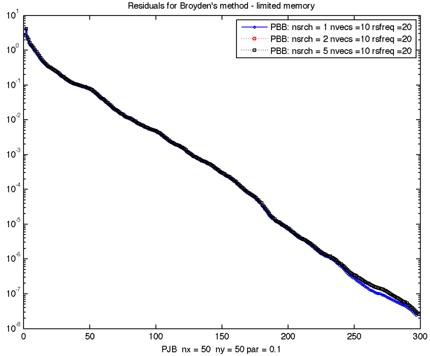
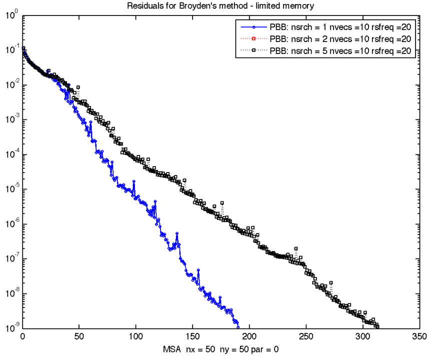
Computational Experiments: Number of Trial Points





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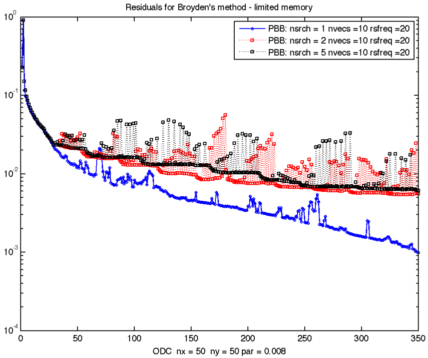
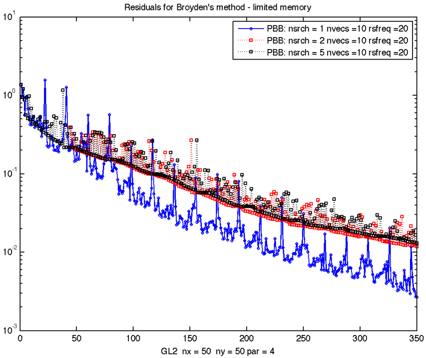
Computational Experiments: Number of Trial Points





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Contributions: Optimization and Performance Analysis

- HFODD majordomo list (January 2007)
- Profile of HFODD using Tuning and Analysis Utilities (TAU)
- HFODD re-structuring (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
- Nuclear Energy Functional workshop (January 2008)
- Optimization in SciDAC Applications, J. of Physics (2007)
- Benchmarking derivative-free optimization algorithms (2007)

Future Work

Year 3

- Development and performance of mass-table algorithms in BG
- Parallelization of HFODD
- Development of model-based derivative-free algorithms

Year 4

- Model and geometry-based optimization algorithms for DFT
- Investigation of performance on new DFT functionals

Year 5

- Fission pathways
- Performance, evaluation, and validation of DFT functional

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