2005 Department Review:

Efficient Large Scale Optimization

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Optimization and Uncertainty Estimation (9211)

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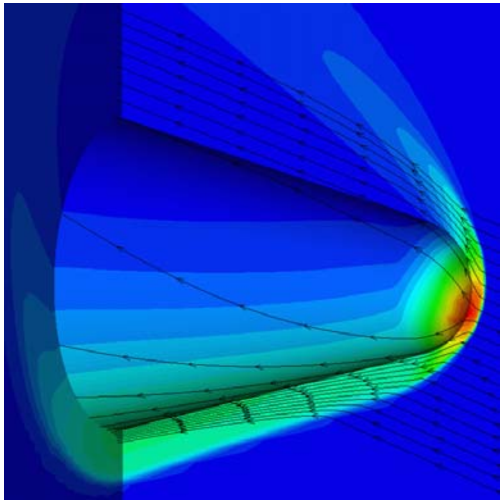
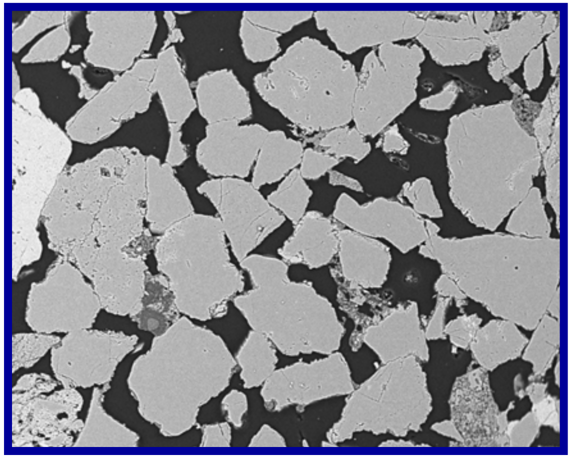
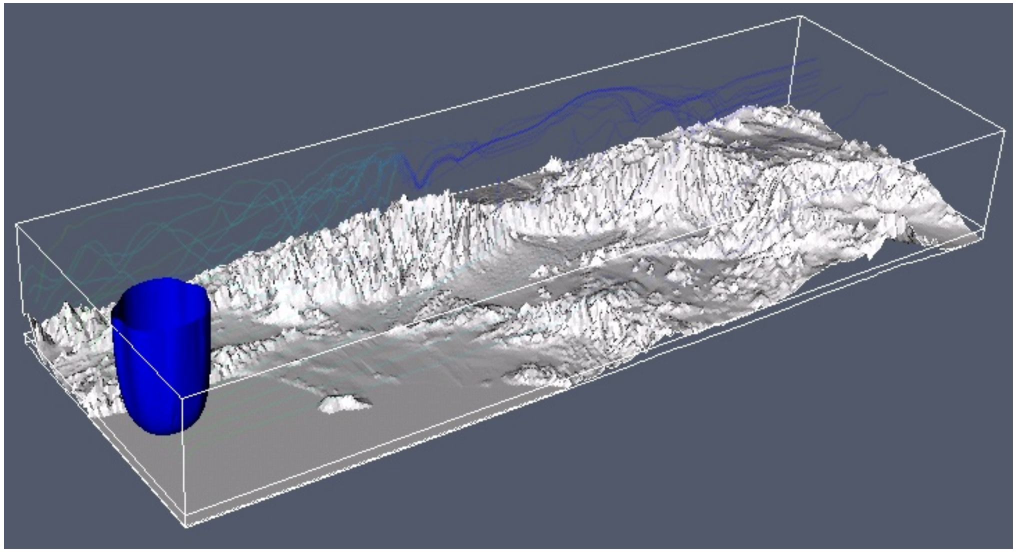
Large Scale Optimization Examples







Mathematical Formulation

Objective function s.t. non-linear contraints

$$\begin{aligned} \min \quad & f(y,u) \\ \text{s.t.} \quad & c(y,u) = 0 \end{aligned}$$

Lagrangian functional

$$L(y,u,\lambda) \equiv f(y,u) + \lambda^T c(y,u)$$

Variations w.r.t. y,u,lambda

$$\begin{aligned} \frac{\partial L}{\partial y} &= \frac{\partial f}{\partial y} + \lambda^T \frac{\partial c}{\partial y} = 0 \\ \frac{\partial L}{\partial u} &= \frac{\partial f}{\partial u} + \lambda^T \frac{\partial c}{\partial u} = 0 \\ \frac{\partial L}{\partial \lambda} &= c(y,u) = 0. \end{aligned}$$

Many Issues:
- Solution mechanism
- Preconditioning
- Inexactness
- software interface
- many inequalities
- etc..

$$\begin{bmatrix} \frac{\partial^2 L}{\partial y^2} & \frac{\partial^2 L}{\partial y \partial u}^T & \frac{\partial c}{\partial y}^T \\ \frac{\partial^2 L}{\partial y \partial u} & \frac{\partial^2 L}{\partial u^2} & \frac{\partial c}{\partial u}^T \\ \frac{\partial c}{\partial y} & \frac{\partial c}{\partial u} & \end{bmatrix} \begin{bmatrix} \delta y \\ \delta u \\ \delta \lambda \end{bmatrix} = - \begin{bmatrix} \frac{\partial L}{\partial y}^T \\ \frac{\partial L}{\partial u}^T \\ c \end{bmatrix}$$

KKT system

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Efficient Large Scale Optimization Technologies

Enabling Technologies

- Reduced Sequential Quadratic Programming (rSQP)
- Full space SQP

Large optimization space

- Automatic differentiation

Exact and efficient derivatives

- Domain decomposition preconditioning (time/space)
- Multigrid preconditioning

Large KKT systems

- Abstract Numerical Algorithms Interfaces – Trilinos/Thyra

Efficient software interfaces

- *Interior point methods*
- *Large scale robust optimization*

Large sets of inequalities and uncertainties

Homeland Security Applications Real Time Efficiency

- Inversion for water networks (Laird, Biegler)
  - Full space, subdomain algorithms
  - Real time inversion for any size networks
  - MIQP reduces uncertainties
- Inversion for internal flows (Shadid, Salinger, Bartlett)
  - Direct sensitivities
  - Offline/online calculations
  - Real time inversion for $O(10^6)$
- Inversion for external flows (Akcelik, Biros, Draganescu, Ghattas, Hill)
  - Reduced Space SQP algorithms
  - Multigrid preconditioning
  - 140 billion KKT unknowns <5 hrs

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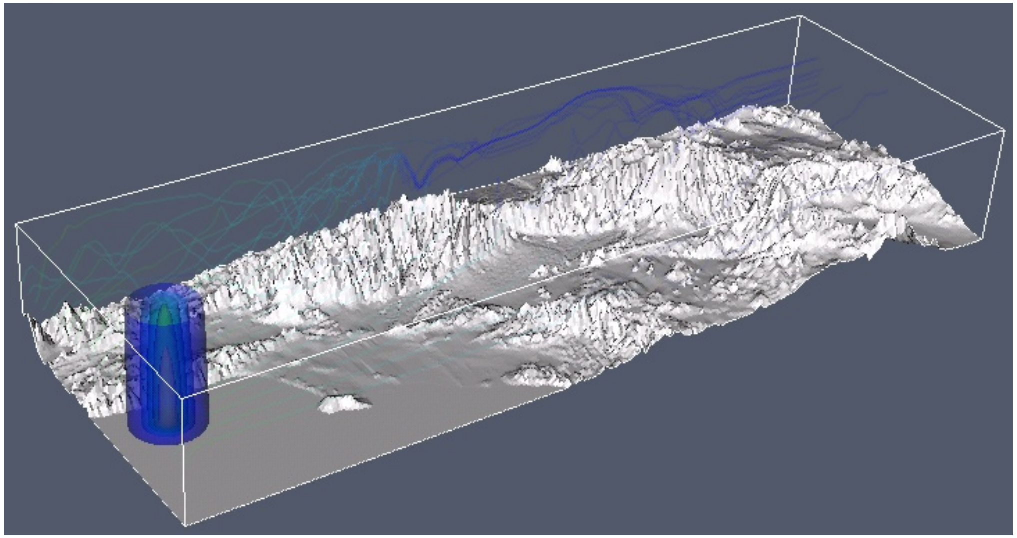
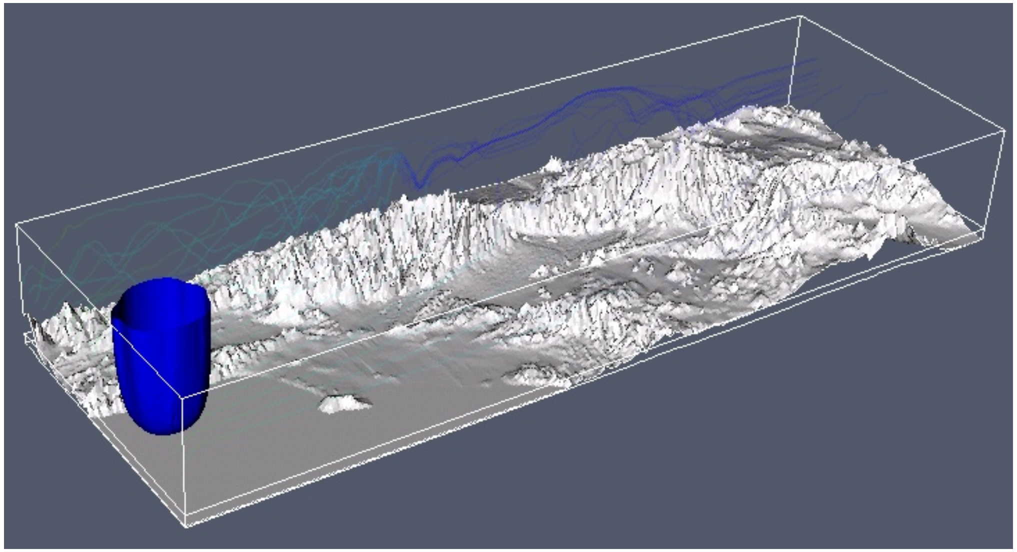
Contamination Identification for External Flows

Typical scenario:
- Greater Los Angeles Basin
- Airflow from mesoscopic weather model (e.g. MM5)
- Sensor readings of contaminant concentration
- Invert for initial condition



"Real" initial condition



Inversion-based reconstruction of initial condition

“Real-time” Inversion for Transport of Contaminant

- Given local velocity field *v* (e.g. from mesoscopic weather model), diffusivity *k*, sensor observations *u**, and a terrain model, estimate initial condition u_0 of a convection-diffusion equation by solving regularized inverse problem:

$$\min_{u,u_0} \sum_j \int_\Omega \int_T (u - u^*)^2 \delta(\boldsymbol{x} - \boldsymbol{x}_j)\, d\boldsymbol{x}\, dt + \frac{\beta}{2} \int_\Omega \boldsymbol{\nabla} u_0 \cdot \boldsymbol{\nabla} u_0 \, d\boldsymbol{x}$$

$$\begin{aligned} \text{subject to} \quad u_t - k\Delta u + \boldsymbol{v} \cdot \boldsymbol{\nabla} u = 0 \;\; &\text{in} \;\; \Omega \times (0,T) \\ u = u_0 \quad &\text{in} \quad \Omega \times \{t = 0\} \\ k\boldsymbol{\nabla} u \cdot \boldsymbol{n} = 0 \quad &\text{on} \quad \Gamma_N \times (0,T) \\ u = 0 \quad &\text{on} \quad \Gamma_D \times (0,T) \end{aligned}$$

- Forward problem can then be solved to predict transport of contaminant

Discrete Optimality System

Discretized optimality system:

$$\begin{bmatrix} \boldsymbol{B}^T\boldsymbol{B} & \boldsymbol{0} & \boldsymbol{A}^T \\ \boldsymbol{0} & \beta\boldsymbol{R} & -\boldsymbol{T}^T \\ \boldsymbol{A} & -\boldsymbol{T} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \\ \boldsymbol{u}_0 \end{bmatrix} = \begin{bmatrix} \boldsymbol{B}^T\boldsymbol{B}\boldsymbol{u}_0^* \\ \boldsymbol{0} \\ \boldsymbol{0} \end{bmatrix}$$

Reduced Hessian system:

$$(\boldsymbol{T}^T\boldsymbol{A}^{-T}\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{T}+\beta\boldsymbol{R})\boldsymbol{u}_0 = -\boldsymbol{T}^T\boldsymbol{A}^{-T}\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{u}_0^*$$

where

$\boldsymbol{A}$: forward operator

$\boldsymbol{A}^T$: adjoint operator

$\boldsymbol{R}$: regularization operator

$\boldsymbol{B}$: observation operator

$\boldsymbol{T}$: extension of Ω into $\Omega \times (0, T)$

- Sensor readings every 3 minutes for 120 minute simulation
- Density of sensor array - 6 £ 6 £ 6, 11 £ 11 £ 11, 21 £ 21 £ 21

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Multigrid Preconditioner for Reduced Hessian

- Unpreconditioned CG is optimal for reduced Hessian – number of iterations is mesh independent
- However, for real-time problems, this is not good enough!
- Problem: need effective preconditioner that does not require H to be explicitly formed
- Standard multigrid smoothers not appropriate
- Appeal to Hackbush/King/Kaltenbacher/Draganescu type multigrid preconditioner for compact operators

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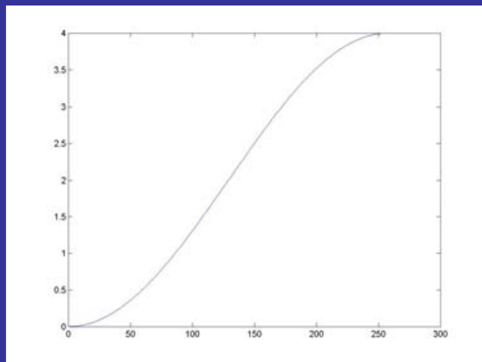
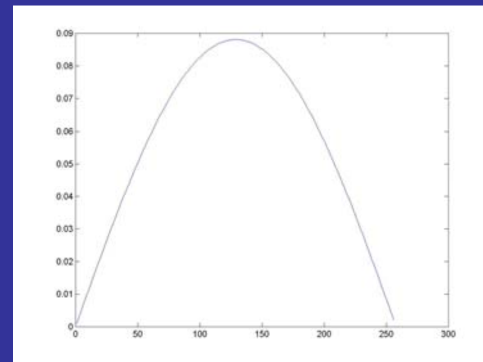
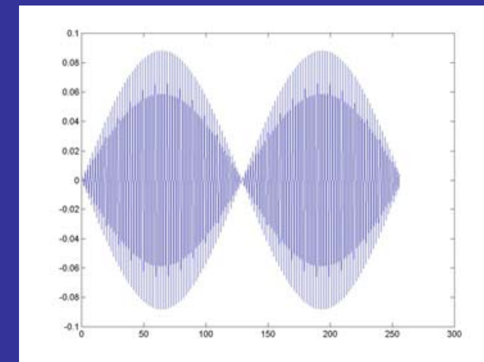
Spectrum of Error for Laplacian vs Reduced Hessian Operator



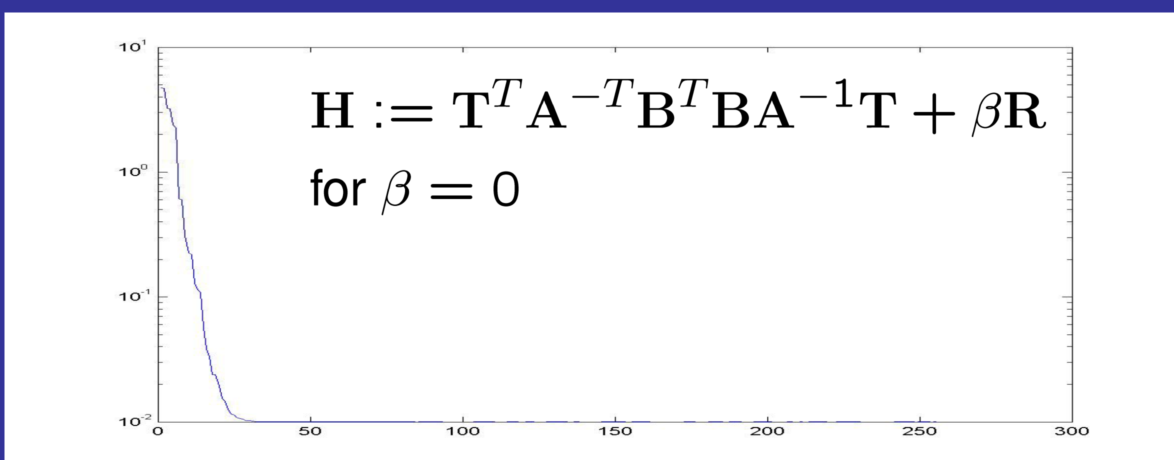
Spectrum of discrete laplacian

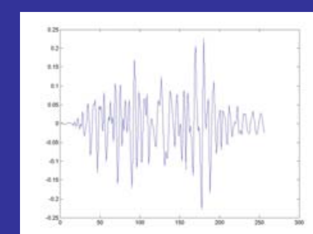


Eigenvector for small eigenvalue

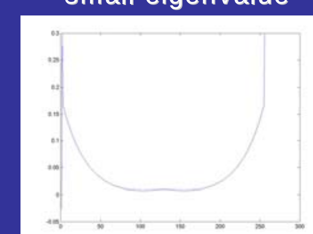


Eigenvectors for large eigenvalue





Eigenvector for small eigenvalue



Eigenvectors for large eigenvalue

Multigrid Preconditioning

Strong smoothing properties of reduced Hessian suggests following preconditioner

$$H_h^{-1} \approx M_h \stackrel{\text{def}}{=} \boxed{\beta^{-1}(I - P_h)} + \boxed{(H_{2h})^{-1} P_h}$$

Resolves high freq
Components in the solution

Resolves low freq
Components in the solution

Recursive preconditioning procedure where preconditioner is solved on the next grid level (2h), until the base level is reached and CG is used as a direct solver..

Parallel Multigrid Performance and Scalability

CPUs	multigrid precond		no preconditioner	
	wallclock (hrs)	parallel efficiency	wallclock (hrs)	parallel efficiency
128	2.22	1.00	5.65	1.00
512	0.76	0.73	1.41	1.00
1024	0.48	0.58	0.74	0.95

Fixed size scalability: 257 x 257 x 257 x 257 space-time grid, 8.7 billion space-time unknowns, 3-level preconditioner, parallelism in space but not time

Grid size	CPUs	multigrid preconditioner		no preconditioner	
		wallclock (hrs)	iterations	wallclock (hrs)	iterations
129^4	16	1.05	8	2.13	23
257^4	128	2.22	6	5.62	23
513^4	1024	4.89	5	—	—

Isogranular scalability: fixed spatial problem size per processor as # of processors increases (largest problem ~140 billion unknowns)`

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Remarks

- Excellent overall scalability (algorithmic + parallel)
- ~17 million parameter inversion problem solved in 29 minutes on 1024 Alpha processors; ~140 billion KKT unknowns solved in <5h on 1K procs
- Overall conclusion is that inversion for very high resolution transport problems can be carried out in time scales sufficiently fast to permit simulation-based response
- Impact: General capability can apply to other large scale optimization problems constrained by dynamical systems, ie control, design, velocity inversion
- Future: implement capability into Trilinos
- However, need reduced model for practical implementations

Summary

FY05 activities:

- IC Reconstuction for external Flows
- Source inversion for water networks, internal facilities
- Reduced order modeling : developed goal oriented model based formulation
- Demain decomposition preconditioners
- Expanded collaborations: CMU, UT, UP, UC, MIT, Brown, Rice
- Papers: 9 Presentations: 4

New activities:

- Large scale robust optimization (workshop Sept, 05)
- Multigrid preconditioning for velocity inversion
- Multiscale algorithms (pending 2 MICS external funding)
- Decontamination using DFT, CDR, ROM and large scale optimization
- Development of interior point methods
- Teach optimization class UNM (fall semester)
- Invited 3 workshops Oberwolfwach, Heidelberg, NSF

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Publications FY05

External Flow

1. Dynamic Data-Driven Inversion For TerraScale Simulations: Real Time Identification of Airborne Contaminants V. Akcelik, G. Biros, A. Draganescu, J. Hill, O Ghattas,, Bart G. van Bloemen Waanders SC05, Seattle, Washington, November, 2005
2. An Optimization Framework for Goal Oriented, Model-Based Reduction of Large Scale Systems, B. Bader, O. Ghattas, B. van Bloemen Waanders, K. Willcox, 44th IEEE Conference on Decisions and Control 2005

Preconditioning of KKT systems:

1. Multigrid Techniques for Inverse Problems Involving Incompressible Flows, A. Dragenescu and B. van Bloemen Waanders, The 15th International Conference on Control and Computer Science, Bucharest May 2005
2. Domain Decomposition Methods for Advection Dominated Linear-Quadratic Elliptic Optimal Control Problems, R.A. Bartlett, M. Heinkenschloss, D. Ridzal, B.G. van Bloemen Waanders, Computer Methods in Applied Mechanics and Engineering (submitted) 2005
3. Domain Decomposition Methods for Advection Dominated Linear-Quadratic Elliptic Optimal Control Problems, R.A. Bartlett, M. Heinkenschloss, D. Ridzal, B.G. van Bloemen Waanders, SAND Report

Water Security:

1. Source Location Inversion and the Effect of Stochastically Varying Demand, Sean A. McKenna, Bart G. van Bloemen Waanders, Carl D. Laird, Steven G. Buchberger, Zhiwei Li, Rob Janke. World Water & Environmental Resources Congress, Anchorage, AL, May 15-19, 2005
2. A Mixed Integer Approach for Obtaining Unique Solutions in Source Inversion of Drinking Water Networks, Carl D. Laird, Lorentz T. Biegler, Bart G. van Bloemen Waanders World Water & Environmental Resources Congress, Anchorage, AL, May 15-19, 2005
3. A Comparison of Navier Stokes and Network Models To Predict Chemical Transport in Municipal Water Distribution Systems, B. van Bloemen Waanders, G. Hammond, J. Shadid, S. Collis, World Water & Environmental Resources Congress, Anchorage, AL, May 15-19, 2005

Large scale sensitivity technologies

1. Sensitivity Technologies for Large Scale Simulation, B. G. van Bloemen Waanders, R. A. Bartlett, S. S. Collis, E.R. Keiter, C.C. Ober, T.M. Smith, V. Akcelik, O. Ghattas, J.C. Hill, M. Berggren, M. Heinkenschloss, L.C. Wilcox. Sandia Report SAND2004-6574, January, 2005