MIPS: A Real-Time Measurement-Inversion-Prediction-Steering Framework for Hazardous Events

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Outline

• Motivation
• MIPS: Measurement-Inversion-Prediction-Steering
• Completed work
  o Massively parallel real-time inversion
• Ongoing work
  o Uncertainty estimation, goal-oriented model reduction
• Future work
  o More complex wind fields and coupling with MM5, uncertainty propagation, optimal steering of sensors
Motivation

• DHS 15 disaster scenarios for emergency planning
• Radiological attack
  o Nuclear detonation (15Ktn)
  o “Dirty Bomb”
• Biological attack (Aerosolized Anthrax)
• Chemical attack
  o Toxic industrial chemicals
  o Nerve, blister agent, chlorine tank explosion
• Natural disasters
  o Hurricanes
Motivation

- 9 cases involving airborne contamination event
- Response
  - Early detection, invert for initial conditions
  - Prediction of transport
  - Sensor steering/uncertainty steering

NYT, March 16, 2005
Typical scenario

- Greater Los Angeles Basin
- Wind from mesoscale models (MM5)
- Sparse sensor readings of concentration
- Inversion for initial condition
MIPS: Measurement, inversion, prediction, steering

- **Measurement**
  - First response: inversion with reduced order model to guide first response teams

- **Inversion**
  - Sensor-data-driven estimation of initial conditions

- **Prediction**
  - Statistical estimation of uncertainty, propagated to future predictions

- **Steering**
  - Sensor steering to minimize uncertainty of prediction
Continual application of MIPS framework

Second-to-minutes decision-making scale
  o Reduced order models (generated by precomputation)
    inversion, prediction, steering

  • Minutes-to-hours decision-making scale
    o High-fidelity, high-resolution PDEs
      Inversion, prediction, steering
Mathematical formulation

• Given wind $v$, diffusivity $k$, observations $u^*$, and a terrain model, estimate initial condition $u_0$:

$$
\min_{u,u_0} \sum_j \int_{\Omega} \int_T (u - u^*)^2 \delta(x - x_j) \, dx \, dt + \frac{\beta}{2} \int_{\Omega} u_0^2 \, dx
$$

subject to

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

• Then forward problem can be used to predict transport contaminant
Inversion example

Inversion
Reconstruction

“Real” initial condition
Inversion example – comparison over time
Optimality conditions – PDE form

State equation:

\[ u_t - k \Delta u + v \cdot \nabla u = 0 \text{ in } \Omega \times (0, T) \]
\[ u = u_0 \text{ in } \Omega \times \{t = 0\} \]
\[ k \nabla u \cdot \mathbf{n} = 0 \text{ on } \Gamma_N \times (0, T) \]
\[ u = 0 \text{ on } \Gamma_D \times (0, T) \]

Adjoint equation:

\[ -p_t - k \Delta p - \nabla \cdot (vp) = - \sum_j (u - u^*) \delta(x - x_j) \text{ in } \Omega \times (0, T) \]
\[ p = 0 \text{ in } \Omega \times \{t = T\} \]
\[ k \nabla p \cdot \mathbf{n} = 0 \text{ on } \Gamma_N \times (0, T) \]
\[ p = 0 \text{ on } \Gamma_D \times (0, T) \]

Inverse equation:

\[ -\beta u_0 - p|_{t=0} = 0 \text{ in } \Omega \]
Optimality conditions – operator form

Discretized optimality system:

\[
\begin{bmatrix}
B^T B & 0 & A^T \\
0 & \beta R & -T^T \\
A & -T & 0
\end{bmatrix}
\begin{bmatrix}
u \\
u_0 \\
p
\end{bmatrix}
= 
\begin{bmatrix}
B^T B u^* \\
0 \\
0
\end{bmatrix}
\]

Reduced Hessian system:

\[(T^T A^{-T} B^T B A^{-1} T + \beta R) u_0 = -T^T A^{-T} B^T B u^*
\]

where

- \(A\): forward operator
- \(A^T\): adjoint operator
- \(R\): regularization operator
- \(B\): observation operator
- \(T\): extension of \(\Omega\) into \(\Omega \times (0, T)\)
Motivation for reduced space CG solver

At iteration $k$, CG solves the weighted least squares problem:

$$
\min_{P_k} ||e_k|| = \sum_i P_k[\lambda_i]^2 \xi_i^2 \lambda_i
$$

where $P_k$ is polynomial of order $k$ and

$$
e_0 = \sum_i \xi_i v_i, \quad Av_i = \lambda_i v_i, \quad i = 1, \ldots, N
$$
Motivation for reduced space CG solver

\[ H := T^T A^{-T} B^T B A^{-1} T + \beta R \]
for \( \beta = 0 \)

Inverse operator

Smooth eigenvector

Rough eigenvector
Multigrid acceleration

• Problems with single level solver
  o Algorithmic scalability ( # of Newton/QN iterations)
  o Global convergence
    Single grid

• Multilevel acceleration
  o Grid continuation
  o Nonlinear Multigrid: full approximation scheme
Full Multigrid

- Restriction
- Interpolation
- High-order Interpolation
Related work on multigrid

Multigrid for elliptic PDEs
  o Brandt, Hackbusch
  o *Standard theory doesn’t apply to Fredholm-type equations* (typical in optimization)

• Multigrid for optimization
  o Ascher & Haber & Oldenburg, Borzi, Borzi & Kunisch, Borzi & Griesse, Chavent, Dreyer & Maar & Schultz, Draganescu, Lewis & Nash, Kaltenbacher, King, Ta’asan, Tau & Xu, Vogel

• Large-scale parallel multigrid/nested iteration
  o Akcelic, Biros & Ghattas, Akcelic et al.
Multigrid preconditioner for reduced Hessian

- Unpreconditioned (or $(\beta R)^{-1}$ preconditioned) CG is optimal for reduced Hessian – number of iterations is mesh independent
- However, for real time problems, this is not good enough – need to reduce constant!
- Problem: need effective preconditioner that does not require $H$ to be explicitly formed
- Appropriate smoothing
2 level multigrid preconditioner

- **Spectral analysis:** (Draganescu, 2004):

\[ H_h^{-1} \approx M_h \overset{\text{def}}{=} \beta^{-1}(I - P_h) + (H_{2h})^{-1}P_h \]

where \( P_h : V_h \rightarrow V_{2h} \) is the \( L^2 \)-orthogonal projection.

- \( \beta^{-1}(I - P_h) \) filters out high frequencies (smoother)

- Recursion \( \rightarrow \) multilevel preconditioner
Reduced Hessian spectra
Discretization/solver details

• Wind: laminar Navier-Stokes
• Solver: Matrix-free conjugate CG on reduced Hessian
  o MatVec(): 1 forward + 1 adjoint
• Forward/adjoint discretization:
  o SUPG/P1 (space), Crank-Nicolson (time)
  o Additive Schwarz-preconditioned GMRES
• No checkpointing
• PETSc (Argonne) implementation
Parallel multigrid performance and scalability on PSC EV68 AlphaCluster

**Fixed size** scalability: $257^4$ space-time
~9 billion unknowns 3-level MG

<table>
<thead>
<tr>
<th>CPUs</th>
<th>multigrid preconditioner</th>
<th>no preconditioner</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>wallclock (hrs)</td>
<td>parallel efficiency</td>
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<td>512</td>
<td>0.76</td>
<td>0.73</td>
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<td>1024</td>
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<td>0.58</td>
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**Isogranular** scalability (fixed size/CPU)
~140 billion unknowns for max size, 3 level MG

<table>
<thead>
<tr>
<th>Grid size</th>
<th>CPUs</th>
<th>multigrid preconditioner</th>
<th>no preconditioner</th>
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<tbody>
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<td></td>
<td>wallclock (hrs)</td>
<td>iterations</td>
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<td>$257^4$</td>
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<td>2.22</td>
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<tr>
<td>$513^4$</td>
<td>1024</td>
<td>4.89</td>
<td>5</td>
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</table>
LA Basin example details

- Topography: USGS GTOPO30 digital elevation (1 km resolution)
- LA Basin: 360 km x 120 km x 5 km
  - 1 km horizontal grid size (max elevation = 3.5 km)
- Topography-conforming logically-rectangular split-hex-based linear tetrahedral mesh
  - 361 \times 121 \times 21 = 917,301 grid points
  - \frac{1}{4} 74M total space-time variables
- Gaussian-shaped plume:
  - \( u_0 = 20 \exp(-0.04|x-x_c|) \)
  - centered at \( x_c = (120,60,0) \) km
- Inflow:
  - \( v_{\text{max}}(z/(5.0-z_{\text{surface}}))^{0.1} \)
  - \( v_{\text{max}} = 30 \text{ km/hr} \)
- Sensors: every 3 minutes for 120 minute simulation
- 64 processors of AlphaCluster at PSC
Numerical studies of inversion sensitivity

- Density of sensor array
  - \(6 \leq 6 \leq 6, 11 \leq 11 \leq 11, 21 \leq 21 \leq 21\)
- Regularization parameter
  - \(\beta = 1, 0.1, 0.01, 0.001\)
- Peclet number
  - \(k = 0.05, 0.1, 0.2, 0.4\)
  - i.e. \(Pe = 10, 5, 2.5, 1.25\)
- Noise level of observations
  - \(\eta = 0\%, 5\%, 10\%\)
Sensitivity to sensor array density

6 × 6 × 6 Sensor Array  11 × 11 × 11 Sensor Array

21 × 21 × 21 Sensor Array  Target Concentration
## Sensitivity to sensors

<table>
<thead>
<tr>
<th>sensor array</th>
<th>$\frac{|u_{\text{target}} - u_{\text{predicted}}|<em>2}{|u</em>{\text{target}}|_2}$</th>
<th>$\frac{|u_{\text{target}} - u_{\text{predicted}}|<em>\infty}{|u</em>{\text{target}}|_\infty}$</th>
<th>time</th>
<th>iterations</th>
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<tbody>
<tr>
<td>$6 \times 6 \times 6$</td>
<td>0.7925</td>
<td>0.9800</td>
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<td>$11 \times 11 \times 11$</td>
<td>0.4953</td>
<td>0.8700</td>
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Sensitivity to regularization

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$|e|_{L_2}$</th>
<th>$|e|_{\infty}$</th>
<th>time</th>
<th>iterations</th>
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<tbody>
<tr>
<td>1</td>
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<tr>
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<td>1.67e+01</td>
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<td>1078</td>
</tr>
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</table>
Sensitivity to diffusion coefficient

<table>
<thead>
<tr>
<th>diffusion coefficient</th>
<th>$| e |_2$</th>
<th>$| e |_\infty$</th>
<th>time</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
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<td>0.05</td>
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<td>1.74e+01</td>
<td>2:18:39.94</td>
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<tr>
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<td>1.91e+01</td>
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<td>275</td>
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</table>
# Sensitivity to noise

<table>
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<tr>
<th>Noise</th>
<th>$|e|_L^2$</th>
<th>$|e|_\infty$</th>
<th>time</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.1077e+02</td>
<td>1.74e+01</td>
<td>2:20:10.29</td>
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<tr>
<td>5</td>
<td>2.1167e+02</td>
<td>1.74e+01</td>
<td>2:40:24.02</td>
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<tr>
<td>10</td>
<td>2.1278e+02</td>
<td>1.75e+01</td>
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<td>581</td>
</tr>
</tbody>
</table>
Summary of completed work

- Simplified model of atmospheric transport
  - Simple wind, no deposition, no chemical reactions
- PETSc based implementation
- Scalability of parallel multigrid preconditioner
- ~17 million parameter inversion problem:
  - 29 minutes on 1024 Alpha processors
- ~140 billion KKT unknowns solved in <5h on 1K procs
  - Parallel systems with 10-100X # of 10X faster processors in use
- **achieved real-time high-resolution inversion**
  - (based on simplified “weather” model)
Ongoing and future work

- Estimate/propagate uncertainty in initial conditions
  - Principal eigenvectors of inverse Hessian approximation of the covariance provide modes of uncertainty
- Reduced order models for rapid response
  - Need reduced models that can handle large initial condition spaces
- Steer sensors to new locations to reduce uncertainty
- Wind velocity from weather model is great source of uncertainty invert for velocity field from sensor data and weather model
  - Turbulent wind fields, couple with MM5, nonlinear inverse problem
Acknowledgments

- DOE: TOPS: Terascale Optimal simulations
  - www.tops-scidac.org
- CSRI Sandia
- NSF ITR, DDDAS
- PSC
- PETSc
Global optimum: Island of Santorini