Dynamic data-driven inversion for terascale simulations:

Real-time identification of airborne contaminants

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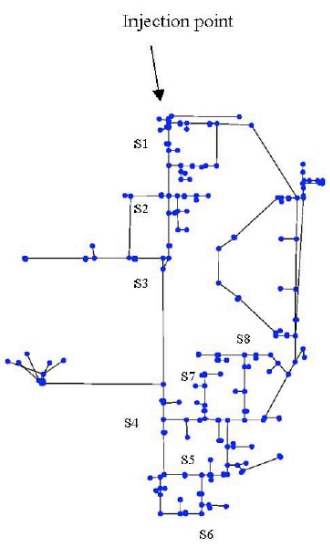
Real time optimization for dynamic inversion & control

DDDAs: MIPS: A Real-Time Measurement –Inversion–Prediction–Steering Framework for HazardousEvents

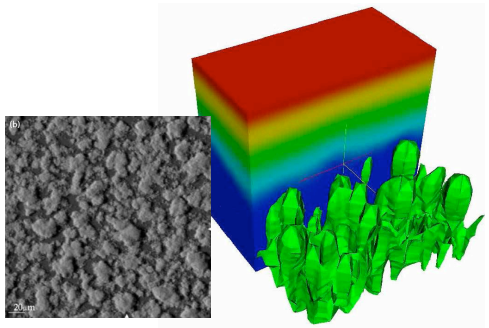
Overview

- **Definition:** An *inverse problem* consists of using the results of actual observations to infer the values of the parameters characterizing the system under investigation.



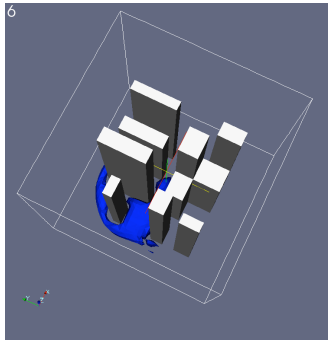
Water Distribution Systems

- *Initial condition inversion*



Computational Biology

- *Material property inversion*



Identification of Airborne Contaminants

- *Initial condition inversion*

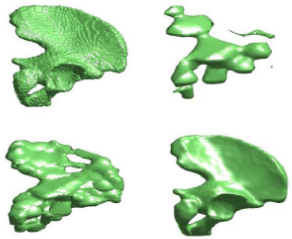
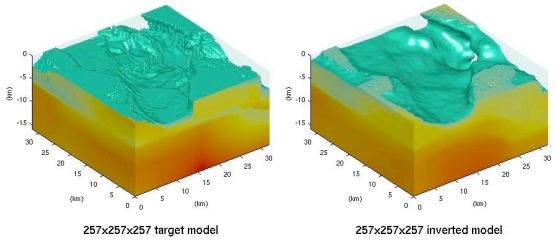


Image Reconstruction

- *Inverse wave-propagation*

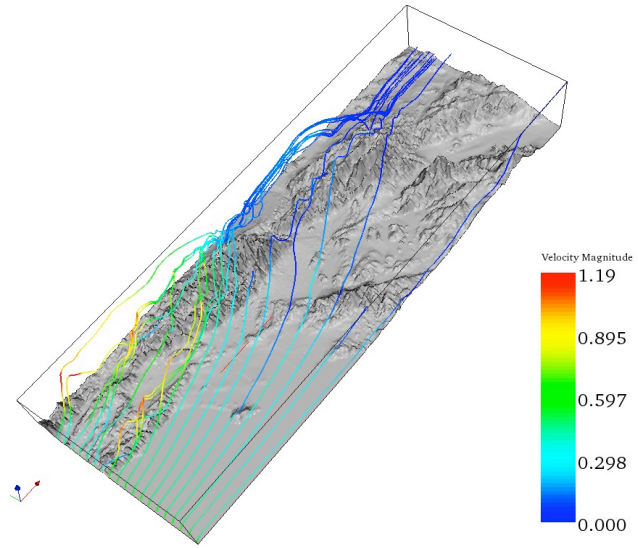


Geologic Properties

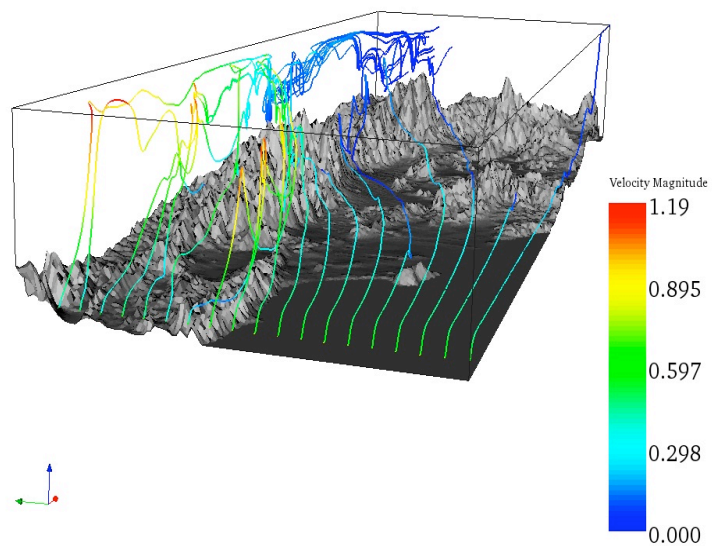
- *Inverse elastic wave propagation*

Scenario

- Class of real-time inversion problems that can be formulated as PDE -constrained optimization problems
  - Emergency response, hazard assessment, structural health monitoring, treaty verification, storm forecasting, image -driven surgery, process control, geophysical exploration, etc.



- Typical scenario
  - Greater Los Angeles Basin
  - Wind from mesoscale models (MM5)
  - Sparse sensor readings of concentration
  - Inversion for initial contaminant location



Motivation

- **The Problem:** Identify the source of the airborne contaminant from sparse sensor measurements

. . . or more generally

Identify *X* from sparse observations

- **Why?**
  - Localizing the contaminant source helps to contain it and mitigate further contamination
  - Improved predictions helps organize evacuation efforts and allocate resources

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Motivation

- **The Problem:** Identify the source of the airborne contaminant from sparse sensor measurements

- **Some Assumptions:**
  - Contaminant is transported by both convection and diffusion
  - Diffusion coefficient is known
  - Velocity field (i.e. winds) in convection operator are exactly known and static

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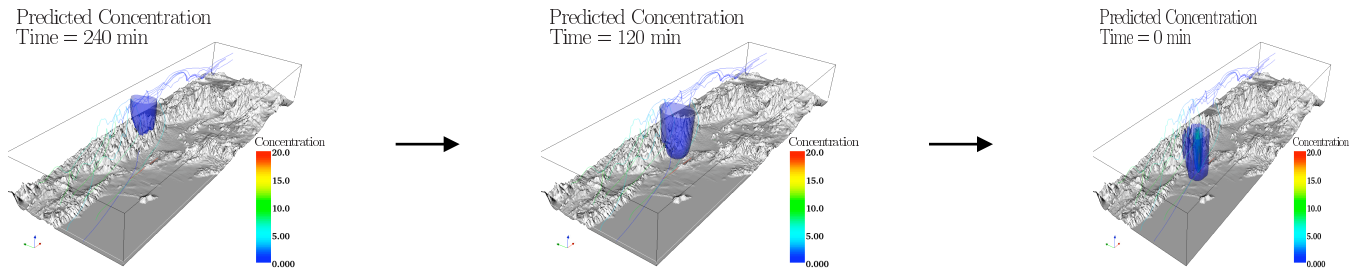
Naïve Solution Approach

- **Potential "Solution":** Run backwards in time



- **Numerical Challenge:** Problem is *ill-posed*
  - The system could be under-determined
  - Solution depends on *discrete* measurements
  - *Solution sensitive to changes in measurements*

  - Well-posedness
    - The problem has a unique solution
    - Small perturbations in the given data yield nearby results

Problem Formulation

- **The Solution:** Formulate this real-time *inversion* problem as a constrained optimization problem

$$
\begin{aligned}
\min_{u,d} \quad & \mathcal{J}(u,d) \\
\text{s.t.} \quad & c_i(u,d) = 0 \qquad i \in \mathcal{E} \\
& h_j(u,d) \geq 0 \qquad j \in \mathcal{I}
\end{aligned}
$$

where the decision variables d are inversion parameters.

Problem Formulation: Source Inversion

- **Problem:** Identify the source of *X* from sparse observations

$$\min_{u,u_0} \ \frac{1}{2}\sum_j \int_\Omega \int_T (u-u^*)^2 \delta(\boldsymbol{x}-\boldsymbol{x}_j)\, d\boldsymbol{x}\, dt + \underbrace{\frac{\beta}{2}\int_\Omega u_0^2\, d\boldsymbol{x}}$$

$$\text{s.t. } c(u,u_0) = 0$$

- **Numerical Challenge:** Optimization problem is also *ill-posed* and requires regularization
  - Solution basin is flat (i.e. many near-solutions close to the minima)
  - **Result:**
    - Good recovery of low frequency components of the solution
    - But, bad recovery of high frequency components

Physical Constraints

- Estimate the initial condition u_0 by solving the inverse problem

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

subject to $u_t - k\Delta u + \boldsymbol{v}\cdot\boldsymbol{\nabla} u = 0$ in $\Omega \times (0,T)$

$$u = u_0 \quad \text{in} \quad \Omega \times \{t=0\}$$

$$k\boldsymbol{\nabla} u \cdot \boldsymbol{n} = 0 \quad \text{on} \quad \Gamma_N \times (0,T)$$

$$u = 0 \quad \text{on} \quad \Gamma_D \times (0,T)$$

Constraints are convection-diffusion transport

given

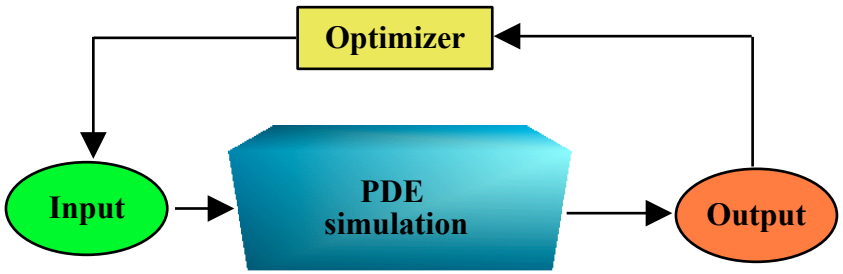
$\boldsymbol{v}$ local velocity field

k diffusion coefficient

u^* sensor observations in space and time

Computational Challenges

- Rapid response is required
  - Variable fidelity models
  - Reduced order modeling



Nested Analysis and Design

Advantages:

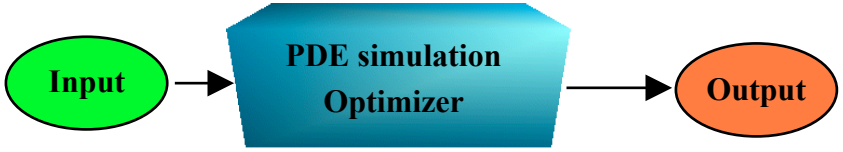
- Requires little change to forward simulation code

Disadvantages:

- Expensive for large design spaces

Computational Challenges

- Rapid response is required
  - Variable fidelity models
  - Reduced order modeling
  - *Fast solution of the optimality conditions via parallelism*



Simultaneous Analysis and Design

Advantages:

- Better scalability to large design spaces
- Computationally efficient

Disadvantage:

- Expensive in development time

KKT System

- The Lagrangian function, a linear combination of the objective function and the constraints, is

$$L(u, \lambda) \equiv \mathcal{J}(u) + \lambda^T c(u)$$

- The point $\widehat{u}$ is a *local minimum* of this problem if there exists *Lagrange multipliers* $\widehat{\lambda}$ such that
  - First-order Karush-Kuhn-Tucker (KKT) conditions are satisfied

$$\begin{aligned} \nabla_u L(\widehat{u}, \widehat{\lambda}) &= 0 \\ c(\widehat{u}) &= 0 \end{aligned}$$

The gradient of the Lagrangian function is zero

  - Second-order KKT conditions are satisfied

$$w^T \nabla_{uu} L(\widehat{u}, \widehat{\lambda}) w > 0$$

Positive curvature indicates a minimum

KKT System: Source Inversion

- **Optimality Conditions: (1st order)**

$$\nabla_u L(u, u_0, \lambda) = 0 \qquad \text{“Adjoint” equation}$$

$$\nabla_{u_0} L(u, u_0, \lambda) = 0 \qquad \text{“Inverse” equation}$$

$$c(u, u_0) = 0 \qquad \text{“State” equation}$$

- **Goal:** Solve this system of equations for an initial condition u_0
- **Numerical Challenges:**
  - Size of the *parameter set* u_0 increases with increasing problem resolution
  - Requires numerous, repeated forward simulations
  - A boundary-value problem in space-time

Computational Challenges

- **Solutions:**
  - *Adjoint Method*
    - Allows computation of the gradient of the cost functional at the cost of two forward solves, *independent* of the number of parameters
  - *Reduced Space Method*
    - Reduces the boundary-value problem in space and time to only space
  - *Matrix-Free Method*
    - Computes the action of the Reduced Hessian, a *very large* linear system, on a vector at the cost of two forward solves
  - *Multigrid Preconditioning and Parallelism*

Numerical Challenges

- **Optimality Conditions:** *(Adjoint Method)*

State equation:

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

Adjoint equation:

$$
\begin{aligned}
-\lambda_t - k\Delta\lambda - \boldsymbol{\nabla}\cdot(\boldsymbol{v}\lambda) &= -\sum_j (u-u^*)\delta(\boldsymbol{x}-\boldsymbol{x}_j) \text{ in } \Omega\times(0,T)\\
\lambda &= 0 \quad \text{in} \quad \Omega\times\{t=T\}\\
k\boldsymbol{\nabla}\lambda\cdot\boldsymbol{n} &= 0 \quad \text{on} \quad \Gamma_N\times(0,T)\\
\lambda &= 0 \quad \text{on} \quad \Gamma_D\times(0,T)
\end{aligned}
$$

Inverse equation:

$$
-\beta u_0 - \lambda|_{t=0} = 0 \text{ in } \Omega
$$

Numerical Challenges

- In compact notation,

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

Large, but sparse

this reduces to (*Reduced Space Method)*

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

Small, but dense

where

$\boldsymbol{A}$: forward operator

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

$\boldsymbol{R}$: regularization operator

$\boldsymbol{B}$: observation operator

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

Numerical Challenges

- **Goal:** Solve the system

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

  - **Challenge:** Impossible to form Reduced Hessian explicitly due to size of the problem
  - **Solution:** *(Matrix-Free Method)* Compute its action on a vector (*never* form it explicitly)

Numerical Challenges

- **Goal:** Solve the system

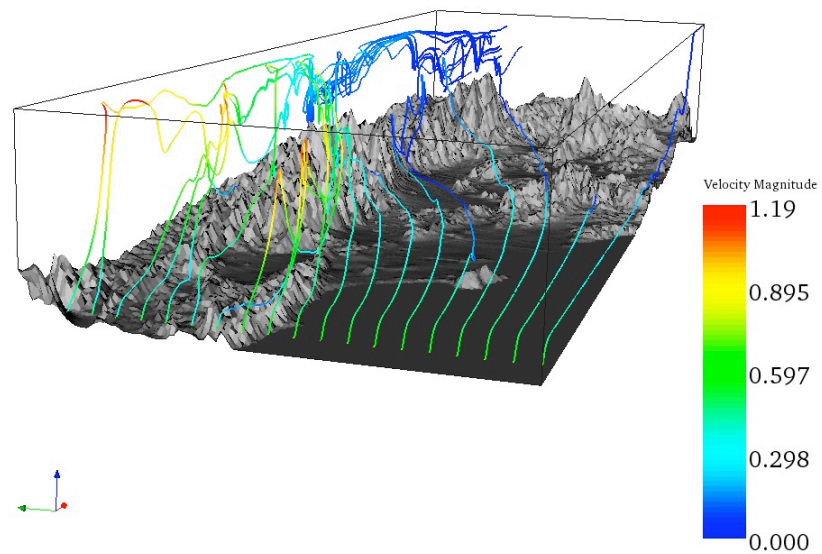
$$(\boldsymbol{T}^T\boldsymbol{A}^{-T}\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{T}+\beta\boldsymbol{R})\boldsymbol{u}_0 = -\boldsymbol{T}^T\boldsymbol{A}^{-T}\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{u}^*$$

  - **Challenge:** Fast computation of the solution
    - Standard iterative methods will solve the problem (Conjugate Gradient), but still not feasible for predictive capabilities
  - **Solution:** Reduced Hessian is well-conditioned for positive beta, but we can do better with special-purpose *Multigrid Preconditioning*

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	—	—

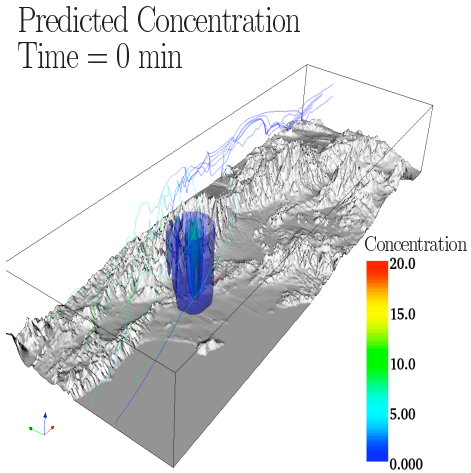
Numerical Results

- Discretization/Solver Details
  - Velocity field pre-computed by laminar Navier-Stokes code
  - Forward/adjoint transport equation discretized by SUPG/P1 in space, Crank-Nicolson in time
  - Data storage and management avoided
    - Typically for a non-linear problem, you need the entire state to compute the adjoints
    - States only needed at the sensor locations
  - PETSc library (Argonne) for parallel implementation



Domain Details

- Surface elevations obtained from USGS GTOPO30 digital elevation model at 1 km resolution
- Topography-conforming logically-rectangular split-hex-based linear tetrahedral mesh
  - 361x121x21 = 917,301 grid points



- Gaussian-shaped plume:

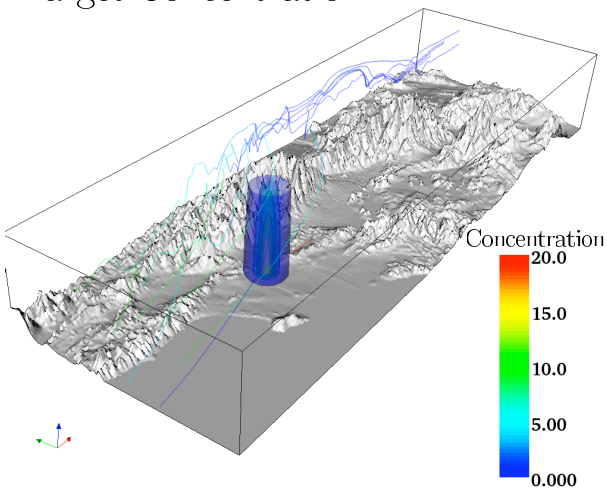
$$u_0 = 20e^{-0.04|x-x_c|}$$

- Inflow: $$v_{\text{in}} = v_{\text{max}} \left(\frac{z}{5.0 - z_{\text{surface}}} \right)^{0.1}$$

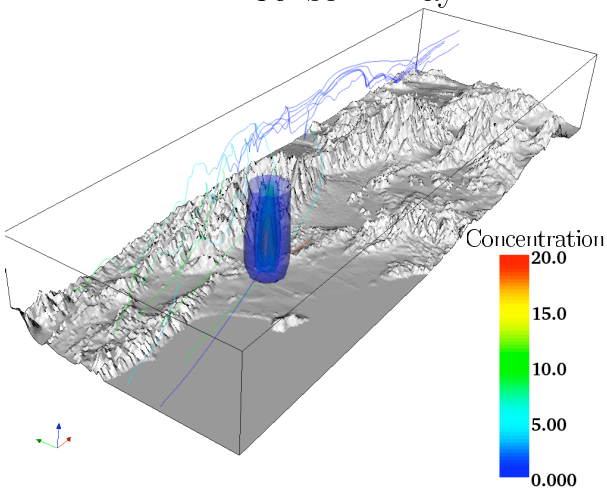
- Synthetic sensor readings every 3 minutes for 120 minute simulation
- Run on 64 processors of AlphaCluster at PSC

Numerical Results: Sensitivity to sensors

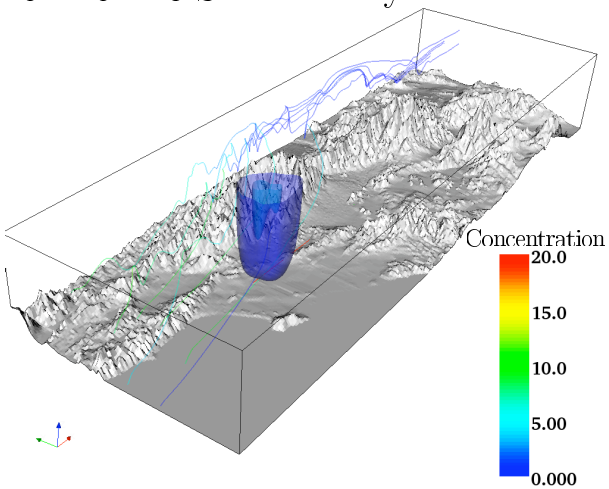
Target Concentration



$21 \times 21 \times 21$ Sensor Array



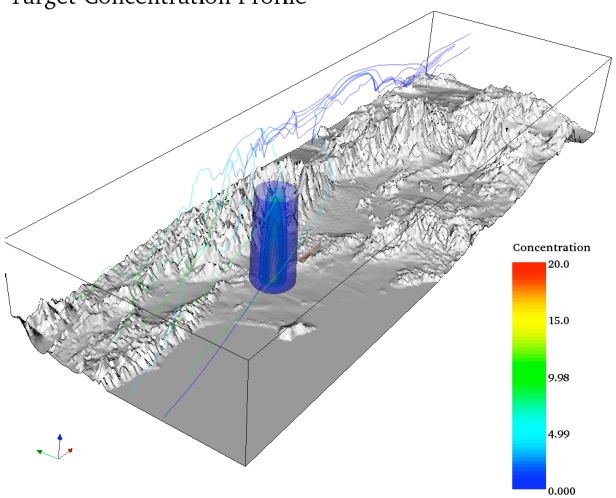
$6 \times 6 \times 6$ Sensor Array



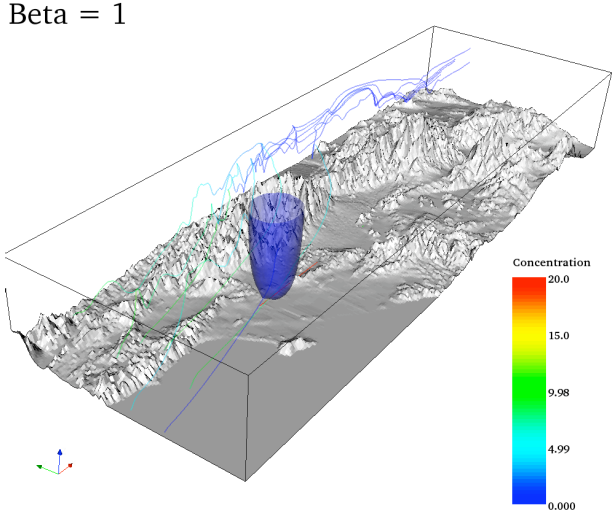
sensor array	$\|e\|_{L_2}^{relative}$	$\|e\|_{\infty}^{relative}$	time	iterations
$6 \times 6 \times 6$	0.793	0.980	2:01:47.11	377
$11 \times 11 \times 11$	0.495	0.870	2:20:02.65	437
$21 \times 21 \times 21$	0.339	0.805	2:33:11.72	484

Numerical Results: Sensitivity to Regularization

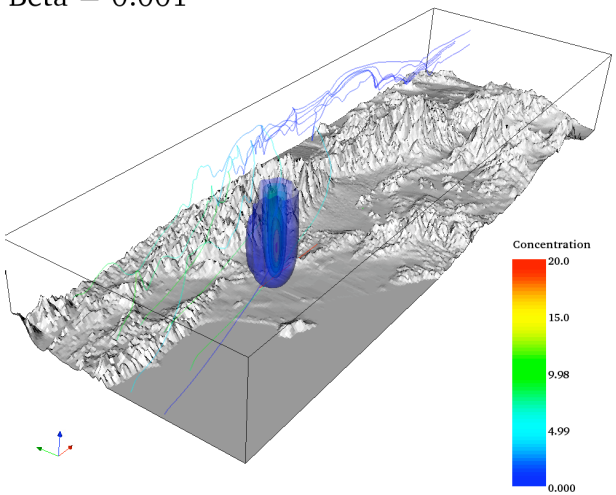
Target Concentration Profile



Beta = 1



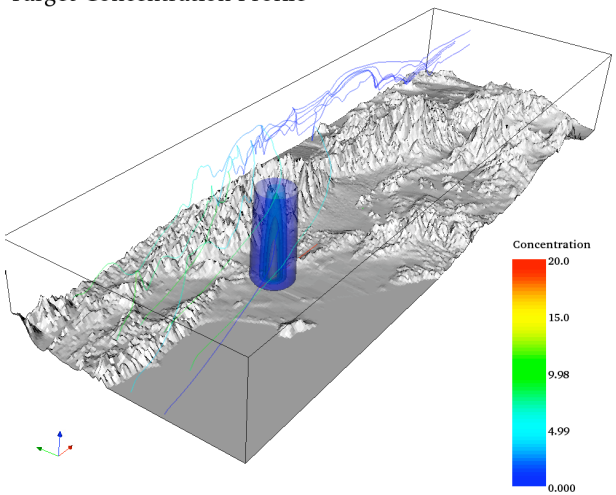
Beta = 0.001



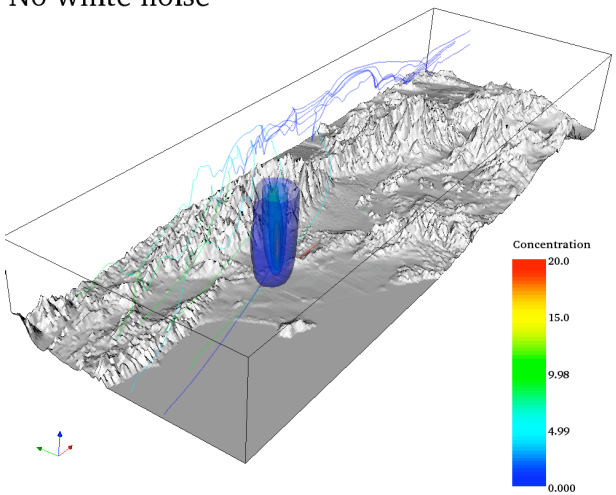
β	$\|e\|_{L_2}^{relative}$	$\|e\|_{\infty}^{relative}$	time	iterations
1	0.852	0.980	1:10:15.81	212
0.1	0.633	0.940	1:14:00.97	211
0.01	0.495	0.870	2:20:10.29	437
0.001	0.435	0.835	5:24:35.65	1078

Numerical Results: Sensitivity to Sensor Noise

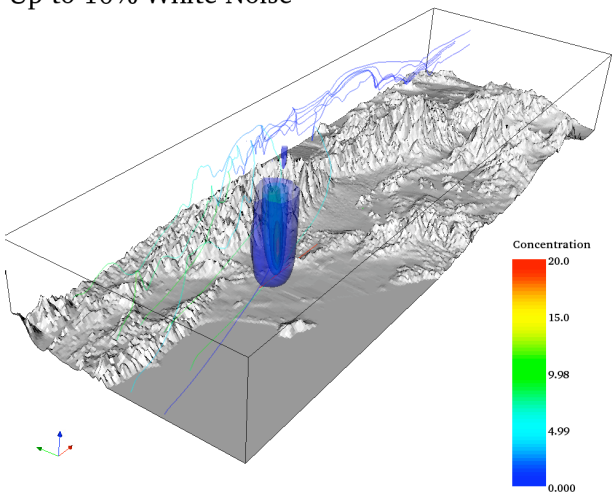
Target Concentration Profile



No white noise

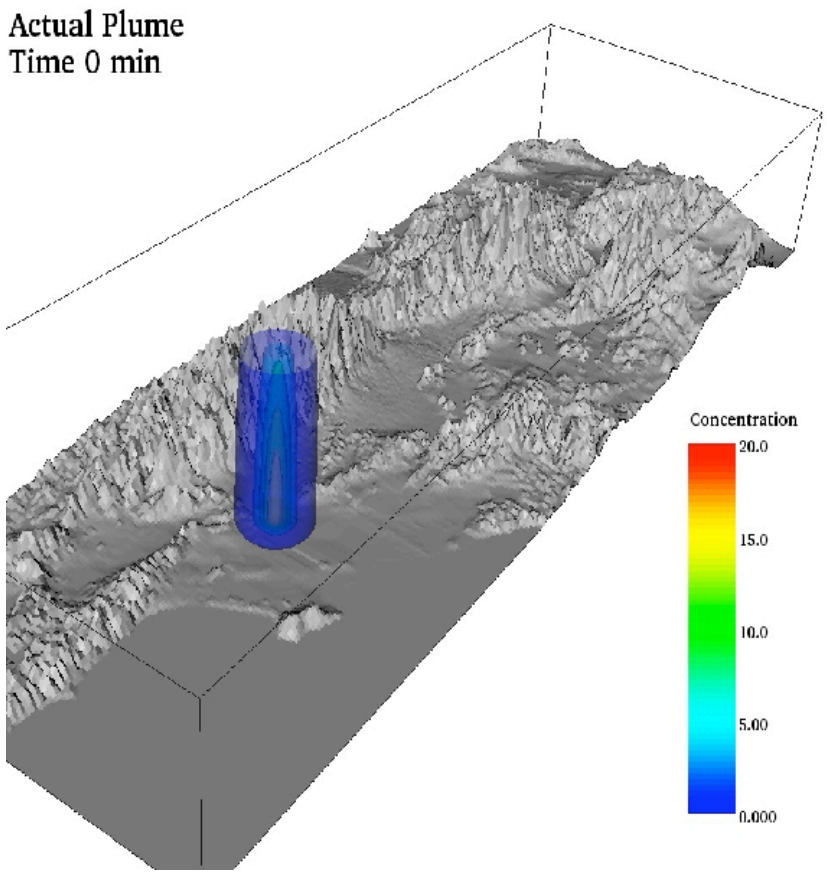


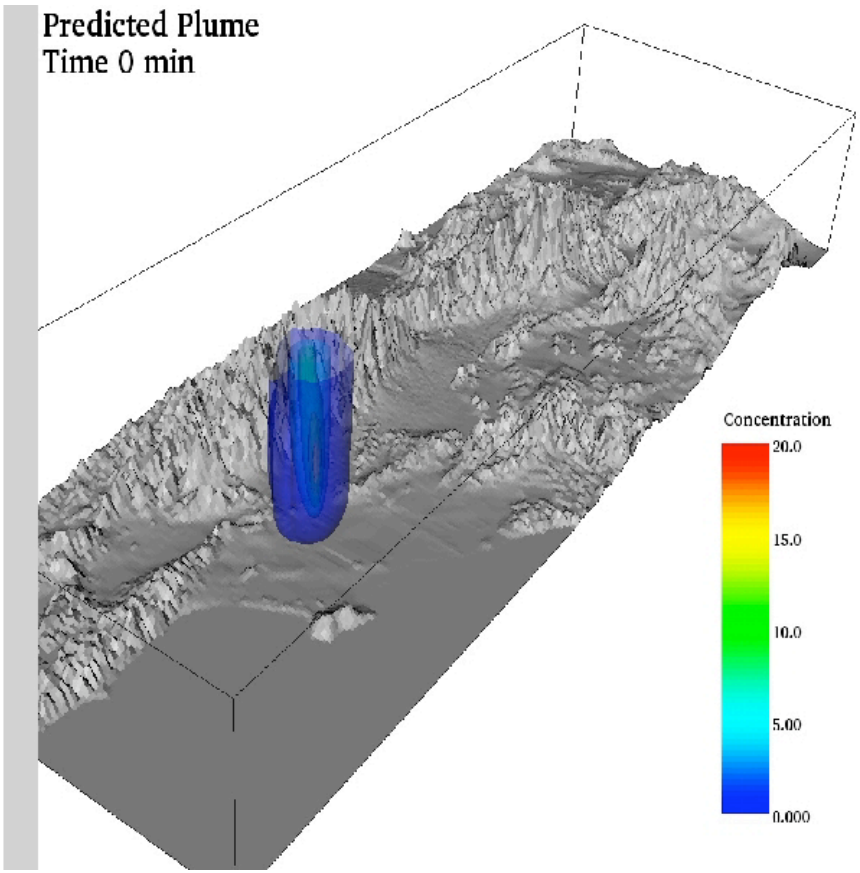
Up to 10% White Noise



Noise	$\|e\|_{L_2}^{relative}$	$\|e\|_{\infty}^{relative}$	time	iterations
0 %	0.495	0.870	2:20:10.29	437
5 %	0.497	0.870	2:40:24.02	506
10 %	0.500	0.875	3:01:52.31	581

Inversion example





Conclusions

- Inversion problems are ill-posed and require special numerical techniques for real-time results
  - Adjoint Methods
  - Reduced Space Methods
  - Matrix-Free Methods
  - Preconditioning and Parallelism

- However, exact concentration values may ***not*** be necessary to invert for the source location

- Nonlinear and multi-physics problems require significant algorithmic work

Remaining Challenges … or Opportunities?

- Demonstrated on a *simple* scalar linear problem
  - Nonlinear problems (*velocity inversion*) require complete history of forward and adjoint problem
    - Too big for memory!
    - Design space is **very** large!
- Multigrid preconditioner was specifically designed for this system and discretization
  - Discontinuous Galerkin methods give us *p*-adaptivity advantages and don't require SUPG stabilization
    - Requires new analysis for MG!

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Questions?

- Contact Information

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Extra Slides

Ill-Posedness

- Consider the heat equation

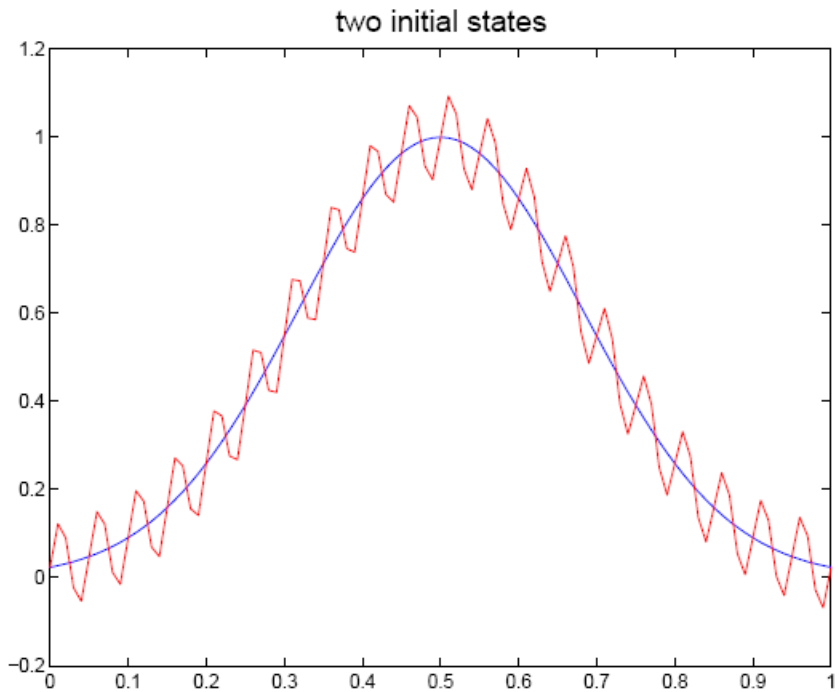
$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$$

$$u(0,t) = u(1,t) \qquad \text{Boundary condition}$$

$$u(x,0) = u_0(x) \qquad \text{Initial condition}$$

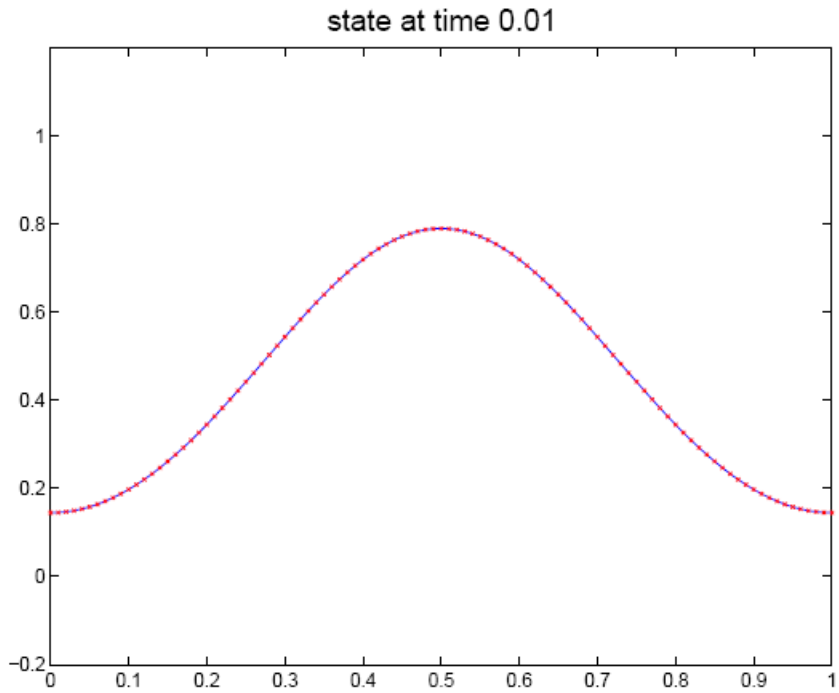
Ill-Posedness

- For two different initial condition states



Ill-Posedness

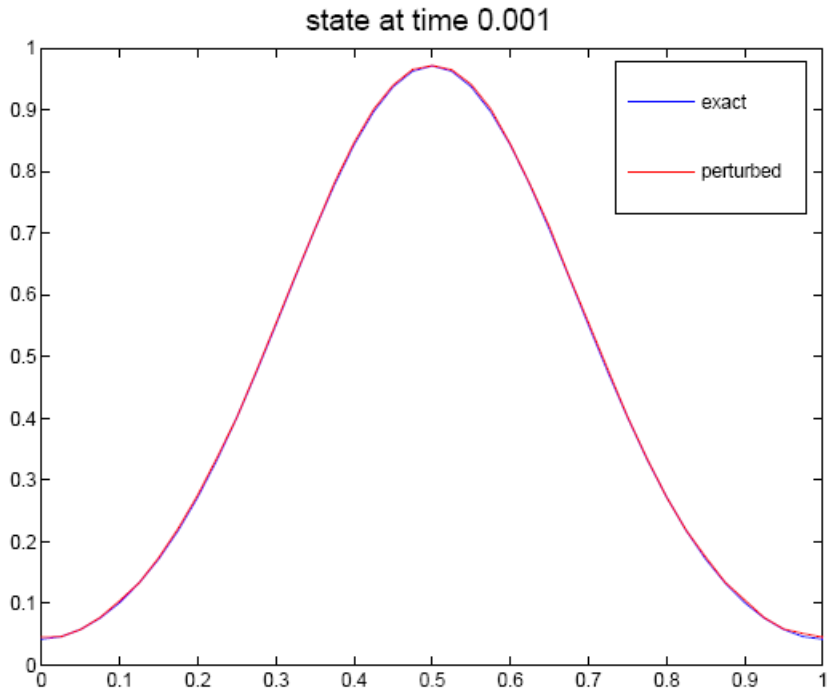
- The resulting end states are virtually identical (non-uniqueness)

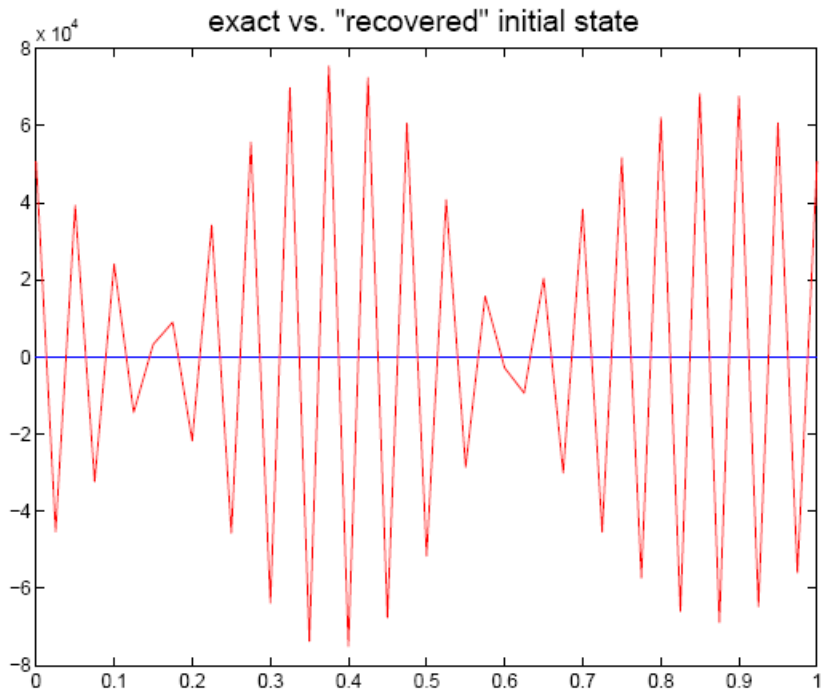


- Recoverir state is impossibl e problem

Ill-Posedness

- Starting from two nearly identical end states



Ill-Posedness

- And running reverse in time yields the following initial states