An Overview of Multiscale Modeling and Optimization Efforts

2006 LTE Review

January 17, 2006

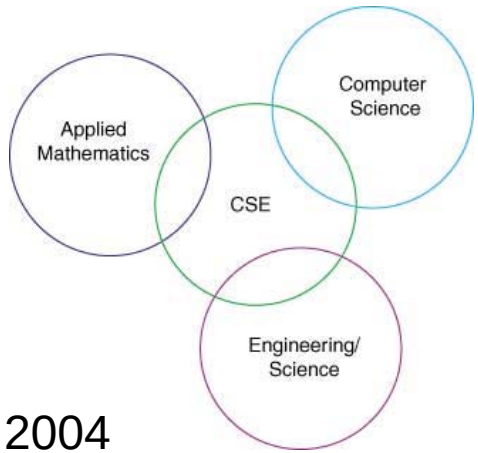
Judith Hill
1411: Optimization & Uncertainty Estimation

SAND2006-0761C

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Biography

- Sandia, September 2005 – present

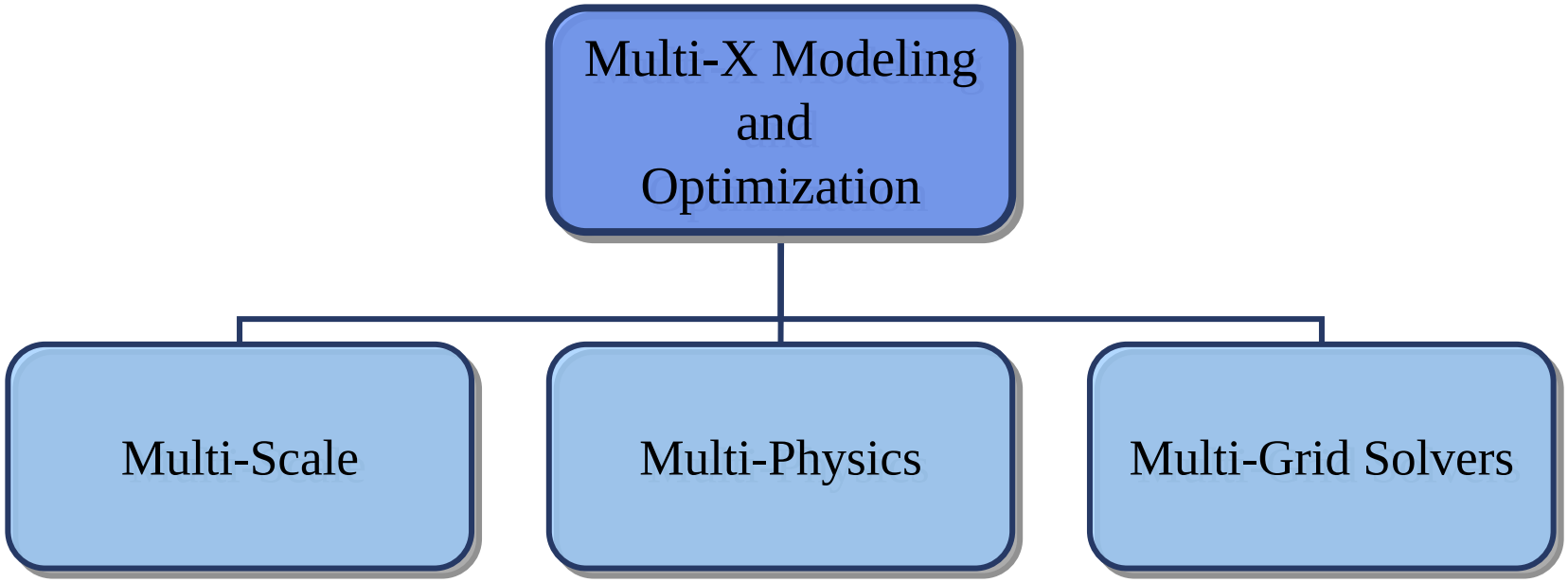


- Postdoctoral Research Associate, Carnegie Mellon University, May 2004 – June 2005
  - Sandia Funded: Real-time identification of airborne contaminants

- Ph.D. Computational Science and Engineering, May 2004
  - Advisors: Omar Ghattas (CEE) & Noel Walkington (Math)
  - Thesis: Phase field methods for flows with elastic membranes
  - Support: DOE Computational Science Graduate Fellowship (CSGF)
    - 2005 Howes Scholar

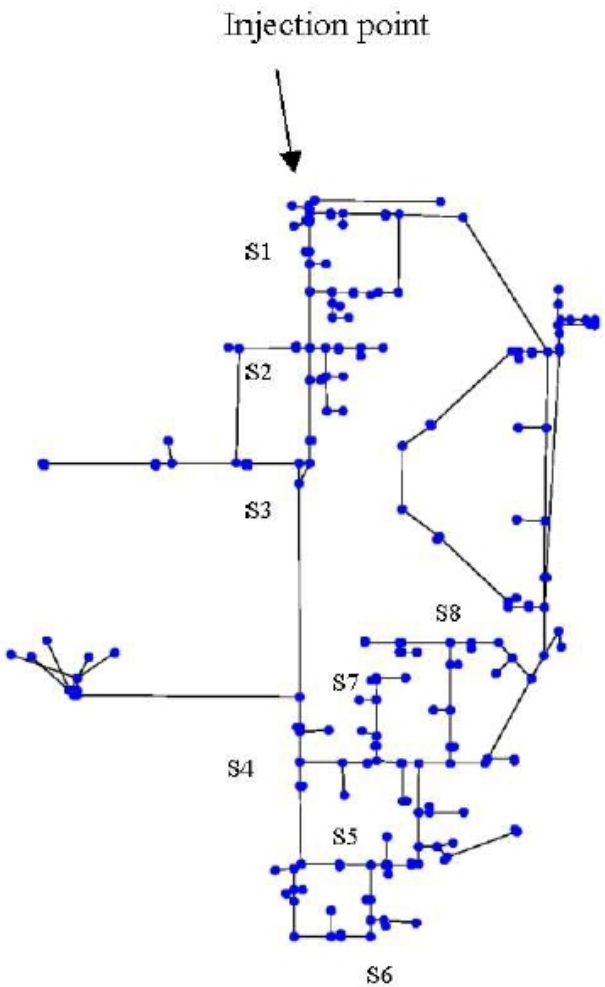
- M.S. Civil and Environmental Engineering, May 1999
  - Thesis: Co-Planar Crack Interactions in Brittle Materials Due to Inclusions
  - Support: NSF Graduate Research Fellowship

Research Interests – Sandia Activities



- Source Inversion in Water Distribution Systems
- Drinking Water Decontamination

Source Inversion in Water Distribution Systems



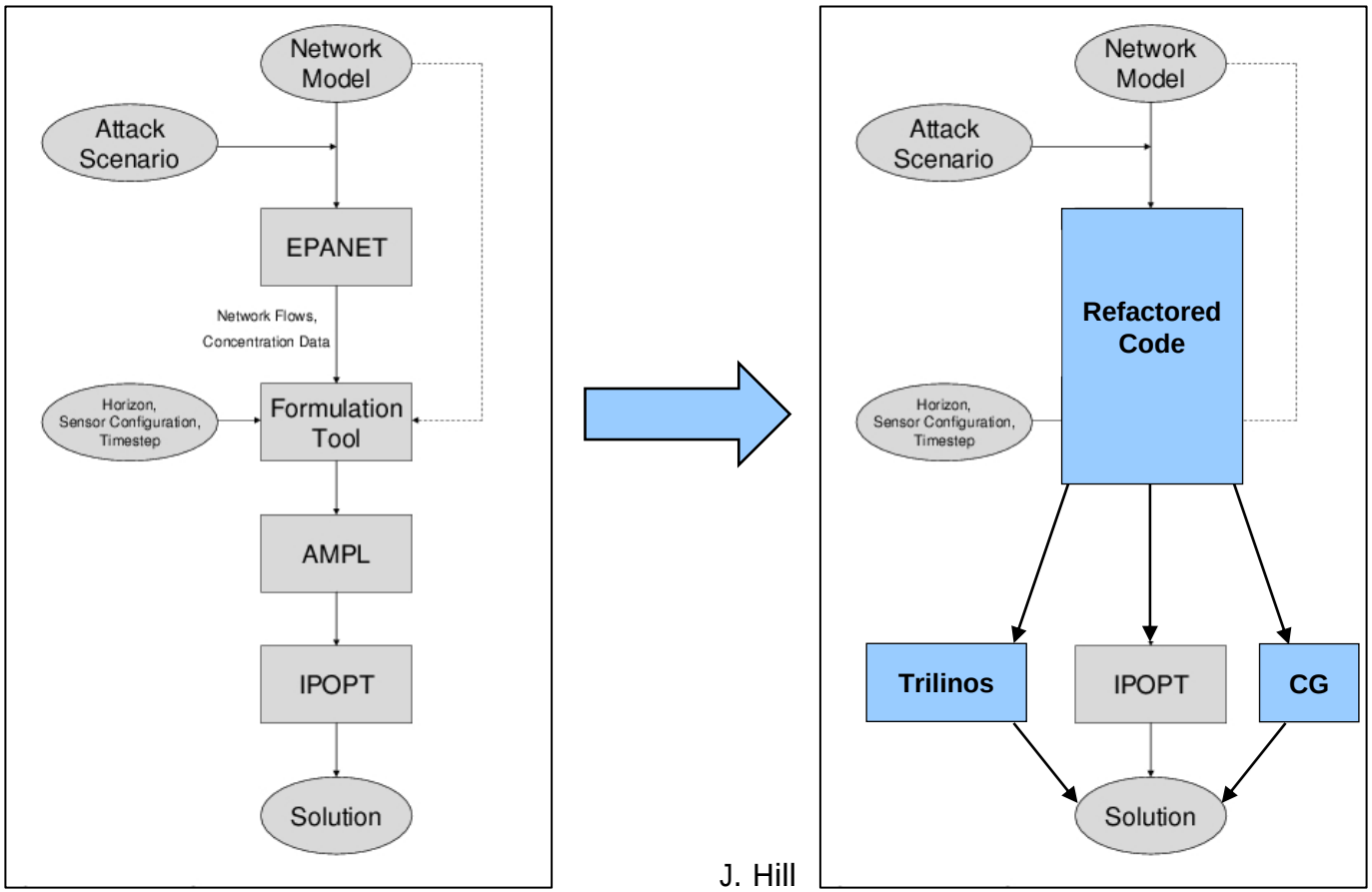
Collaborators:
B. Van Bloemen Waanders (1411)
EPA Water Security Project Team

Funding:
EPA WFO

- Applications:
  - Homeland security concerns
    - Terrorist attack on a water system
  - Monitoring of water utility equipment
    - Accidental surge of chlorine
- Leverages background in PDE-constrained optimization

Source Inversion in Water Distribution Systems

- Tasks and Contributions:
  - Refactor existing source inversion tool.
    - Refactored code is significantly more robust and efficient.



Source Inversion in Water Distribution Systems

– Algorithmic improvements have resulted in more accurate results.

$$\min_{\bar{c}^{\mathcal{I}},\bar{c}^{\mathcal{O}},\hat{c},m} \quad \frac{1}{2}\left[\hat{c}-\hat{c}^{\star}\right]^{T} W \left[\hat{c}-\hat{c}^{\star}\right] + \rho\frac{1}{2} m^{T} R m$$

$$\text{s.t.} \quad \bar{c}^{\mathcal{I}} - P^{\mathcal{I}}\hat{c} = 0,$$

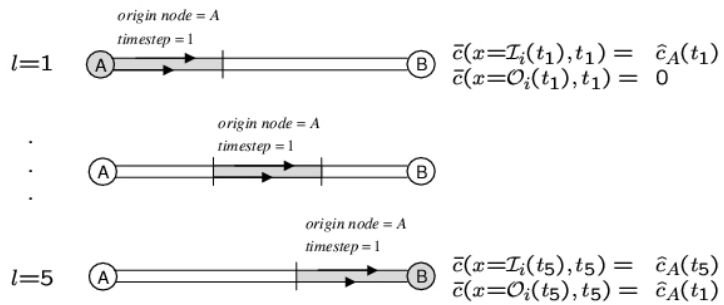
$$\bar{c}^{\mathcal{O}} - P^{\mathcal{O}}\hat{c} = 0,$$

$$\bar{N}\bar{c} + \hat{N}\hat{c} + Mm = 0,$$

$$m \geq 0,$$

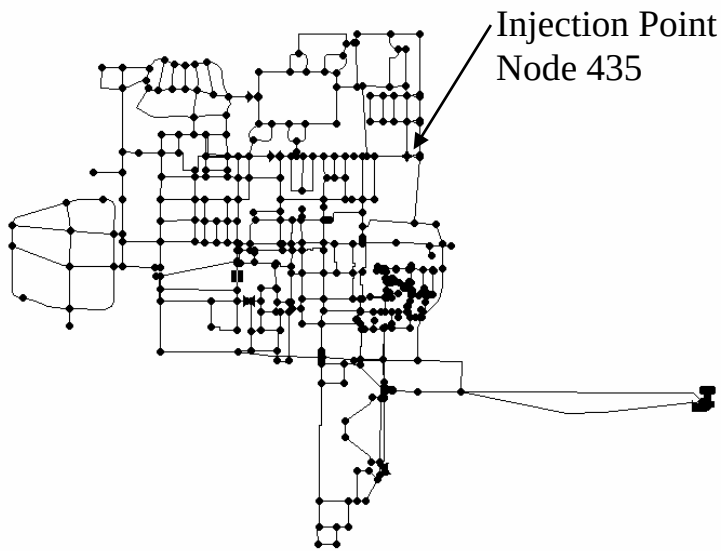
(Reformulated)
Flow through a pipe

Mass Balance at node



Source Inversion in Water Distribution Systems

ORIGINAL TOOL		REFACTORED TOOL	
Node	**Contaminant**	**Node**	**Contaminant**
2301	36.91%	**435**	**99.12%**
435	**20.53%**	4381	0.27%
4381	11.35%	2301	0.26%
2501	8.68%	437	0.25%
437	7.28%	416	0.04%
431	5.42%	430	0.03%
2401	5.06%	2601	0.02%
5673	0.02%	412	0.01%



- Investigate the effectiveness of inversion for Boolean (0/1) sensors.
  - Conference proceeding for EWRI conference in progress.

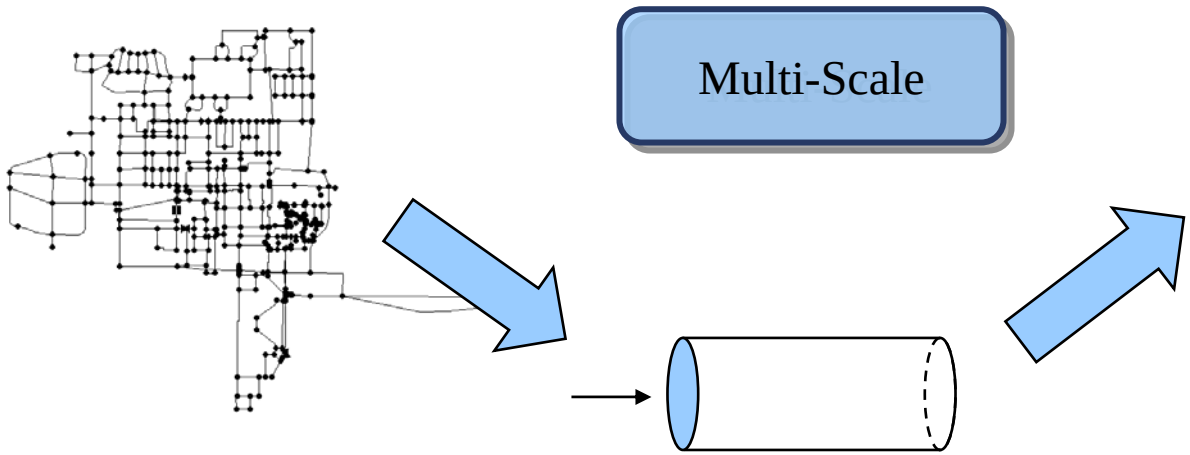
Multi-Scale | Multi-Physics

Drinking Water Decontamination

- Natural extension to the source inversion in water distribution systems
- Leverages background in fluid dynamics

Collaborators:
S. Altman (6115)
B. Bader (1416)
L. Frink (8333)
B. Van Bloemen Waanders (1411)

Funding:
LDRD joint w/ Bio IAT, EIA IAT



Drinking water systems requires network-scale simulations

Pipe flow requires continuum-scale simulations

Biofilms in water systems requires molecular-scale simulations

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Multi-Scale | Multi-Physics

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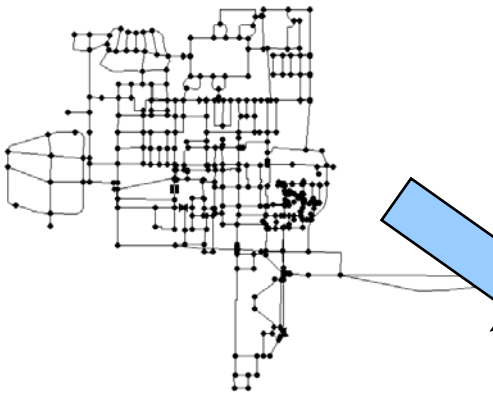
Multi-Physics



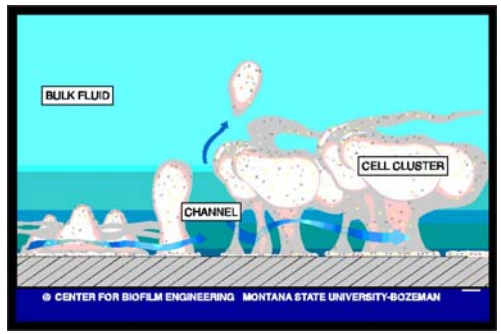
Hydraulics simulation for network flows

Reactions for contaminants

Optimal decontamination strategy

Navier-Stokes with turbulence for pipe flow

Convection-diffusion-reaction for contaminants in the water



Surface reactions for action of biofilm

(Modified) Navier-Stokes model to account for water flow

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Drinking Water Decontamination

- Tasks and Contributions:
  - Couple Navier-Stokes model for fluid to a convection-diffusion-reaction model for contaminants..
    - Requires a turbulence model.
    - One-way coupling.

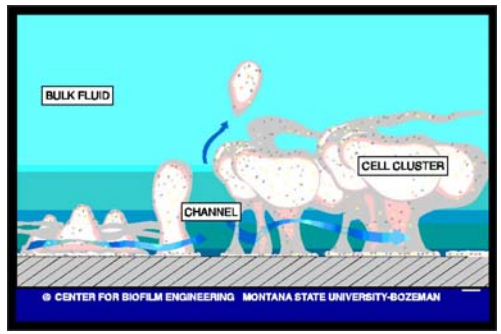
Navier-Stokes with turbulence for pipe flow

Convection-diffusion-reaction for contaminants in the water

$$\begin{aligned} \rho\left(v_t + (v\cdot\nabla)\,v\right) - div\left(pI + \mu D(v)\right) &= \rho f \quad \text{in } \Omega \\ div(v) &= 0 \quad \text{in } \Omega. \end{aligned}$$

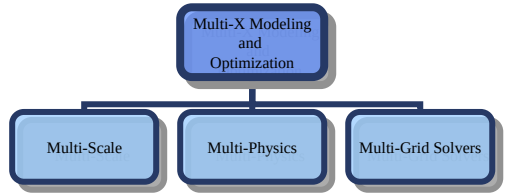
$$\frac{\partial u}{\partial t} - \nu\Delta u + \boldsymbol{v}\cdot\nabla u = 0 \quad \text{in} \quad \Omega\times(0,T),$$

Drinking Water Decontamination



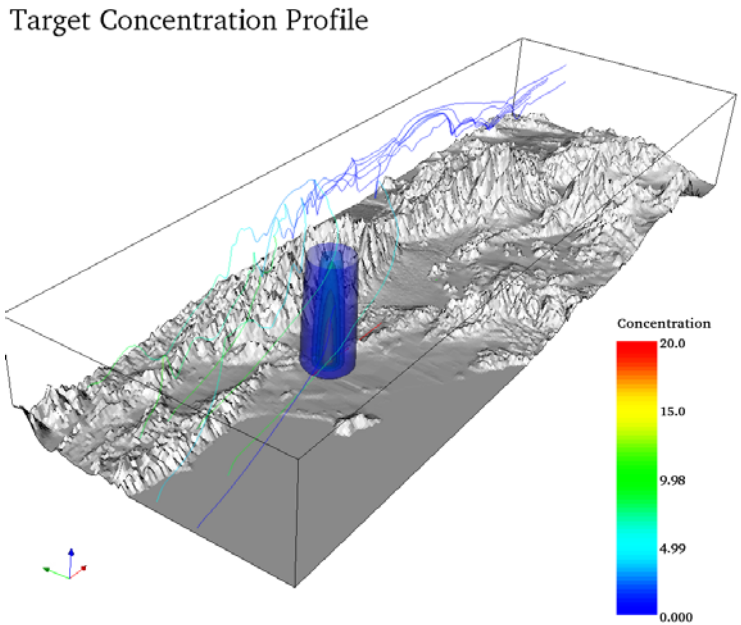
- Couple a (modified) Navier-Stokes model for the bulk fluid to a DFT model for the biofilm.
  - DFT is a method for deterministically finding the density distribution of a fluid
  - New territory – little previous work has been done in the area of transport of interfacial fluids.
    - Diffusion studied by Frink, Thompson & Salinger
  - Heterogeneous fluid requires modification of the density and viscosity terms in the Navier-Stokes model.

$$\begin{aligned} \rho\left(v_t + (v \cdot \nabla)\, v\right) - div\left(pI + \mu D(v)\right) &= \rho f \quad \text{in } \Omega \\ div(v) &= 0 \quad \text{in } \Omega. \end{aligned}$$



Thoughts for Future Work

- Uncertainty in inversion

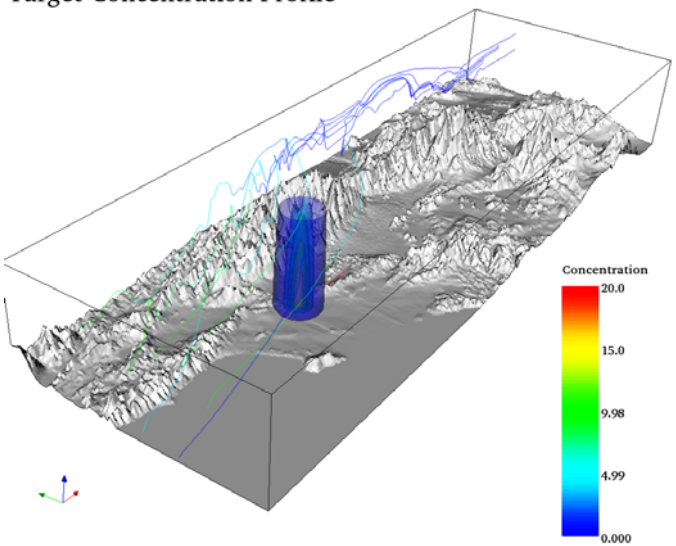


Collaborators:
V. Akcelik (SLAC)
G. Biros (Penn)
A. Draganescu (1411)
O. Ghattas (UT-Austin)
B. Van Bloemen Waanders (1411)
K. Willcox (MIT)

- Sources of Uncertainty:
  - Correctness of model
  - Faulty (incorrect or unreliable) sensor measurements
  - Ill-posedness of the problem

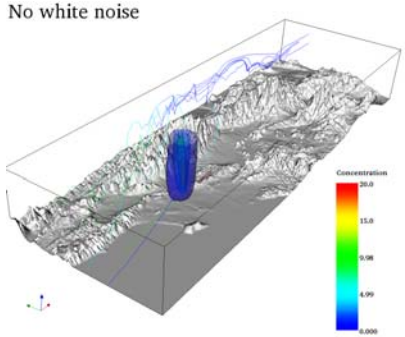
Uncertainty in inversion

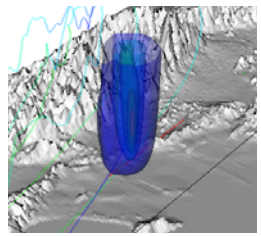
Target Concentration Profile



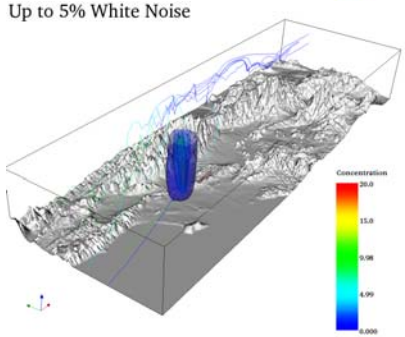
Noise	$\|e\|_{L_2}^{relative}$	$\|e\|_{\infty}^{relative}$	time	iterations
0 %	0.495	0.870	2:20:10.29	437
5 %	0.497	0.870	2:40:24.02	506
10 %	0.500	0.875	3:01:52.31	581

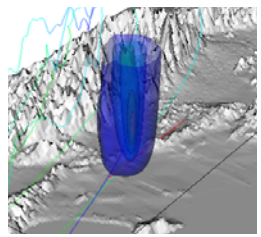
No white noise



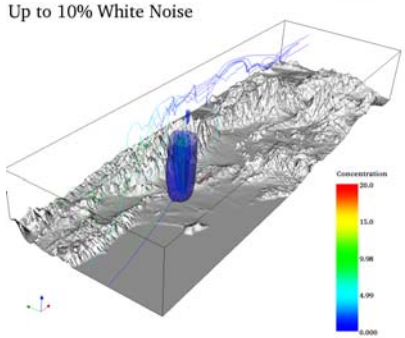


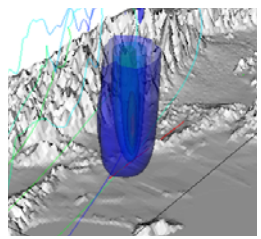
Up to 5% White Noise





Up to 10% White Noise





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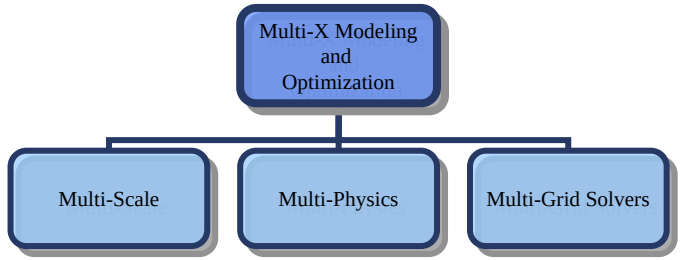
Uncertainty in inversion

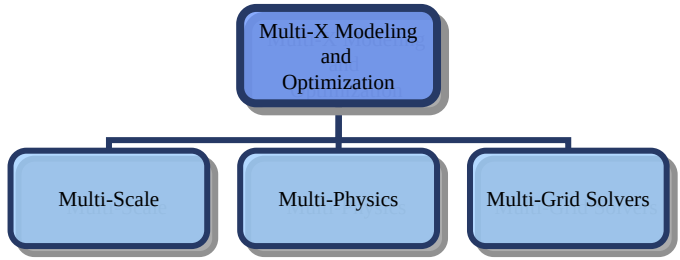
- Technical challenges:
  - Statistical representation of confidence in inversion
  - Analytical representation of uncertainty.

- Programmatic Impacts:
  - Well-positioned to answer the recent **DTRA call**.
  - Inversion under uncertainty will play a role in an upcoming **Sci-DAC proposal**.
  - University collaborators received an NSF collaborative research grant to continue research (Co-PI).
  - Conference proceeding in progress.



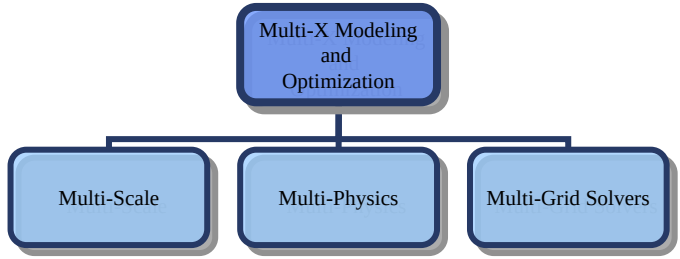
Summary

- Source Inversion in Water Distribution Systems (EPA)
- Drinking Water Decontamination (LDRD)
- Continuum to Continuum Multiscale Math Effort (MICS)
  - With S. Collis (1414)
- Simulation of a Chemically-Reacting Laser (AFRL)
  - With T. Madden (AFRL), L. Musson (1437), R. Pawlowski (1416), A. Salinger (1416)



Summary

- Professional Accomplishments this year:
  - 1 book chapter
    - V. Akcelik, G. Biros, O. Ghattas, J. Hill, D. Keyes, and B. van Bloemen Waanders, "Parallel algorithms for PDE-constrained optimization", in Frontiers of Parallel Computing, M. Heroux, P. Raghaven, H. Simon, eds, SIAM, 2006, to appear.
  - 1 conference proceeding (2 in progress)
    - V. Akcelik, G. Biros, A. Draganescu, O. Ghattas, J Hill, and B. van Bloemen Waanders, Dynamic data-driven inversion for terascale simulations: Real-time identification of airborne contaminants, Proceedings of SC2005, Seattle, WA, November 2005.
  - 1 SAND report
    - 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. Sensitivity Technologies for Large Scale Simulation, Sandia Report SAND2004-6574, January, 2005.
  - 2 conference presentations (1 invited)
  - 2 journal papers under preparation



Questions