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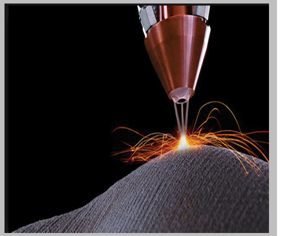

RAPID OPTIMIZATION LIBRARY

# Multiscale optimization under uncertainty

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Sandia National Laboratories

Optimization & UQ, Org. 1441

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February, 2017

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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# PDE-constrained optimization

$$\min_{u,x} \; f(u,x) \quad \text{subject to} \quad c(u,x) = 0$$

where $u$ is the state, $x$ are the control variables,

# Objective function formulations

- Design $$f(u,x) = \frac{1}{2}\int_{\Omega} \chi d\Omega$$
- Inverse $$f(u,x) = \frac{1}{2}\int_{\Omega} (u-u^*)^2 \delta(y-y^*) d\Omega + \frac{\beta}{2}\int_{\Omega} x^2 d\Omega$$
- OED $$f(u,x,q) = tr\ C^{-1}(q)$$
- Control $$f(u,x) = \frac{1}{2}\int_{\Omega} (u-\overline{u})^2 d\Omega + \frac{\beta}{2}\int_{\Omega} x^2 d\Omega$$
- OUU $$f(u,x,\eta) = \frac{1}{2}\sigma\int_{\Omega} (u(\xi)-\overline{u})^2 d\Omega + \frac{\beta}{2}\int_{\Omega} x^2 d\Omega$$

# Equality constraints

- Phase field

$$\frac{\partial \phi_i}{\partial t} + L\left\{16 * W_\phi \phi_i \left[-\phi_i + \sum_{j=0}^{n_\phi} \phi_i^2\right] - \epsilon^2 \nabla^2 \phi_i\right\} = \quad 0, \quad i = 1, ..., n_\phi$$

- Thermal

$$\frac{\partial u}{\partial t} - D\Delta u = f$$

- Linear elasticity

$$-\nabla \cdot \sigma(u) = f$$

- Molecular dynamics

$$m\frac{d^2 u_i}{dt^t} + F_i(u_1, u_2, ..., u_N), \quad i = 1, 2, ...., N$$

- AM processes

Powered bed, LENS, Direct Write, etc.

# Solution strategy

$$\min_{u,x} \; f(u,x)$$

$$\text{subject to: } c(u,x) = 0$$

Optimization Formulation

$$\mathcal{L}(u,x,\lambda) = f(u,x) + \lambda c(u,x)$$

Lagrangian

$$\begin{Bmatrix} \mathcal{L}_u \\ \mathcal{L}_x \\ \mathcal{L}_\lambda \end{Bmatrix} = \begin{Bmatrix} J_u + \lambda c_u \\ J_x + \lambda c_x \\ c \end{Bmatrix} = 0$$

Optimality conditions

$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{ux} & c_u^T \\ \mathcal{L}_{xu} & \mathcal{L}_{xx} & c_x^T \\ c_u & c_x & 0 \end{bmatrix} \begin{Bmatrix} \delta u \\ \delta x \\ \lambda^* \end{Bmatrix} = - \begin{Bmatrix} f_u \\ f_x \\ c \end{Bmatrix}$$

KKT after Newton iteration

# Risk averse optimization

$$\min_{u,x} F(u(\xi),x) \equiv \sigma\left[||f(u(\xi),x))||^2\right] + \frac{\alpha}{2}||x||^2$$

$$\text{s.t.} \quad c(u(\xi),x) = 0$$

where $u$ is the state, $x$ are the control variables,

$\xi$ are stochastic components, and $\sigma$ is a risk measure

# Trilinos packages

| Linear Algebra |
|---|
| Epetra |
| EpetraExt |
| Tpetra |
| Jpetra |
| Kokkos |

| Preconditioners |
|---|
| ML |
| Ifpack |
| Teko |

| Mesh Partitioning / DD |
|---|
| Claps |
| Moertel |
| Isorropia |
| Zoltan |

| Solvers |
|---|
| AztecOO |
| Belos |
| Pliris |
| Komplex |
| Amesos |
| NOX |
| LOCA |
| ROL |
| Piro |
| Rythmos |
| TriKota |
| Globipack |
| Optipack |
| Anasazi |

| PDE Tools |
|---|
| Phalanx |
| Intrepid |
| Shards |
| Panzer |

| Tools |
|---|
| Teuchos |
| SEACAS |
| STK |
| Sacado |
| Stokhos |

| Interfaces |
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| Thyra |
| PyTrilinos |
| Stratimikos |

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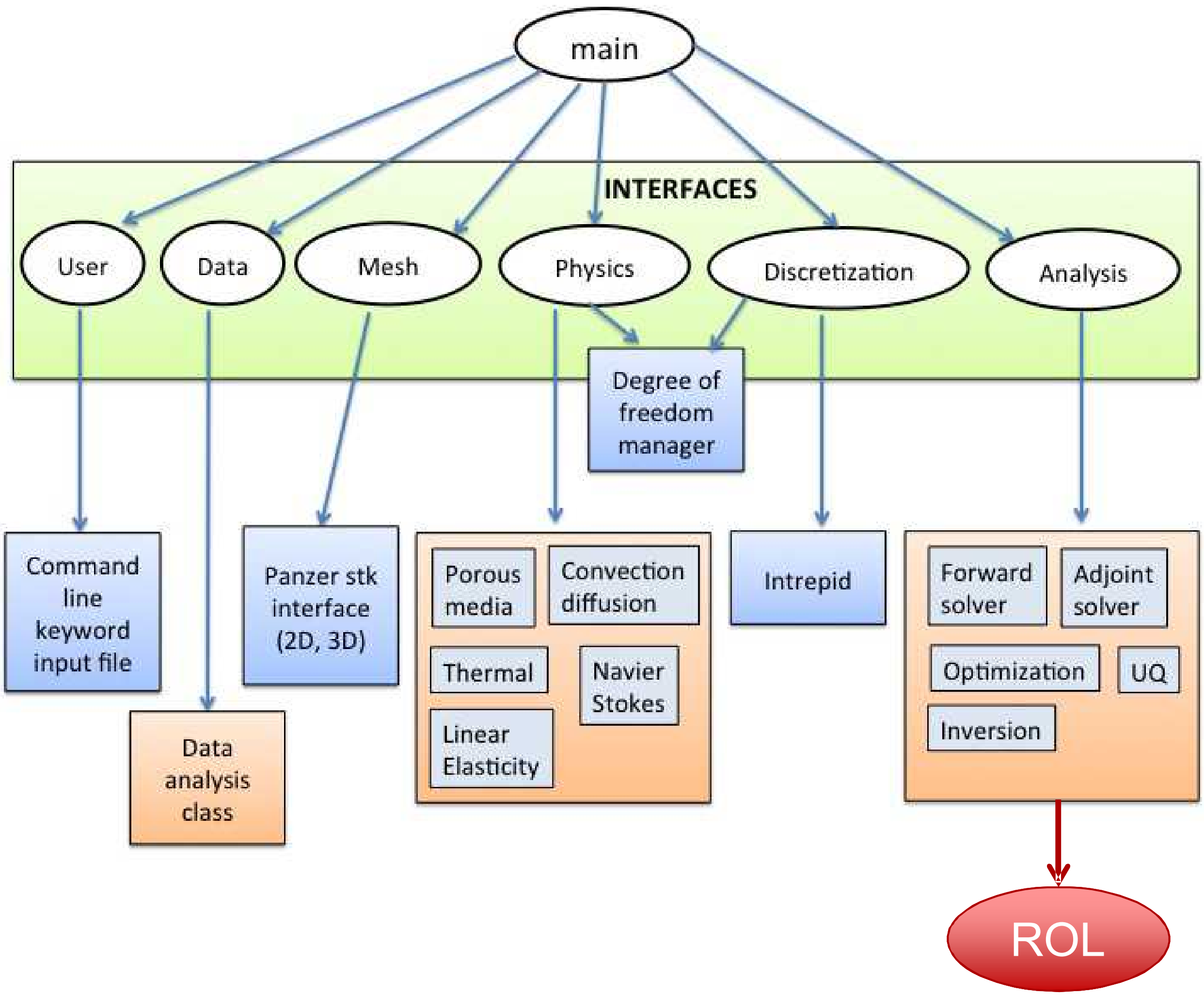
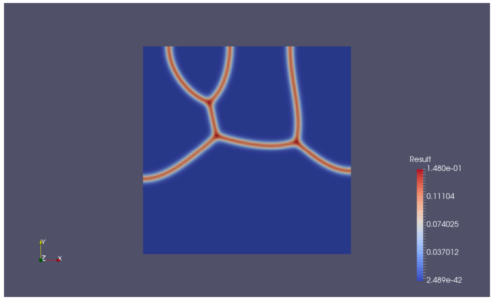
# Multi scale/physics Interface for Large scale Optimization (MILO)



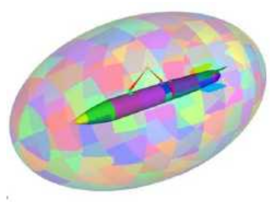



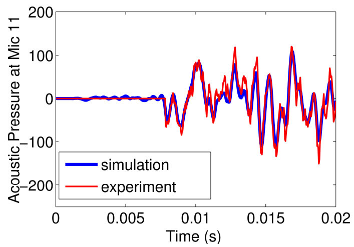
**Automates:**

- 2D/3D Parallel
- Adjoints
- Opt under uncertainty
- Unstructured
- Multiscale
- Multiphysics

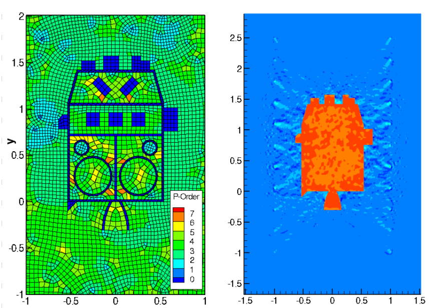
# Example use cases

## Inversion acoustics / elasticity.



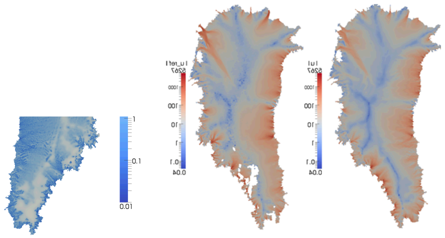



1M optimization variables
1M state variables



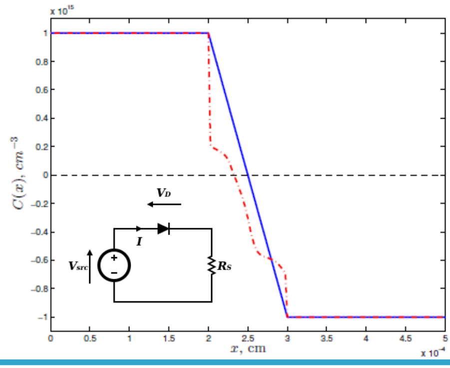
- 175K opt variables
- 525K state variables

## Estimating basal friction of ice sheets.



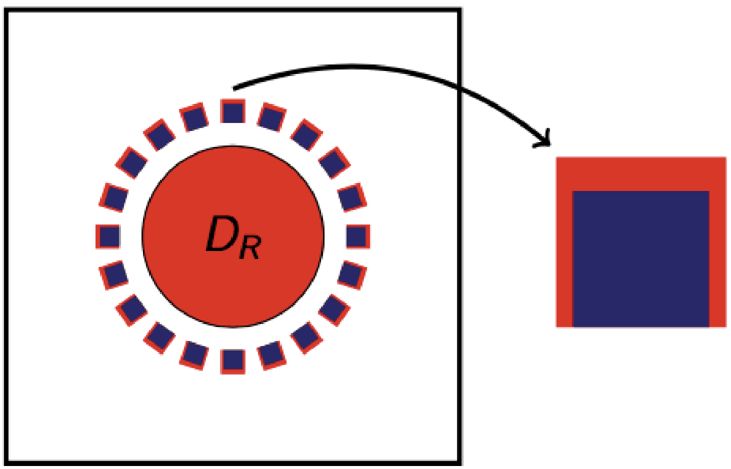
- 65K opt variables
- 700,000 state variables

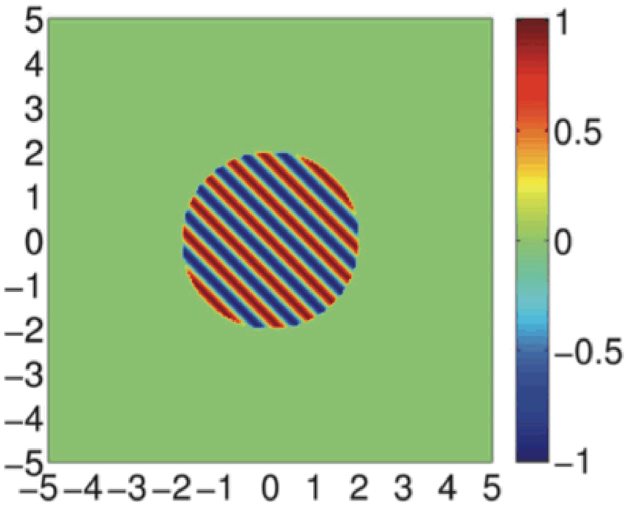
## Calibration of electrical device models.



- 50 opt variables

# Risk Averse Optimal control



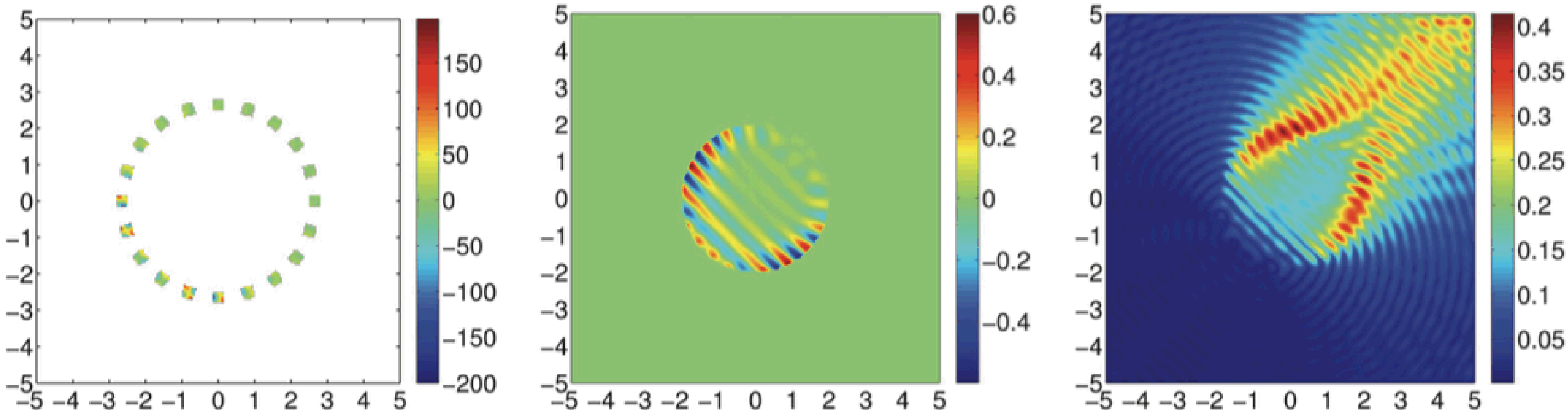

**Note:**
- Region of interest is stochastic
- Region around the speakers are stochastic
- Parameterized with KL expansion



$\xi \leftarrow \mathbb{E}[\xi]$

# Solution (real part)





# Scalability in the stochastic dimension

| $dim$ | PDE Solves | $CP_{obj}$ | $CP_{grad}$ | Obj. Value |
|---|---|---|---|---|
| 42 | 11,543 | 145 | 145 | 5.2542 |
| 44 | 32,739 | 233 | 481 | 5.2637 |
| 46 | 60,617 | 243 | 1,453 | 5.2641 |
| 48 | 79,221 | 247 | 2,961 | 5.2641 |
| 50 | 90,157 | 251 | 4,569 | 5.2641 |
| 60 | 100,911 | 271 | 7,621 | 5.2641 |
| 70 | 103,979 | 291 | 8,233 | 5.2641 |
| 80 | 105,607 | 311 | 8,253 | 5.2641 |

***Scalable performance as dim is increased!***

D. P. Kouri, M. Heinkenschloss, D. Ridzal, and B. G. van Bloemen Waanders , "*Inexact Objective Function Evaluations in a Trust-Region Algorithm for PDE-Constrained Optimization under Uncertainty",* SIAM Journal on Scientific Computing, 2014, Vol. 36, No. 6,

# Key Points

- State-of-the-art PDE constrained optimization
- Finite element based framework that automates the necessary optimization objects and interfaces
- Complete range of optimization formulations
- Optimization under uncertainty via risk averse methods

# Application to Hydraulic Fracturing

- Map uncertainty from reconstructed material properties to control under uncertainty
- FWI and EM inversion for material properties
- Fracture inversion using peridynamics
- Control of operating conditions to steer towards optimal fracture patterns
- Optimal experimental design to guide data acquisition
- Develop real time feedback control

# Challenges

- Coupled physics: Non-Newtonian fluid flow, peridynamics
- Multiscale inversion/control
- Quantification of uncertainties
- Implement inversion/control with real data and operating conditions
- Real time will require reduced order modeling and feedback control

# Inversion and control

$$\min_{z} \quad \mathcal{J} = \frac{1}{2}\int_0^T \int_\Omega (u - \boxed{y_d)^2 \delta(x - x^*, t - t^*)\ d}x\ dt + \frac{\beta}{2}\int_0^T \int_\Omega z^2\ dx\ dt$$

$$\text{where } u \text{ solves: } \frac{\partial u}{\partial t} - D\Delta u + v \cdot \nabla u = \boxed{f(z)}^* \quad \in \Omega \times (0,T)$$

$$u = \tilde{u} \qquad \text{on} \quad \Gamma \times (0,T)$$

$$u = u_0 \qquad \in \Omega, \ T = 0$$

$$\min_{z} \quad \mathcal{J} \boxed{=\sigma} \left[\frac{1}{2}\int_0^T \int_\Omega (u \boxed{- \bar{u})^2}\ dx\ dt)\right]$$

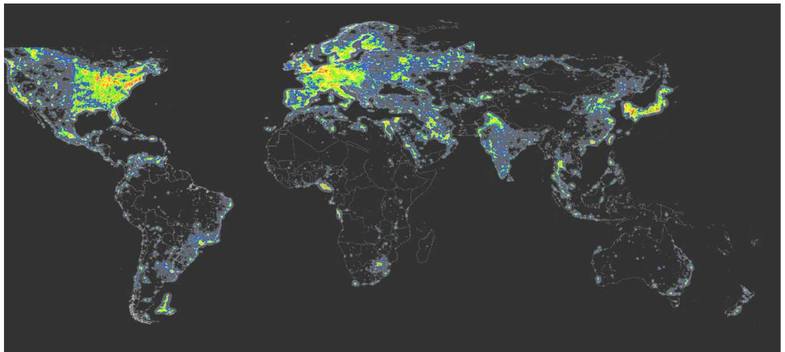
$$\text{where } c \text{ solves: } \frac{\partial u}{\partial t} - D\Delta u + v \cdot \nabla u = \boxed{f(\zeta, z)^*} \quad \in \Omega \times (0,T)$$

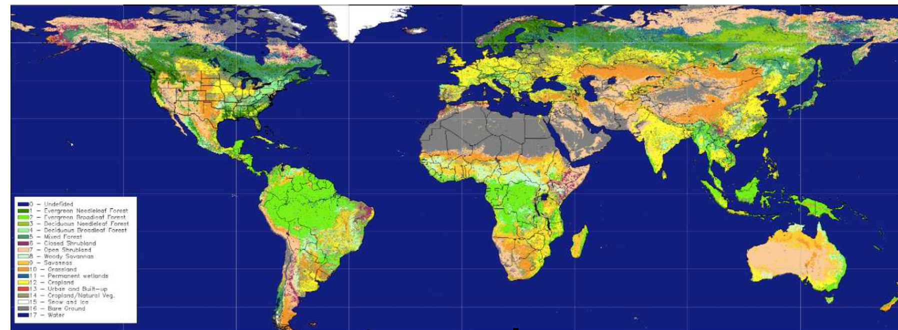
$$u = \tilde{u} \qquad \text{on} \quad \Gamma \times (0,T)$$

$$u = u_0 \qquad \in \Omega, \ T = 0$$

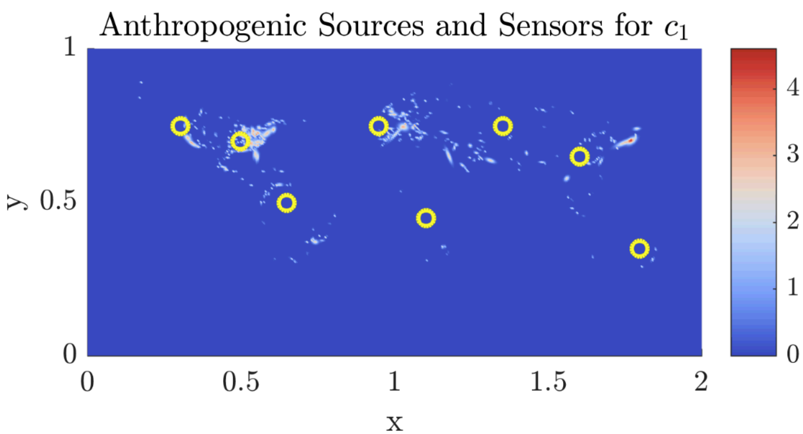
* SUPG stabilized

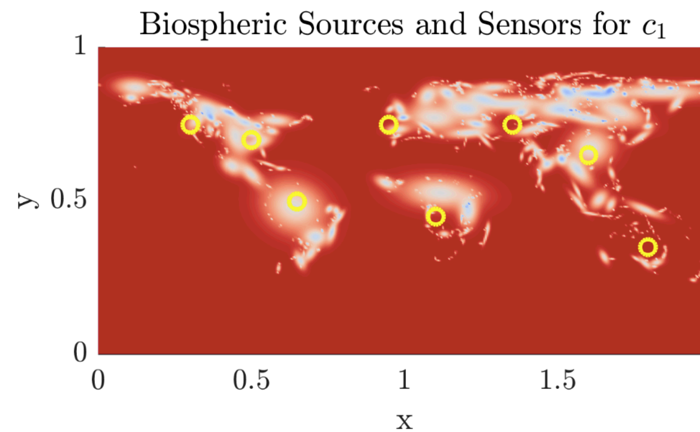
# Anthropogenic and biospheric sources





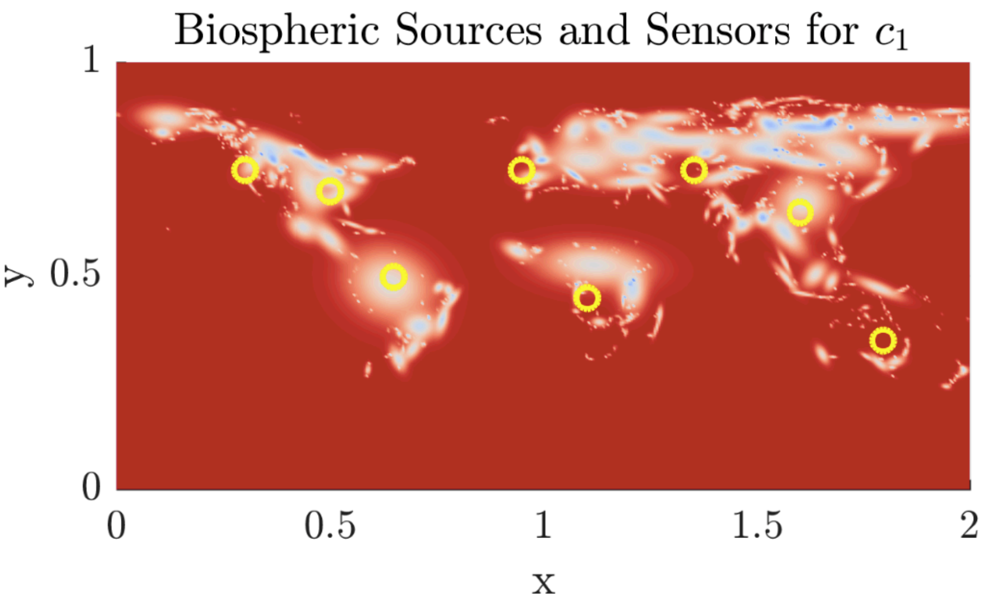
$$f(x) = s\exp((x-m)^T\Sigma^{-1}(x-m))$$

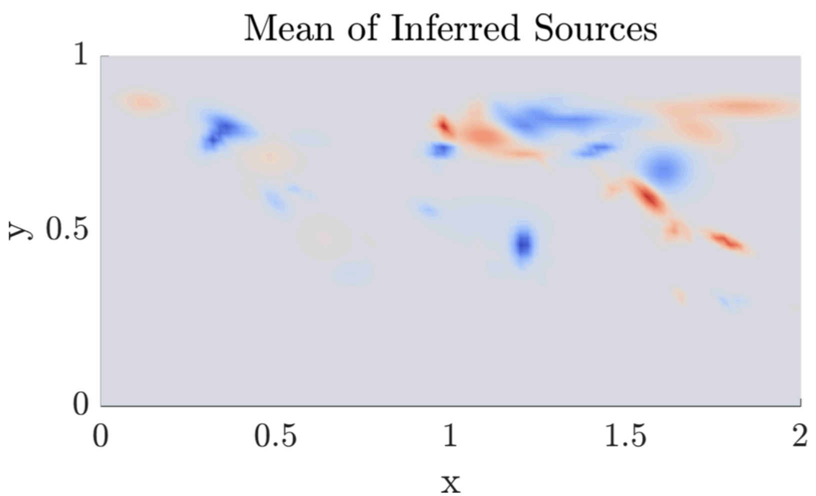


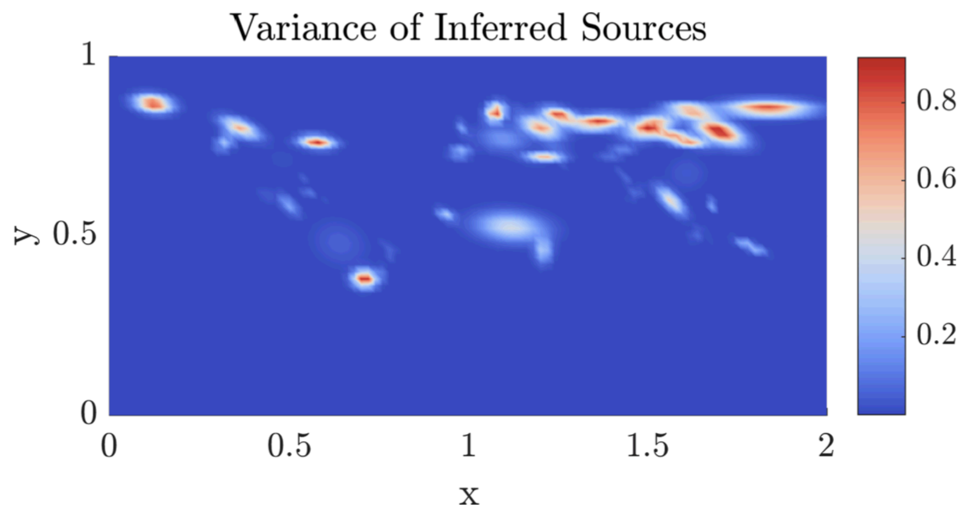



# Inversion of biospheric sources

- 100 Gaussian kernels
- constant initial guess
- Gaussian noise $\sigma^2 = 10^{-4}$
- two temporal measurements for each of 16 sensors
- noisy solution: few sensors, noisy data, sparse source terms

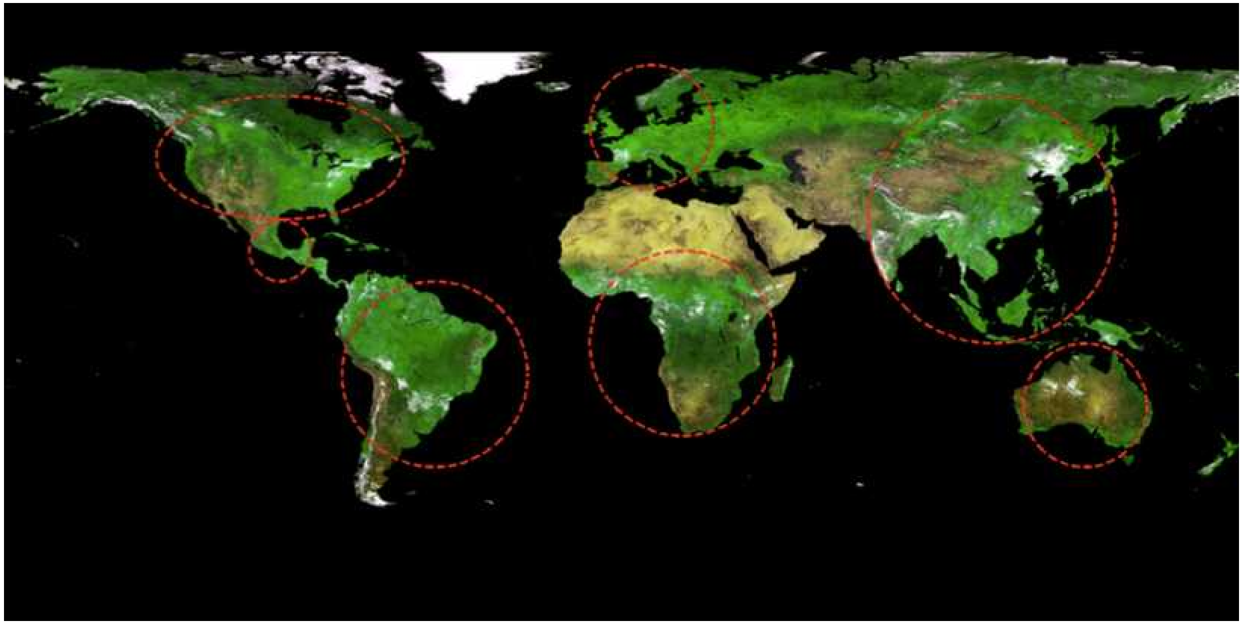


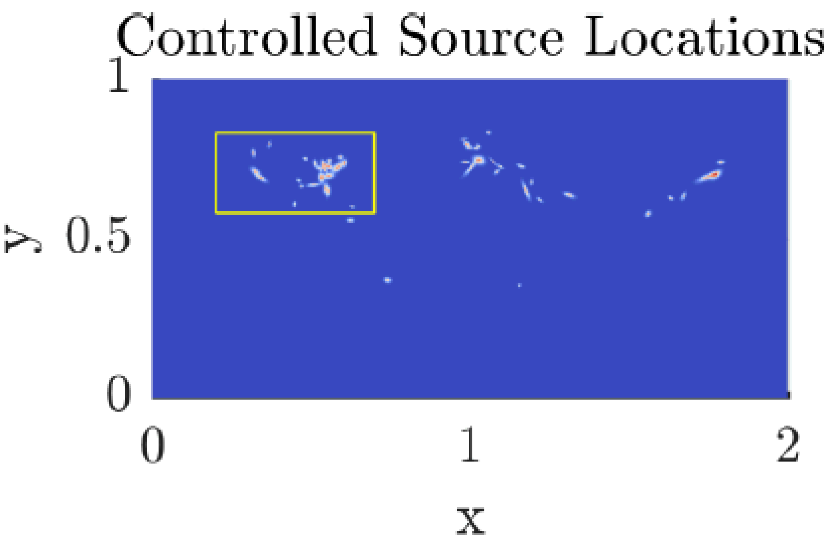



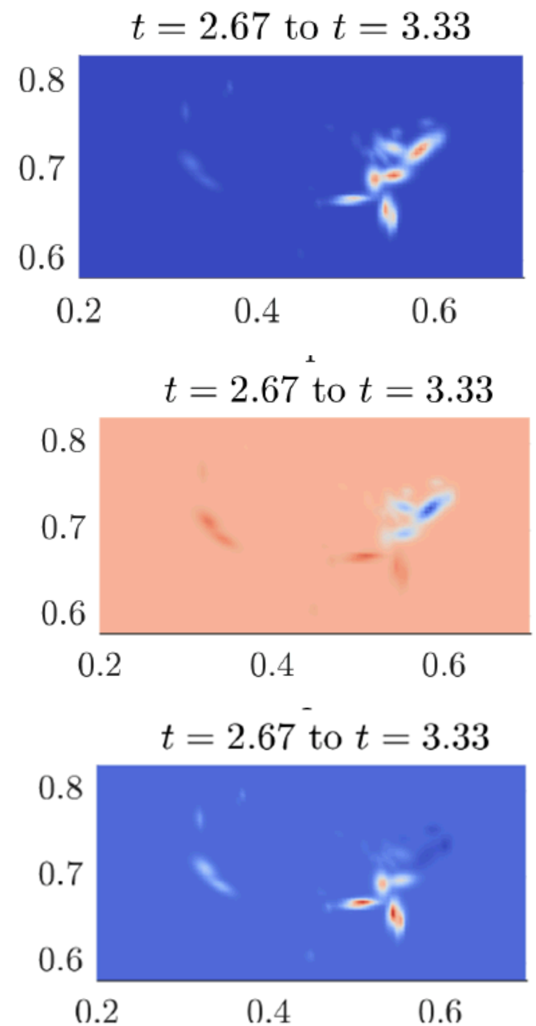
# Control problem

- constant spatial subregion and single temporal targets
- 50 spatial control points with three temporal periods
- evaluate risk neutral and CVaR



# Differences between RN and CVaR controls




Risk Neutral

Differences

CVaR