# *Atmospheric Source Estimation with Uncertainty Quantification for Urban Scales*

**Don Lucas, Akshay Gowardhan, Gardar Johannesson**
**Ron Baskett , Philip Cameron-Smith**

**Lawrence Livermore National Laboratory**

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**LLNL-PRES-656016**

# Atmospheric Source Estimation Team

**Ron Baskett, PI** (AEED/Atm Sci)

Overall responsibility for the project

**Philip Cameron-Smith, Co-PI** (AEED/Climate)

Guide implementation and technical lead

**Akshay Gowardhan** (AEED/Atm Sci)

AEOLUS model and urban case study

**Don Lucas** (AEED/Atm Sci)

Ensemble modeling and UQ methods

**Gardar Johannesson** (Engr/Statistics)

Monte Carlo source inversion methodology

**Matthew Simpson** (AEED/Atm Sci)

WRF modeling





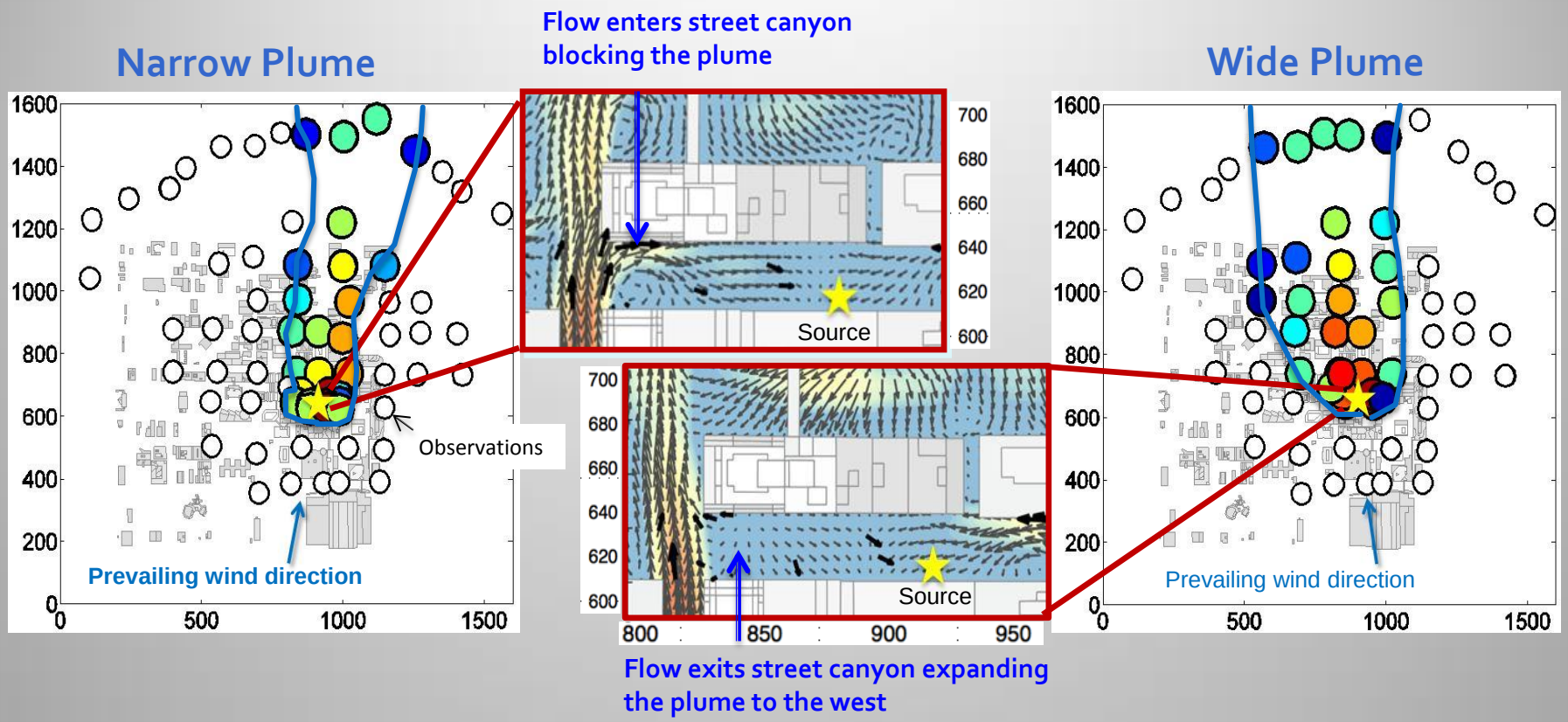








# Small changes in wind direction affect urban plumes



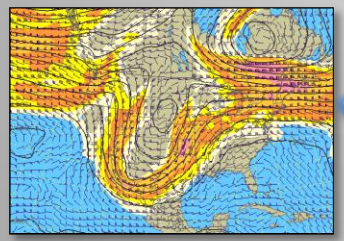

Accounting for meteorological uncertainty will help advance source estimation methodologies

# Atmospheric Source Estimation Using Monte Carlo

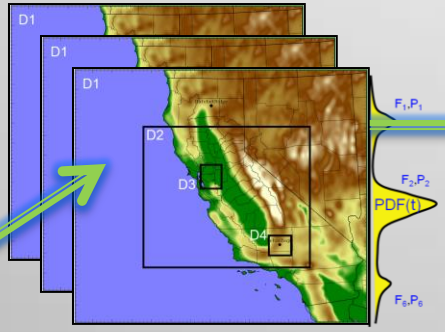
observations | source | measurement error

$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{\theta}, \boldsymbol{X}) + \boldsymbol{\delta}(\tau) + \boldsymbol{\varepsilon}(\sigma)$$

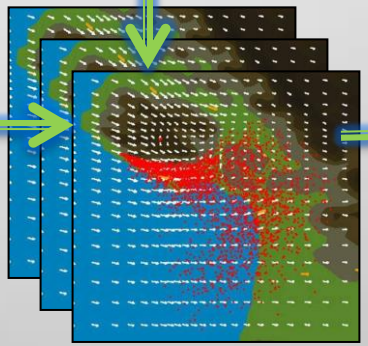
dispersion code | meteorology | model error



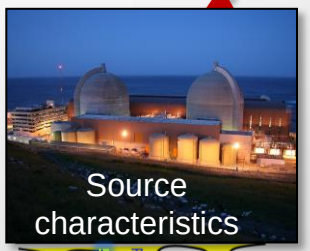
Gridded analyses




WRF regional model

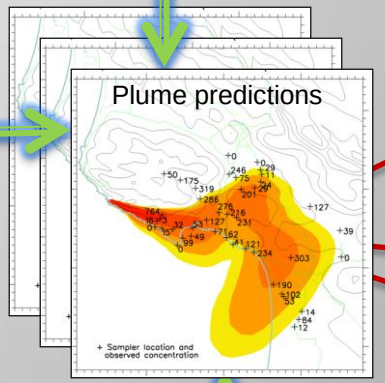


Dispersion model

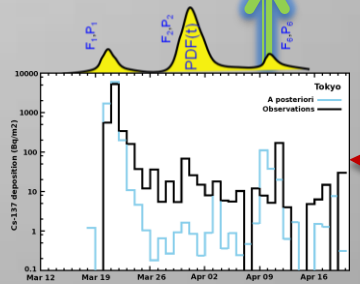





Field observations




Apply Monte Carlo optimization




Uncertainty & bias of model & obs

A

B

C

A = source loop

B = meteorology loop

C = discrepancy loop

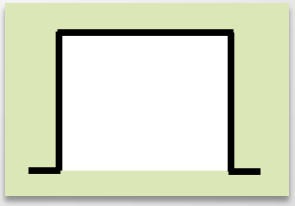
# Bayesian computation via Monte Carlo simulations

Bayes' Rule

$$P(X|Y) \propto P(Y|X)\ P(X)$$

posterior likelihood prior

Prior distribution of $X$

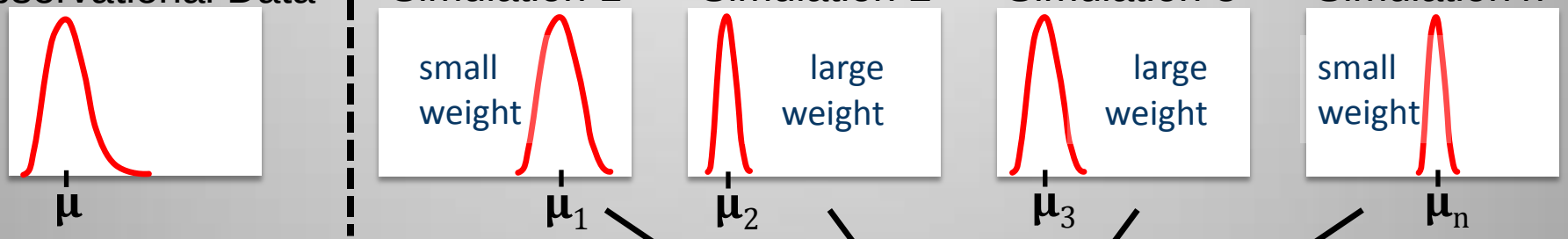


❷ Sample prior distribution

❶ Define observational target

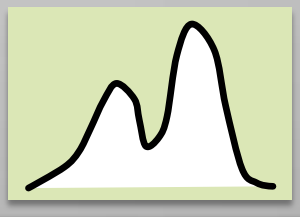
$X_1$ $X_2$ $X_3$ $X_n$

Observational Data | Simulation 1 | Simulation 2 | Simulation 3 | Simulation *n*




❸ Compute likelihood distance weights between simulations and observations

Posterior distribution of $X$



❹ Use likelihood weights to approximate posterior distribution

# OKC case study: source estimation for Joint Urban 2003

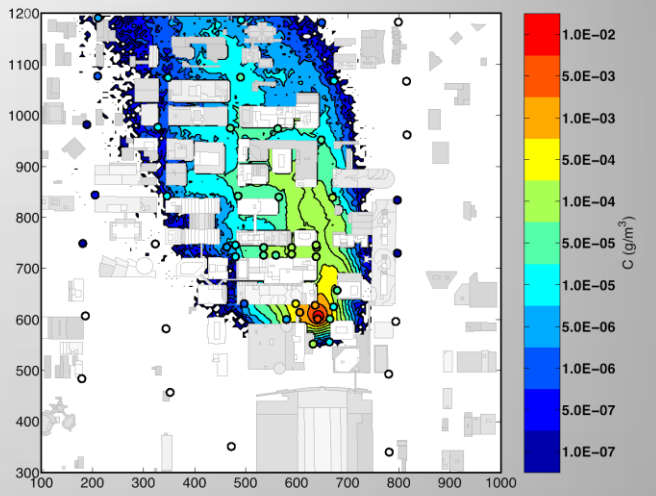
Aeolus Atmospheric Simulation Tool

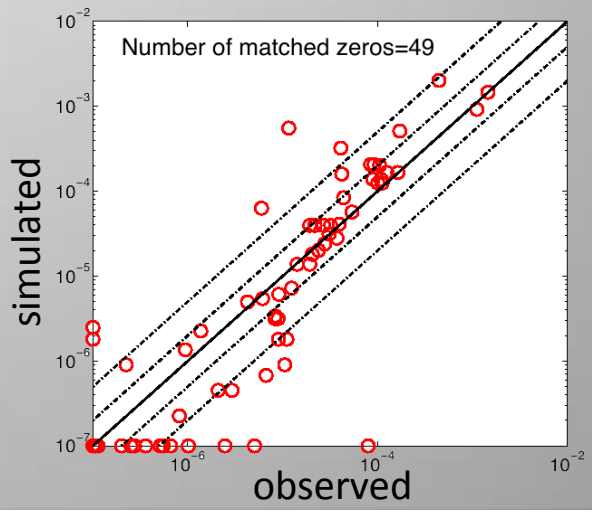
- AEOLUS [RANS + Lagrangian particles] was used to simulate 12 trials of Joint Urban 2003
- Previous: predicted and measured concentrations in "good" agreement
- Current goals: 1) use wind and concentration data to determine source location and strength and 2) add error bars to model predictions

| IOP# | FAC2 (%) | FAC5 (%) | FAC 10 (%) | Wind Model runtime* (sec) | Plume Model runtime* (sec) | Total runtime* (sec) |
|---|---|---|---|---|---|---|
| IOP2, Trial3 | 46.67 | 61.67 | 70.00 | 203.7 | 82.70 | 286.40 |
| IOP3, Trial1 | 38.71 | 67.74 | 72.58 | 202.7 | 67.10 | 269.80 |
| IOP3, Trial2 | 53.33 | 70.67 | 86.67 | 207.72 | 85.88 | 293.60 |
| IOP3, Trial3 | 60.87 | 86.95 | 89.85 | 203.53 | 78.93 | 282.46 |
| IOP8, Trial1 | 35.41 | 60.41 | 79.16 | 204.12 | 83.76 | 287.88 |
| IOP8, Trial2 | 47.69 | 75.38 | 86.15 | 211.17 | 82.14 | 293.13 |
| IOP8, Trial3 | 45.45 | 68.18 | 71.21 | 202.25 | 74.93 | 277.18 |
| IOP9, Trial1 | 54.05 | 64.86 | 78.37 | 204.23 | 83.54 | 287.77 |
| IOP9, Trial2 | 60.41 | 79.16 | 85.41 | 201.55 | 79.21 | 280.76 |
| IOP9, Trial3 | 47.62 | 66.67 | 80.95 | 198.62 | 72.33 | 270.95 |
| IOP10, Trial1 | 46.67 | 68.89 | 82.22 | 199.64 | 78.09 | 277.73 |
| IOP10, Trial2 | 37.78 | 55.55 | 73.33 | 208.27 | 84.62 | 292.89 |
| - | **47.88** | **68.84** | **79.65** | **203.95** | **79.43** | **283.38** |

IOP 8, Trial 2

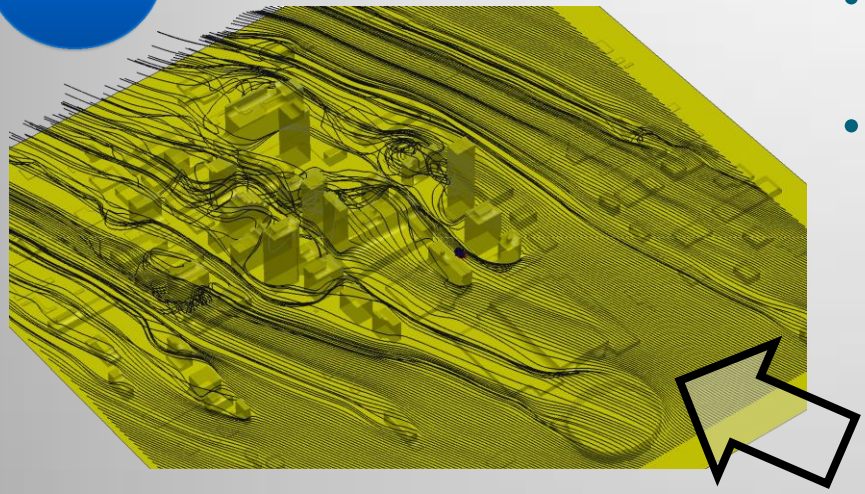
## Previous Validation Studies



# OKC case study: source estimation for Joint Urban 2003

Aeolus Atmospheric Simulation Tool

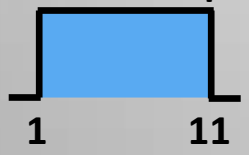


## Uncertainty in Inflow Conditions

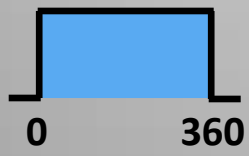
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- Now infer a distribution of inflow conditions using wind data collected from many sensors *within* the computational domain

Prior Distribu-tions

**inflow wind speed**



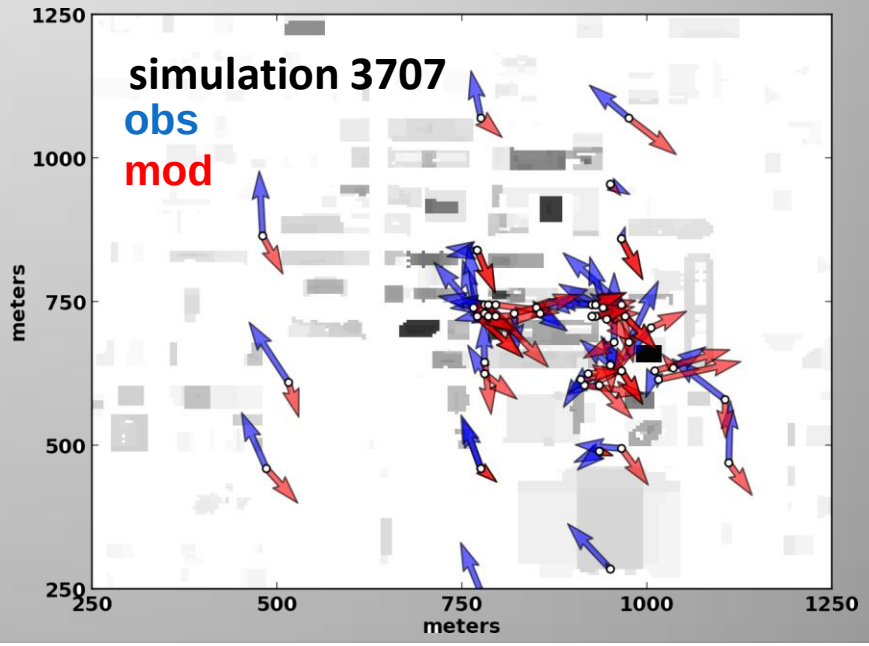

**inflow wind direction**




draw *N* samples

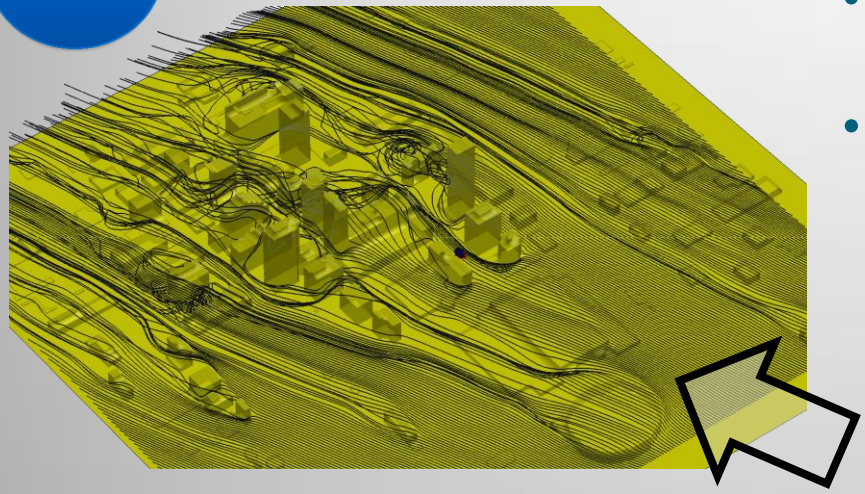
run AEOLUS at each sample

[25,000 samples simulated to date]



# OKC case study: source estimation for Joint Urban 2003

Aeolus Atmospheric Simulation Tool

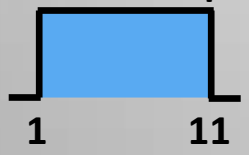


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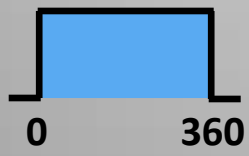
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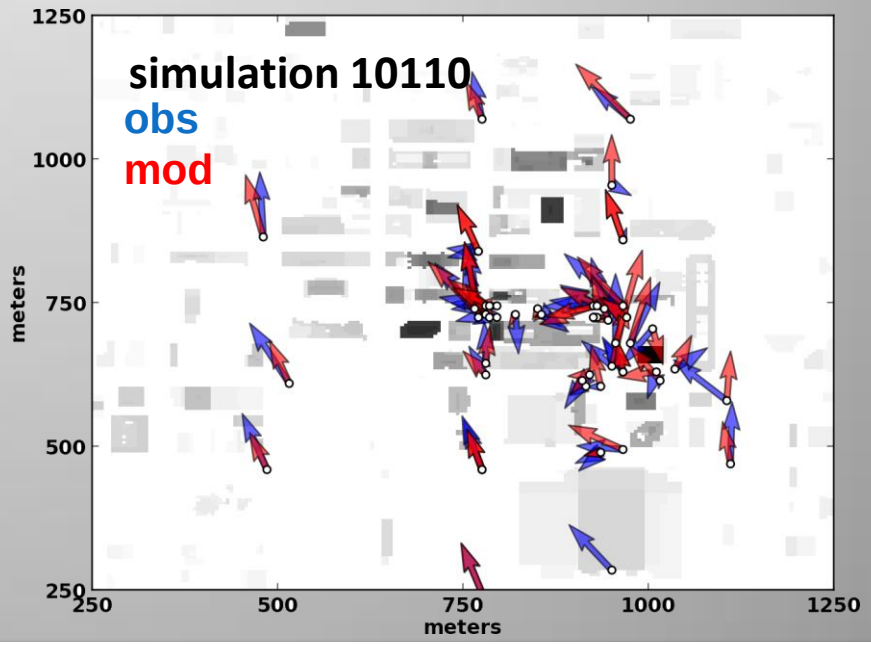

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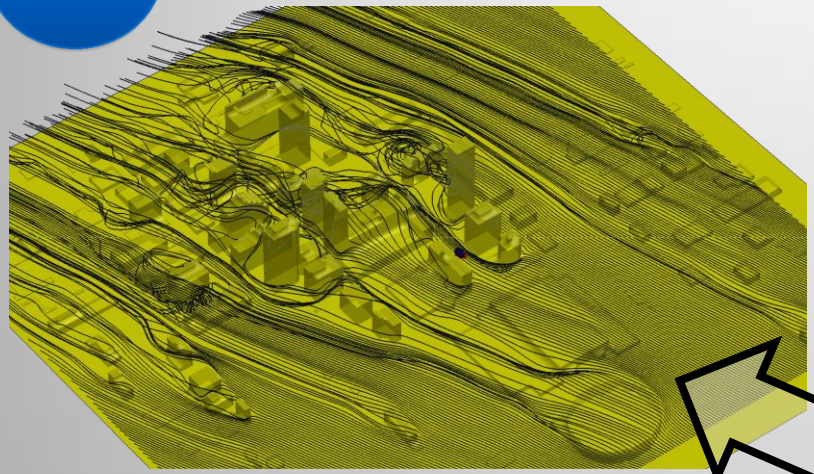
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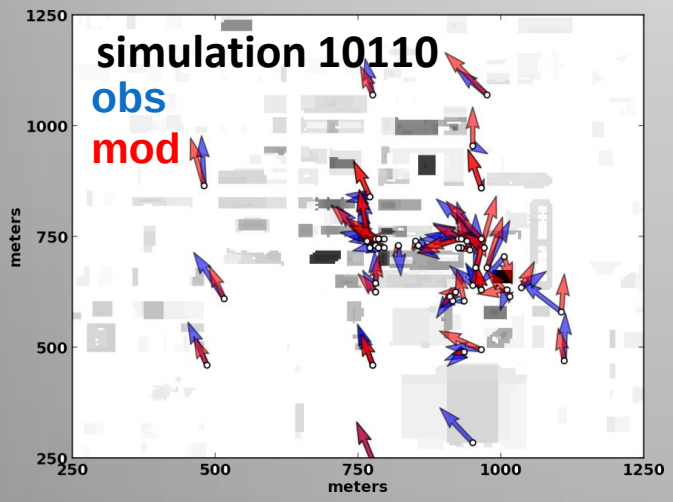
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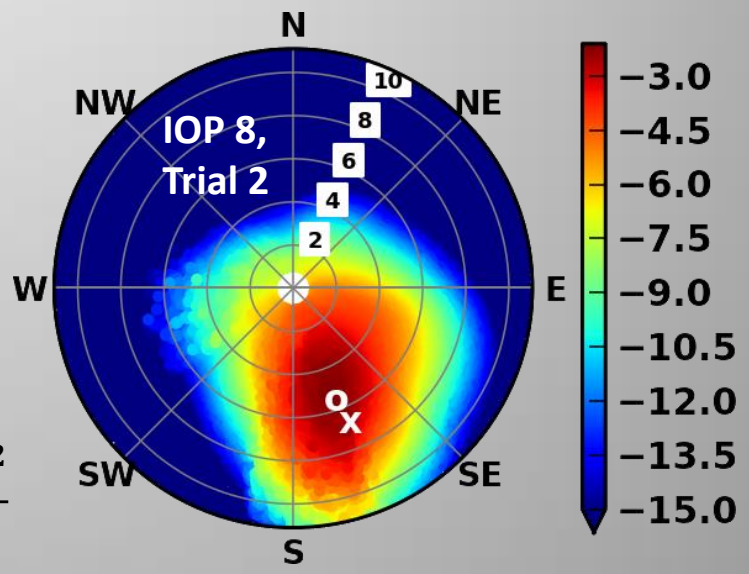
## Uncertainty in Inflow Conditions

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compute likelihood weights

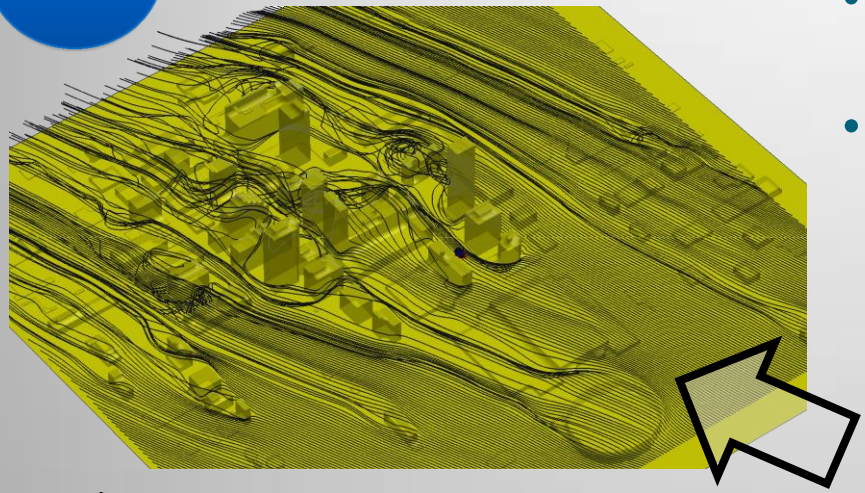
$$\log L \propto \sum \frac{-(y_m - y_o)^2}{2\sigma^2}$$




x = upstream [6.8 m/s, 157 deg]
o = inferred [5.6 m/s, 159 deg]

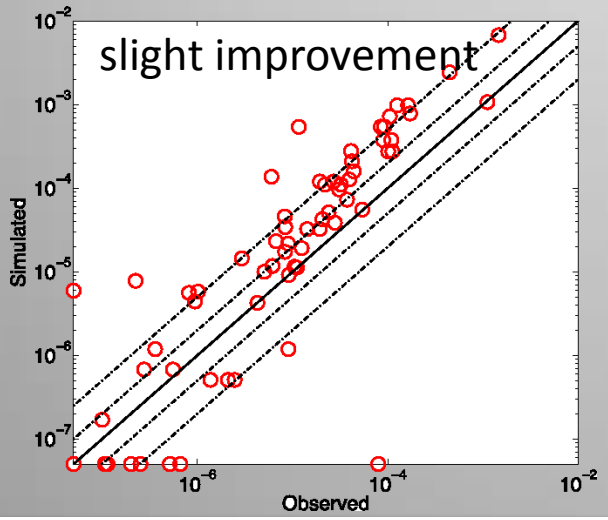
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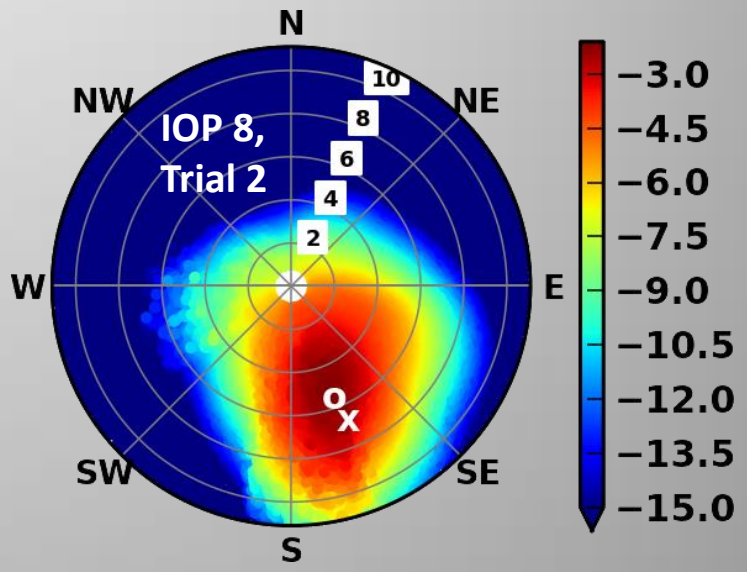


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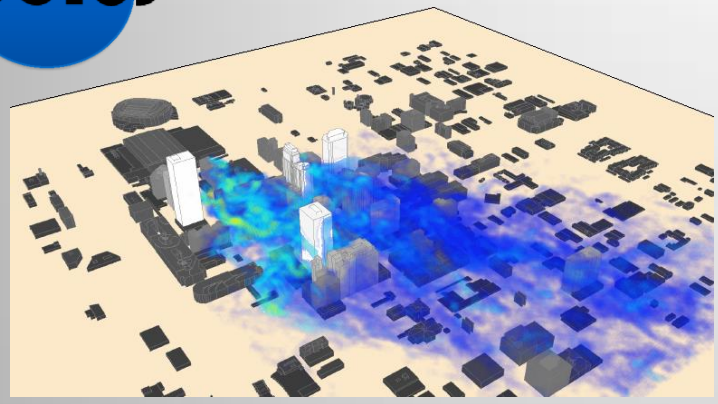

particle simulation at maximum likelihood winds




**x = upstream [6.8 m/s, 157 deg]**
**o = inferred [5.6 m/s, 159 deg]**

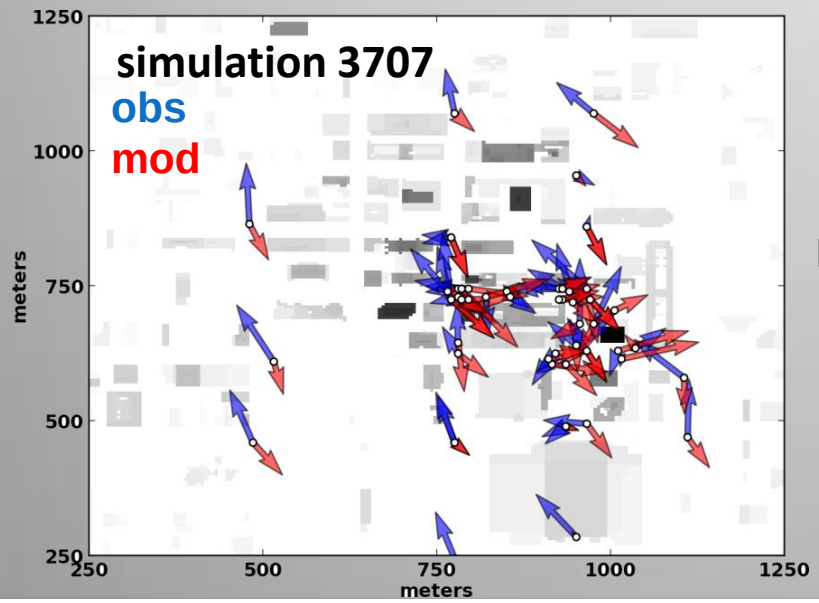
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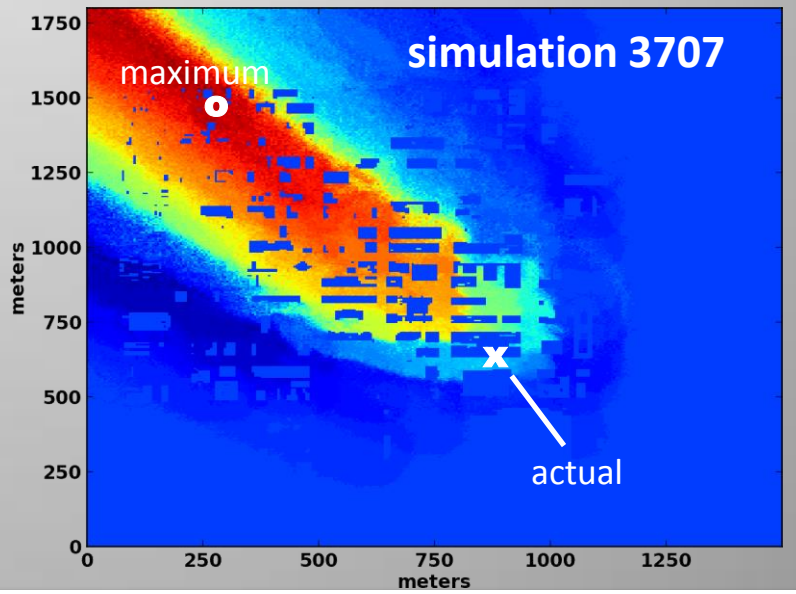


## Source location via back trajectory ensemble

- Run back trajectories for each simulation in the wind ensemble
- Concentration sensors
  - "hit" sensors have +1 source
  - "miss" sensors have -1 source
- Apply wind likelihood weights to back trajectories

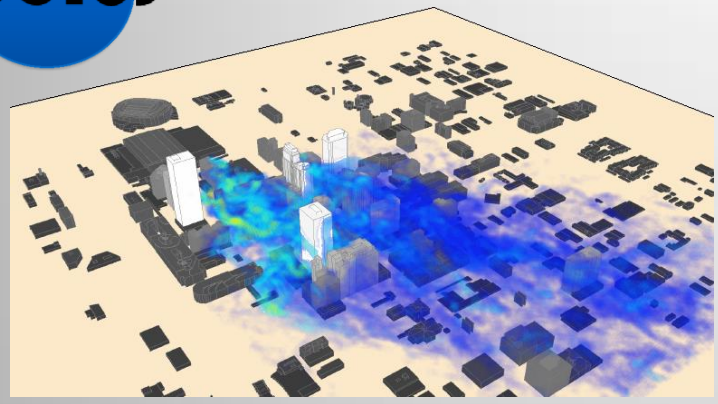



low likelihood



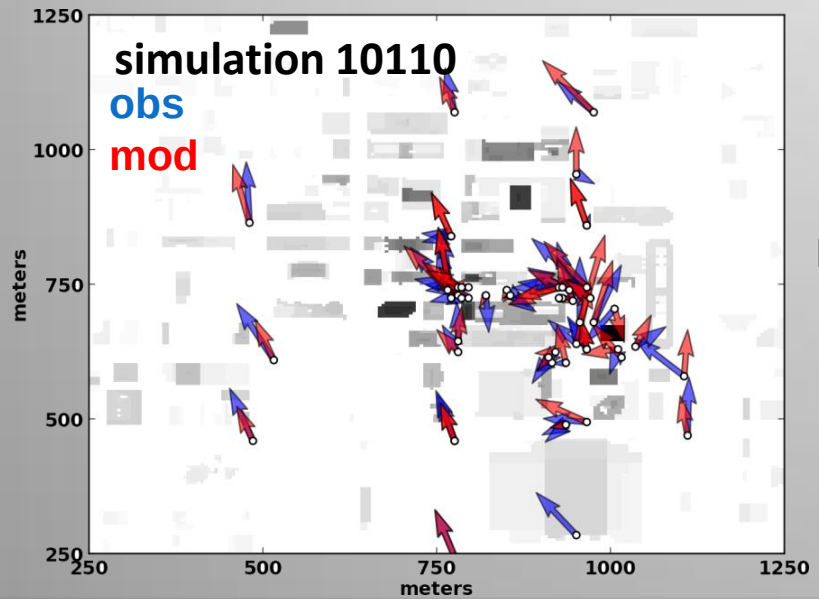
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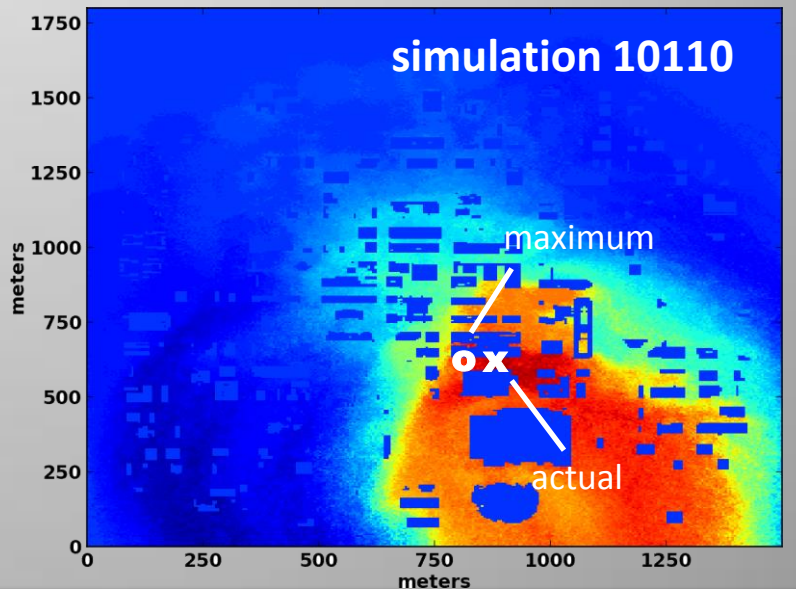


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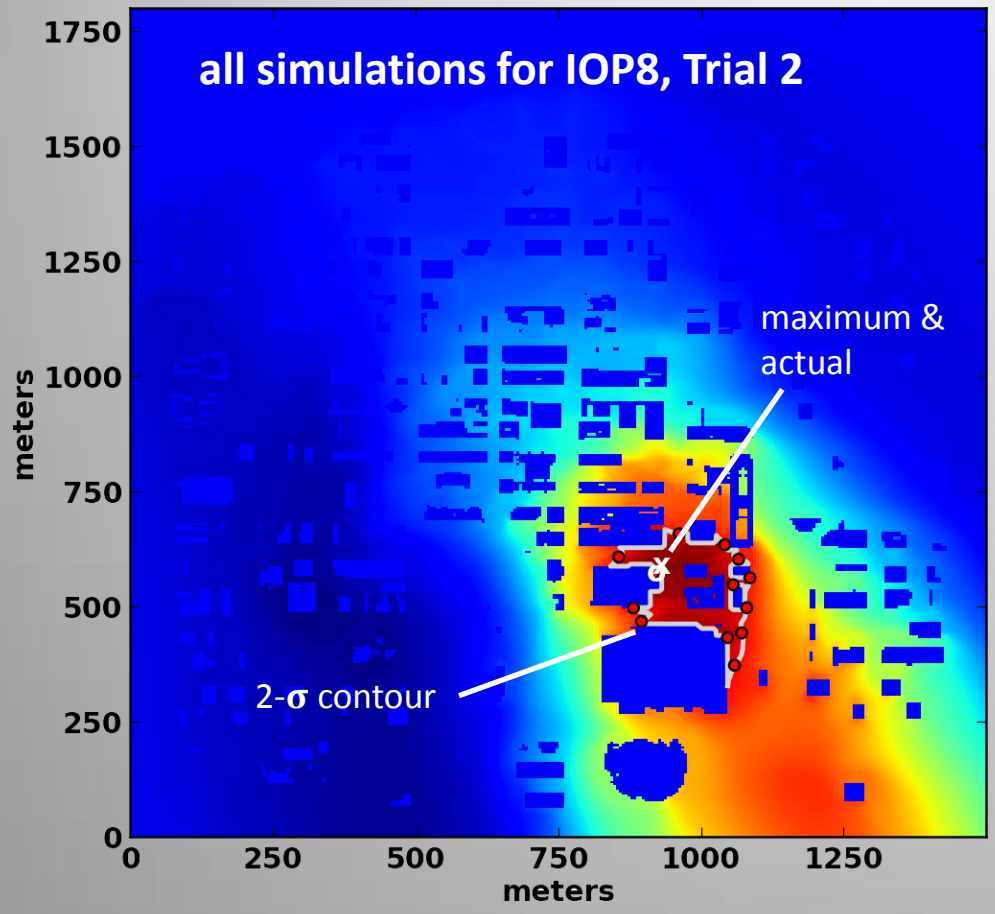

high likelihood



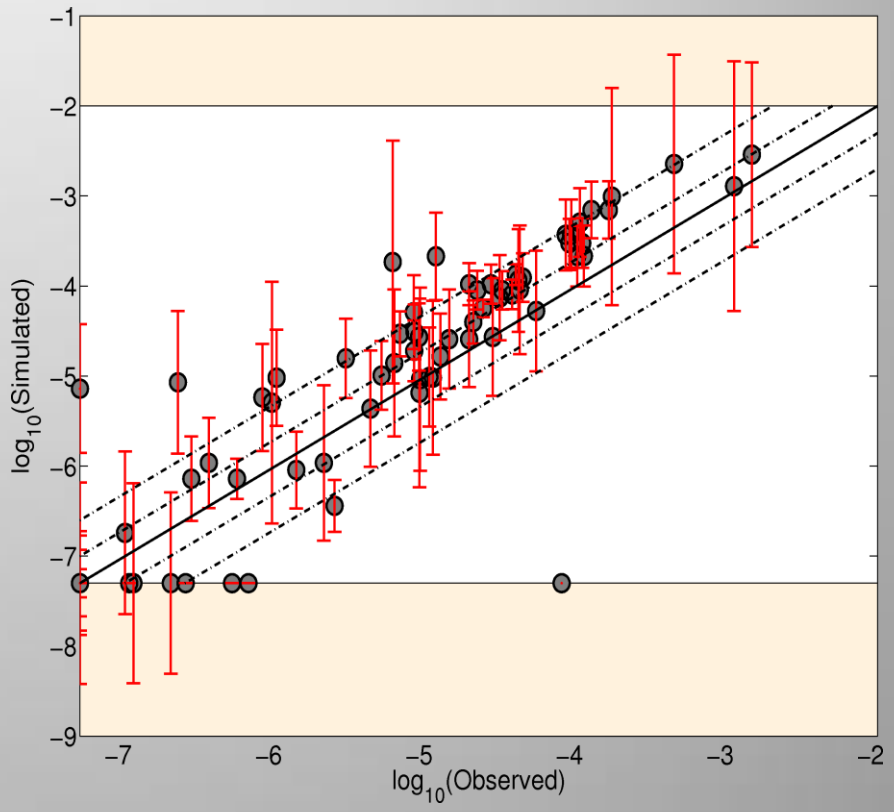
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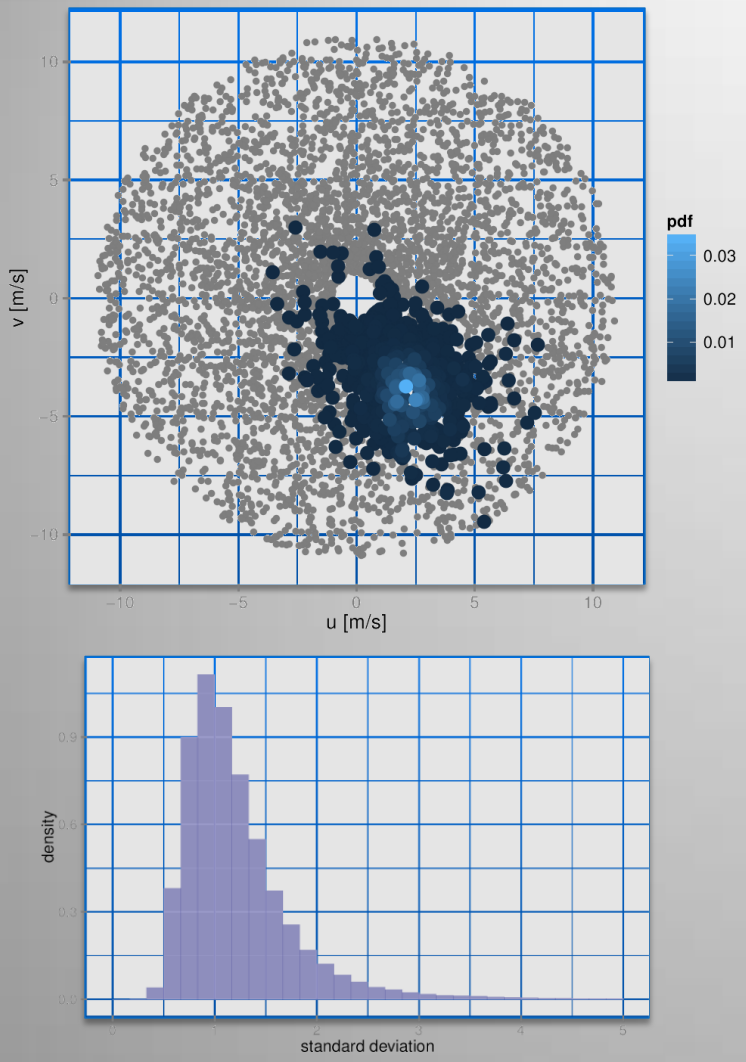
## Source location via back trajectory ensemble




Validation plot for IOP8, Trial 2



# Looking forward



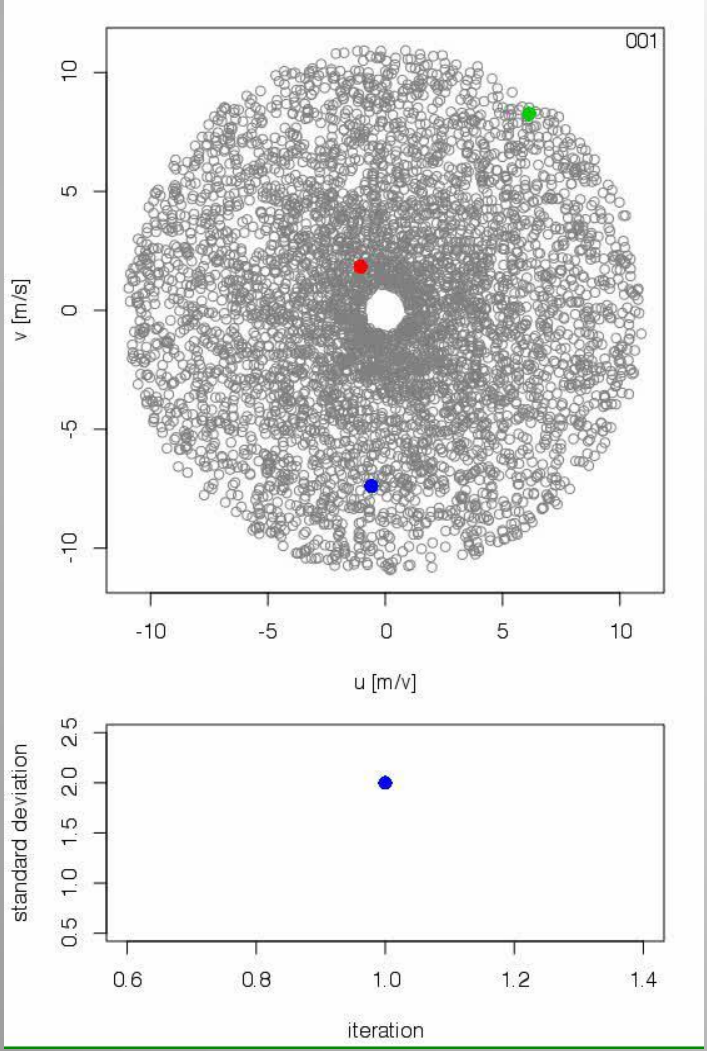

Need to estimate observation error and prediction bias parameters

Use MCMC to jointly sample posterior distribution of:

- meteorological input parameters
- meteorological observation error and bias parameters
- dispersion source parameters
- concentration observation error and bias parameters

*Example:* sample met u-v input parameters and standard deviation parameters for a Gaussian error model for the difference in predicted and observed u-v wind components

# Looking forward




Need to estimate observation error and prediction bias parameters

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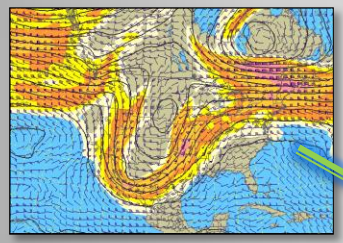
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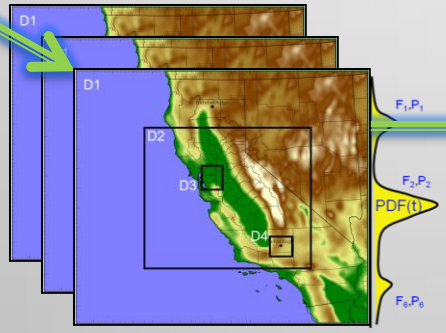
# *Questions?*



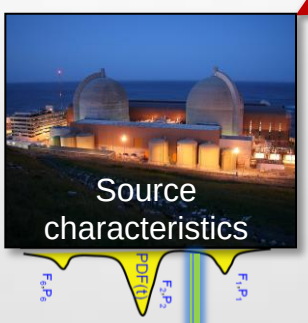
# Atmospheric Source Estimation Using Monte Carlo

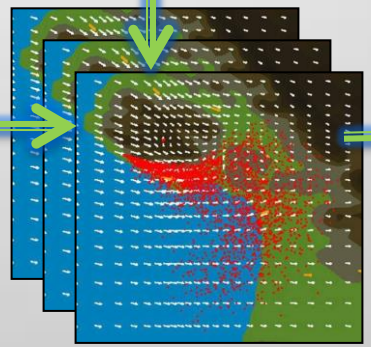


Gridded analyses




WRF regional model

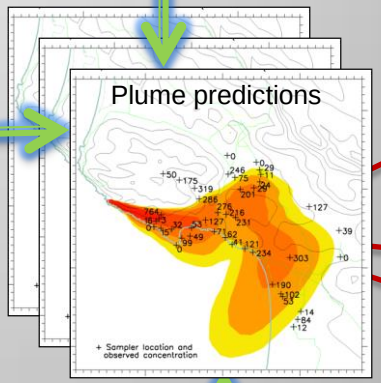


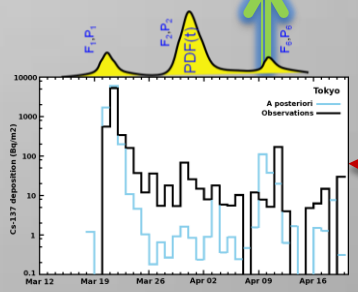



Dispersion model



Field observations




Uncertainty & bias of model & obs

A

B

C

Apply Monte Carlo optimization

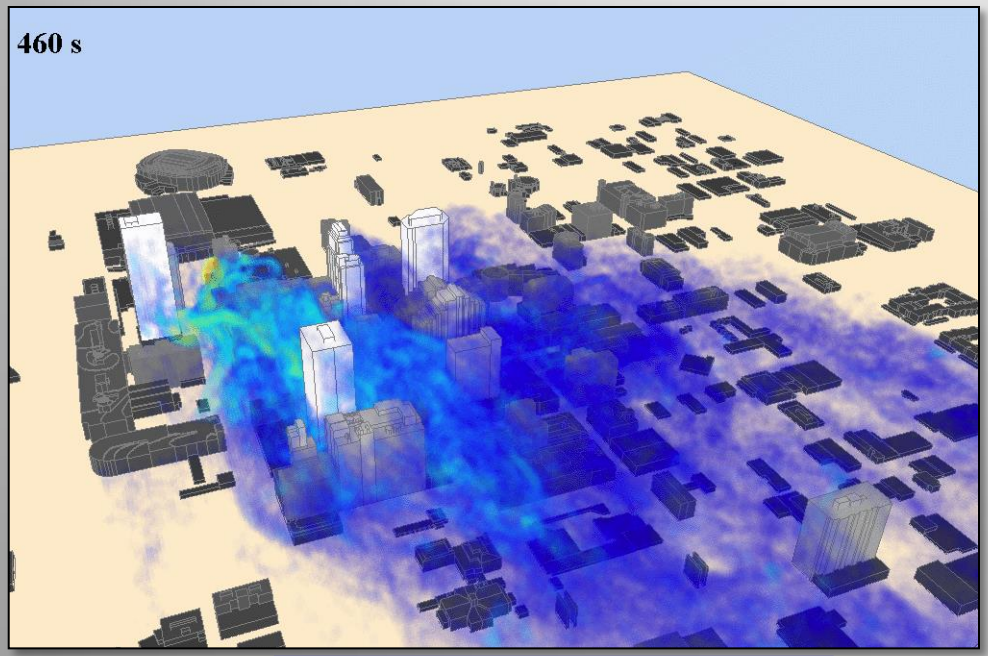
A = source loop
B = meteorology loop
C = discrepancy loop

# Phase one: source characteristics

observations | **source characteristics** | dispersion model error

$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{\theta}, \boldsymbol{X}) + \boldsymbol{\delta}(\tau) + \boldsymbol{\varepsilon}(\sigma)$$

dispersion code | meteorology | measurement error




2003 Oklahoma City test case

## A Source Inversion

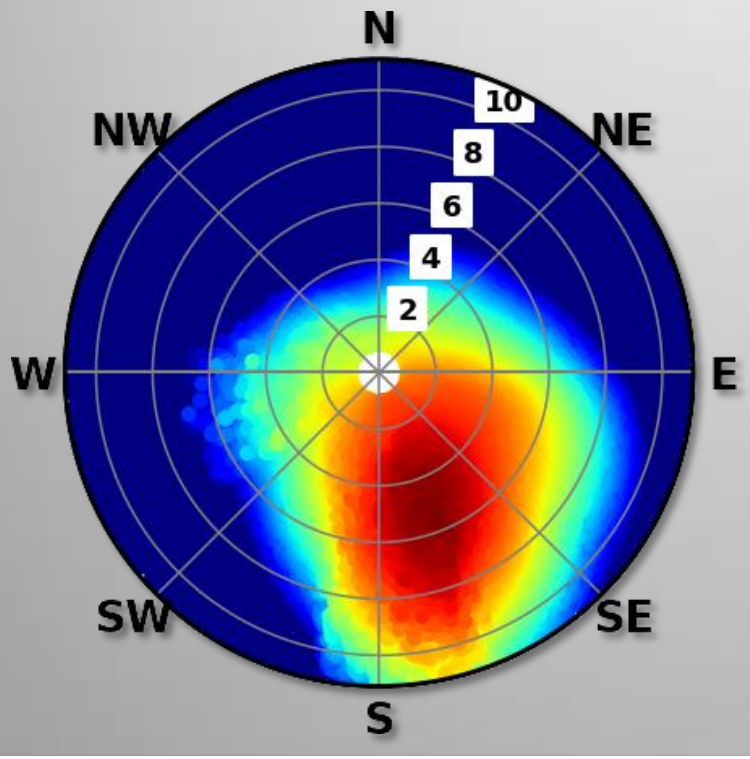
Developing efficient and adaptive Bayesian Monte Carlo methods to estimate the probability distributions of the source properties.

# Phase two: uncertainty in meteorology

observations | source characteristics | dispersion model error

$$y = F(\theta, X) + \delta(\tau) + \varepsilon(\sigma)$$

dispersion code | **meteorology** | measurement error




## B Uncertainty in Meteorology

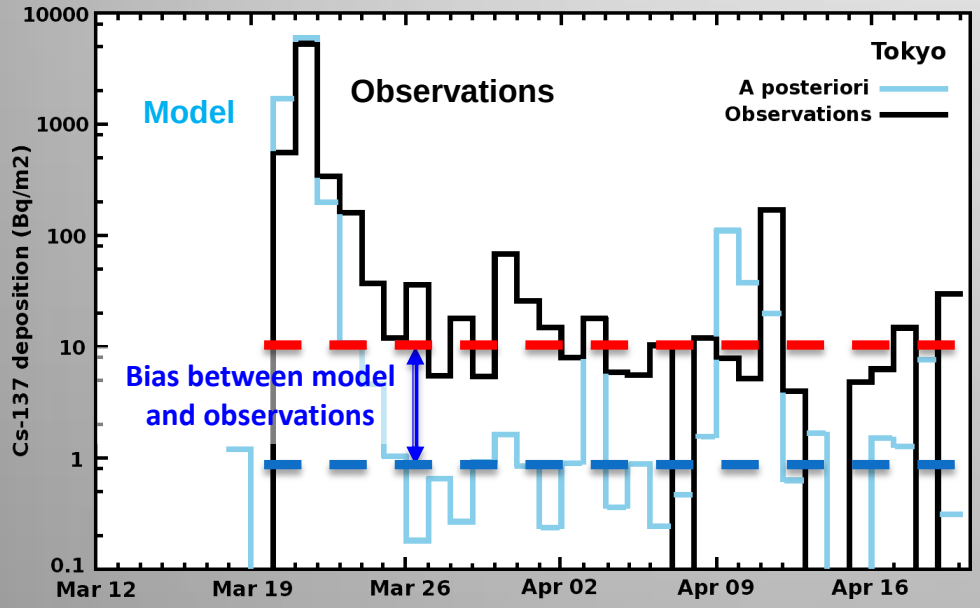
Determining ways to sample meteorological uncertainty (initial state, inflow and lateral boundary meteorology, and model physics) in a computationally efficient way.

# Phase three: model and measurement biases

observations | source characteristics | **dispersion model error**

$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{\theta}, \boldsymbol{X}) + \boldsymbol{\delta}(\tau) + \boldsymbol{\varepsilon}(\sigma)$$

dispersion code | meteorology | **measurement error**




C

## Model and Measurement errors

Models and measurements are imperfect, which causes residual errors between the observations and model predictions. We are developing methods to identify the biases and intrinsic variability.