RADIONUCLIDE ATMOSPHERIC TRANSPORT

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Radionuclide transport modeling: Outline

- Overall objectives
- Atmospheric transport model (ATM) description
  - Forward and adjoint formulations
  - Bayesian updating of source estimation
- Preliminary ATM code benchmarking with volcanic ash data
- Source estimation study with synthetic binary source
- Access to IMS radionuclide data

Radionuclide transport modeling for CTBT verification

- Support NNSA GNDD Technology Roadmap
  - Develop accurate radionuclide (RN) atmospheric transport modeling (ATM) capability to monitor clandestine nuclear fuel cycle activities
  - Assess uncertainties in RN source estimation
- Compare and benchmark ATM codes with atmospheric transport data
- Benchmark ATM codes with available RN data from IMS stations
- Coordinate with seismic and infrasound data

Atmospheric Transport Model

- Advection-diffusion equation for RN concentration χ:

$$L\chi = \frac{\partial\chi}{\partial t} + \mathbf{u}\cdot\nabla\chi - \nabla\cdot k\nabla\chi - \alpha\chi = q$$

$\alpha =$ scavenging/deposit, radioactive decay/buildup

$q =$ RN source

Lagrangian formulation: $L\chi = \frac{d\chi}{dt} - \nabla\cdot k\nabla\chi - \alpha\chi = q$

- Adjoint (backward) formulation for observation R:

$R = \langle h, \chi\rangle$, with $L^{+}\chi^{+} = h =$ detector response

$$R = \langle L^{+}\chi^{+}, \chi\rangle = \langle \chi^{+}, L\chi\rangle = \langle \chi^{+}, q\rangle$$

$$\Rightarrow L^{+}\chi^{+} = -\frac{d\chi^{+}}{dt} - \nabla\cdot k\nabla\chi^{+} - \alpha\chi^{+} = h$$

$\Rightarrow$ Calculate responses to multiple sources through single χ^{+}.

Bayesian updating of source estimation

- Reaction rate for detector response $h(\mathbf{r}_i)$ and source $q(\mathbf{r}_j) \equiv q_j$:

  $$R(\mathbf{r}_i \mid q_j) = \left\langle h(\mathbf{r}_i), \chi(\mathbf{r}_i) \right\rangle = \left\langle \chi^+(\mathbf{r}_i), q(\mathbf{r}_j) \right\rangle$$

- Initial estimate for PDF for source $P[q(\mathbf{r}_j)] \equiv P(q_j)$

  Relationship between source and reaction rate $P[R(\mathbf{r}_i \mid q_j) \mid q_j]$

  Bayes theorem provides updated estimate for source

  $$\Rightarrow P[q_j \mid R(\mathbf{r}_i \mid q_j)] = \frac{P(q_j) P[R(\mathbf{r}_i \mid q_j) \mid q_j]}{\int P(q_j') P[R(\mathbf{r}_i \mid q_j') \mid q_j'] dq_j'}$$

  Markov chain Monte Carlo (MCMC) algorithm used.

- Alternately, may use the likelihood function

  $P[\chi^+(\mathbf{r}_i) \mid q_j]$ instead of $P[R(\mathbf{r}_i \mid q_j) \mid q_j]$.

HYSPLIT and FLEXPART atmospheric transport codes

- Lagrangian transport model
- Removal processes: deposition, radioactive decay
- Forward and adjoint modeling

<u>HYSPLIT</u>

- Used in PNNL and others
- Graphical user interface
- Available through NOAA ARL
- Supports many meteorological data sets with conversion

<u>FLEXPART</u>

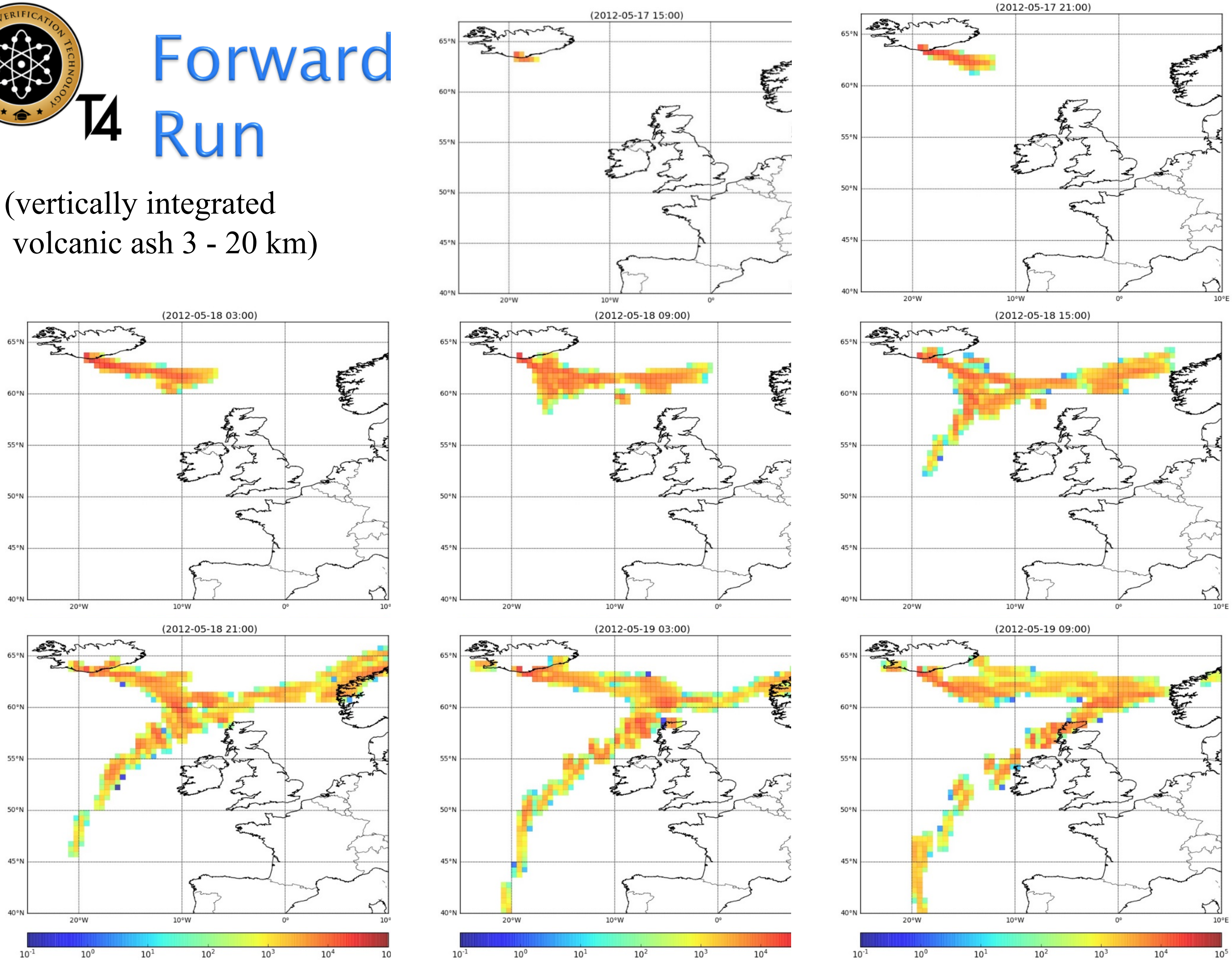
- Used by CTBTO and others
- Command-line interface
- Open source
- Supports ECMWF and NCEP GFS meteorological data

Verifying FLEXPART simulations

- Compared our simulation output (v9.0) with a known volcanic study case output (v8.2)
- Employed same input and weather data (GFS)
- Information of volcanic study case:
  - Location and release particles based on the eruption of the volcano Eyjafjallajokull in Iceland
  - Employed weather data on a different period from actual volcanic eruption
  - Forward run for 72 hours and output averaged over 3 hours

Forward Run

(vertically integrated volcanic ash 3 - 20 km)



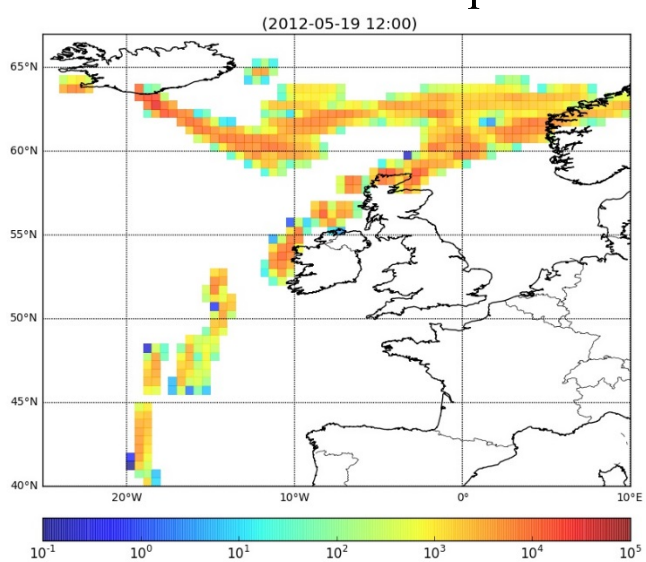
Verifying FLEXPART output

1. Plume centroid latitude position comparison

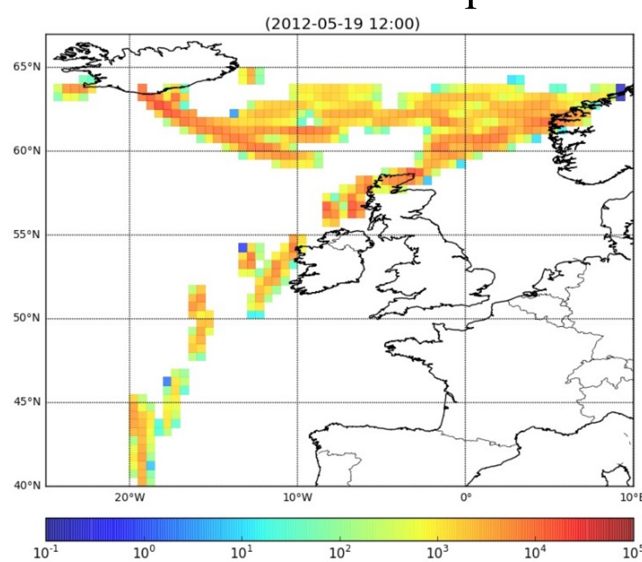
Cluster #10	Benchmark	Simulation	Diff %
Day 0	63.35	63.35	–
Day 1	62.11	62.10	0.016%
Day 2	61.88	61.83	0.081%
Day 3	62.55	62.53	0.032%

2. Final dispersion snapshot after 72 hours

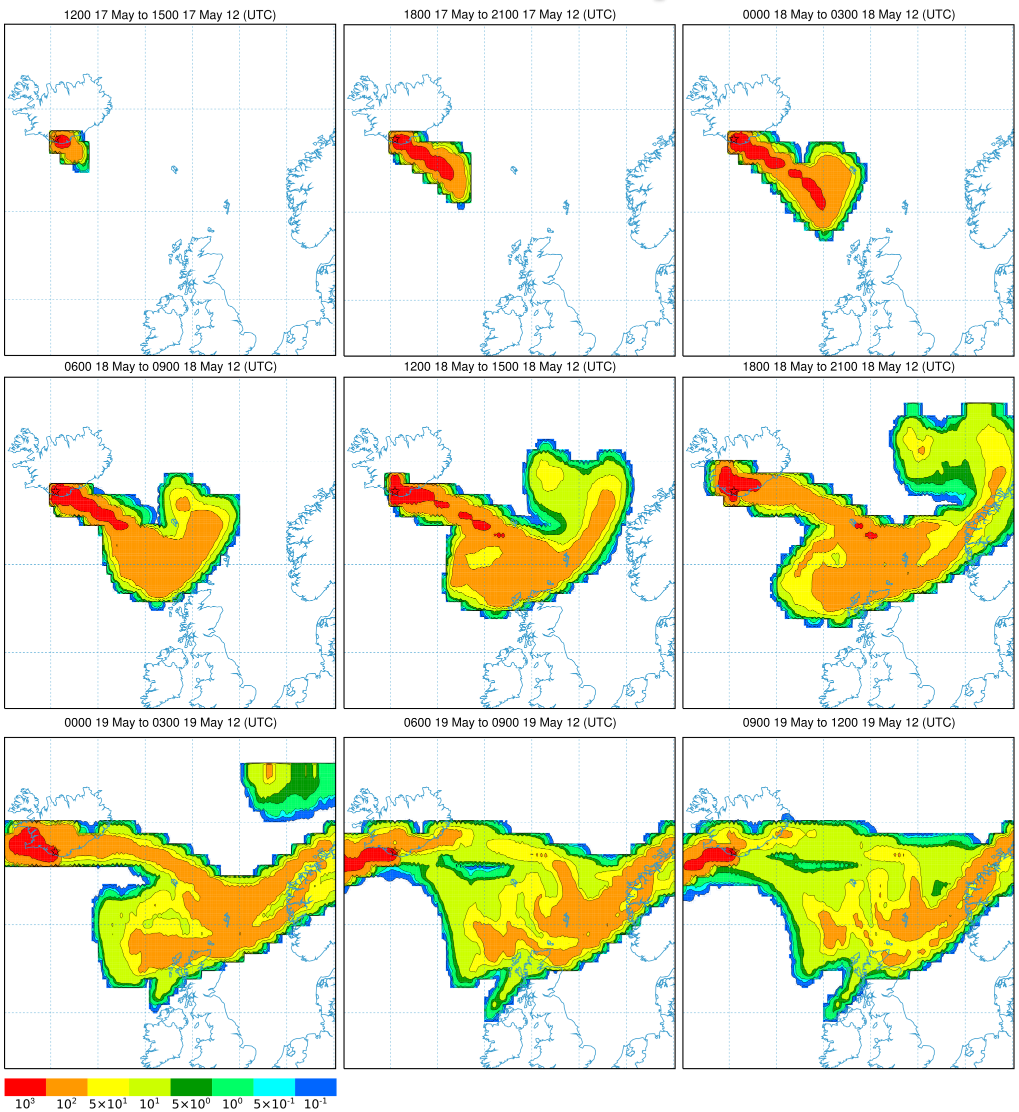
Benchmark output



Simulation output



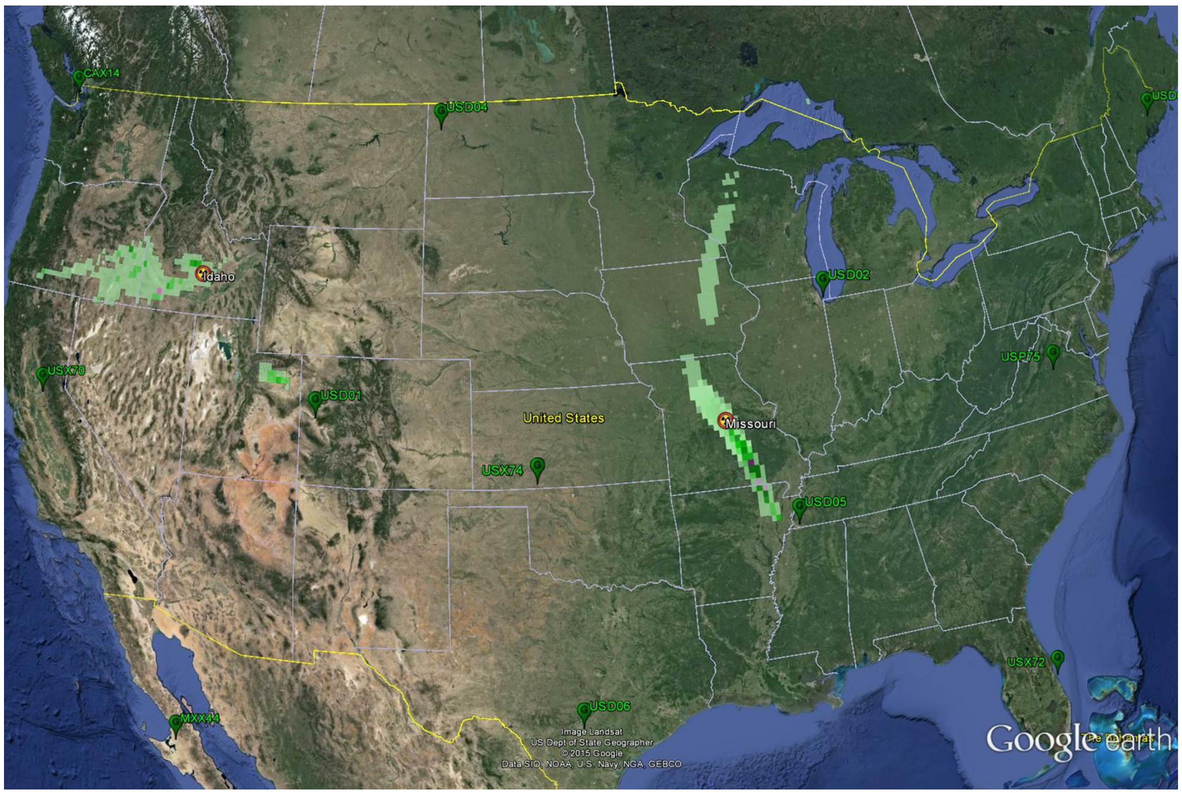
HYSPLIT simulation of volcanic ash study



- FLEXPART shows south-west plume movement not seen in HYSPLIT
- Magnitudes are on same order
- Quantitative analysis to come
- Different meteorological data set

Bayesian data assimilation methods with synthetic data

- Generate synthetic data using 120-144 hours of forward ATM and 11 measurement locations
- Determine source parameter distribution using backward ATM up to 96 hours before initial detect

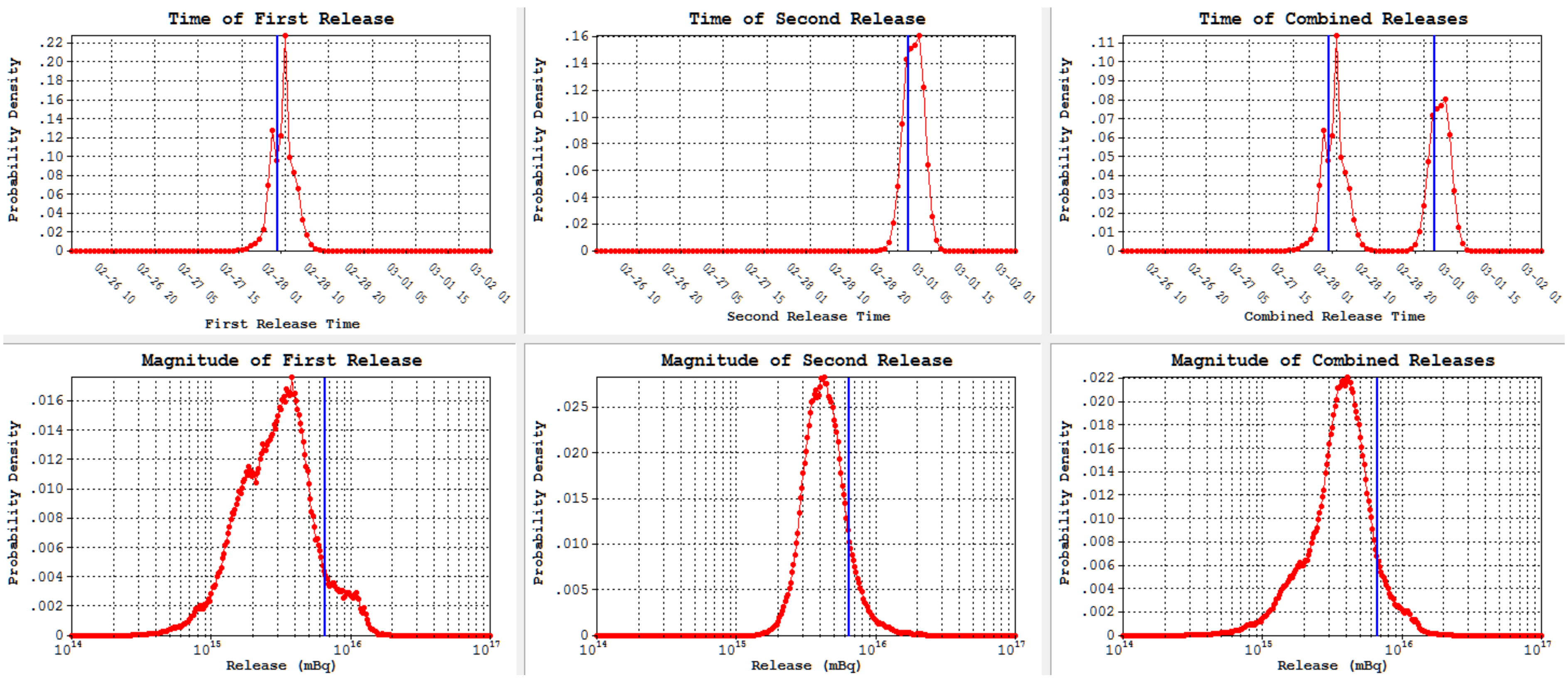


Two sources, disjoint plumes:

- 6.45×10^{15} mBq
- 1 hour release
- Idaho: 2/28/13
- Missouri: 3/1/13

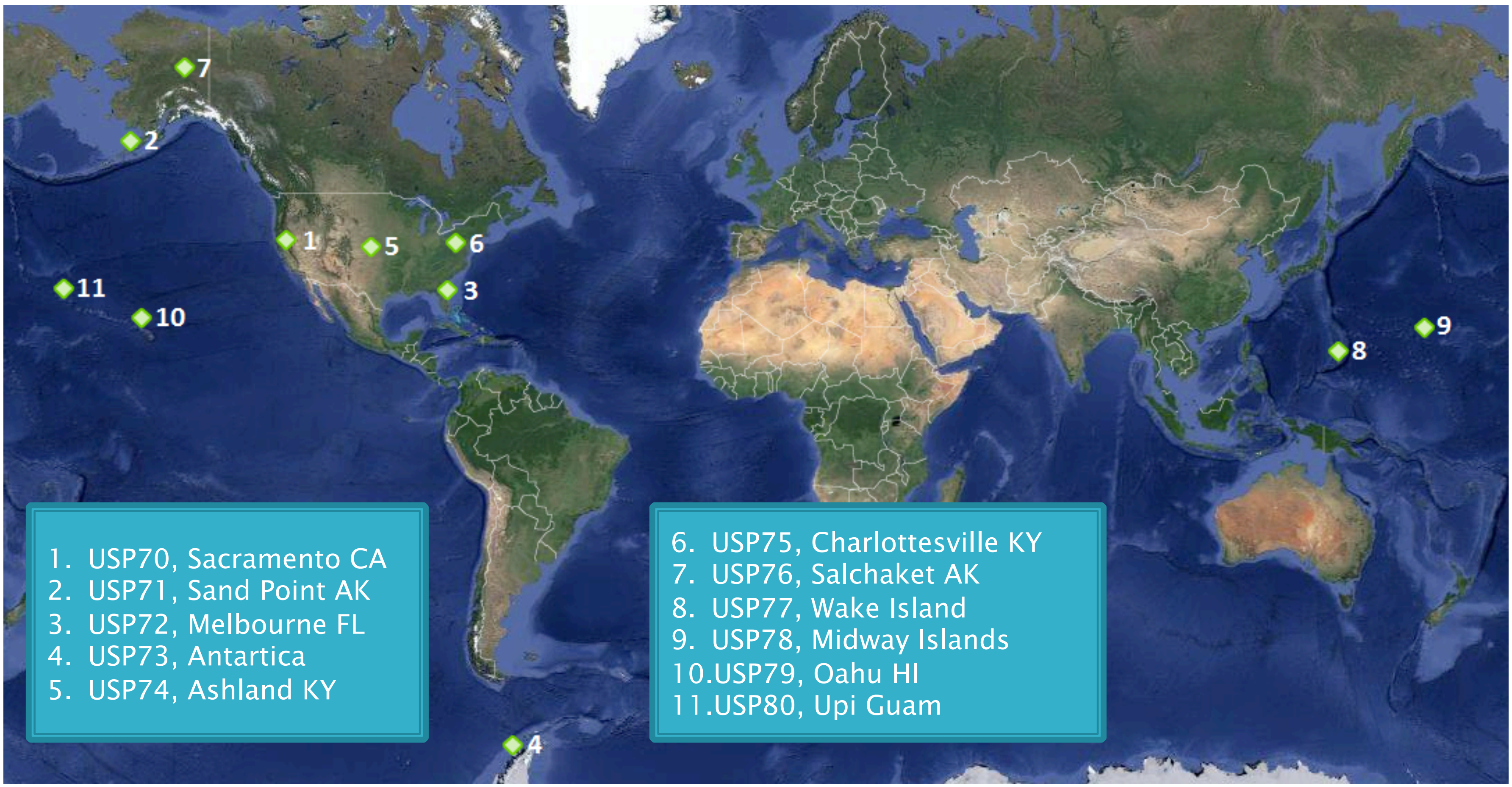
Adjoint MCMC analysis

- Uniform source parameter prior distribution
- Sample from posterior distribution



International Monitoring System (IMS)

- Obtained access to Fukushima radionuclide data for 11 U.S. IMS stations
- Initial simulation of Cs and I data is in progress



Future tasks

- Complete benchmarking the HYSPLIT and FLEXPART codes for volcanic ash data
- Simulate Fukushima IMS radionuclide data with the ATM codes
- Reconstruct radiological source using adjoint ATM with IMS data
- Characterize uncertainties in ATM and source reconstruction
- Explore maximum likelihood estimation (MLE) or Kalman filter algorithms for optimal source estimation