Sensor Data Fusion Working Group
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Tracking Atmospheric Plumes Using Stand-off Sensor Data

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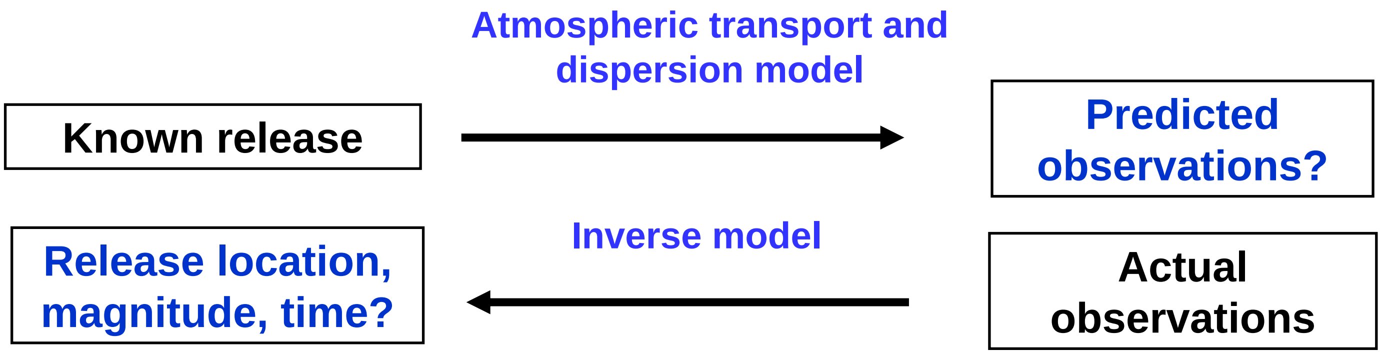
The Inverse Problem



C. Wunsch, The Ocean Circulation Inverse Problem, Cambridge University Press,1996:

“An inverse problem, is one that is the inverse to a corresponding forward or direct one, interchanging the roles of at least some of the knowns and unknowns”.

Fundamental aspect: the quantitative combination of theory and observation

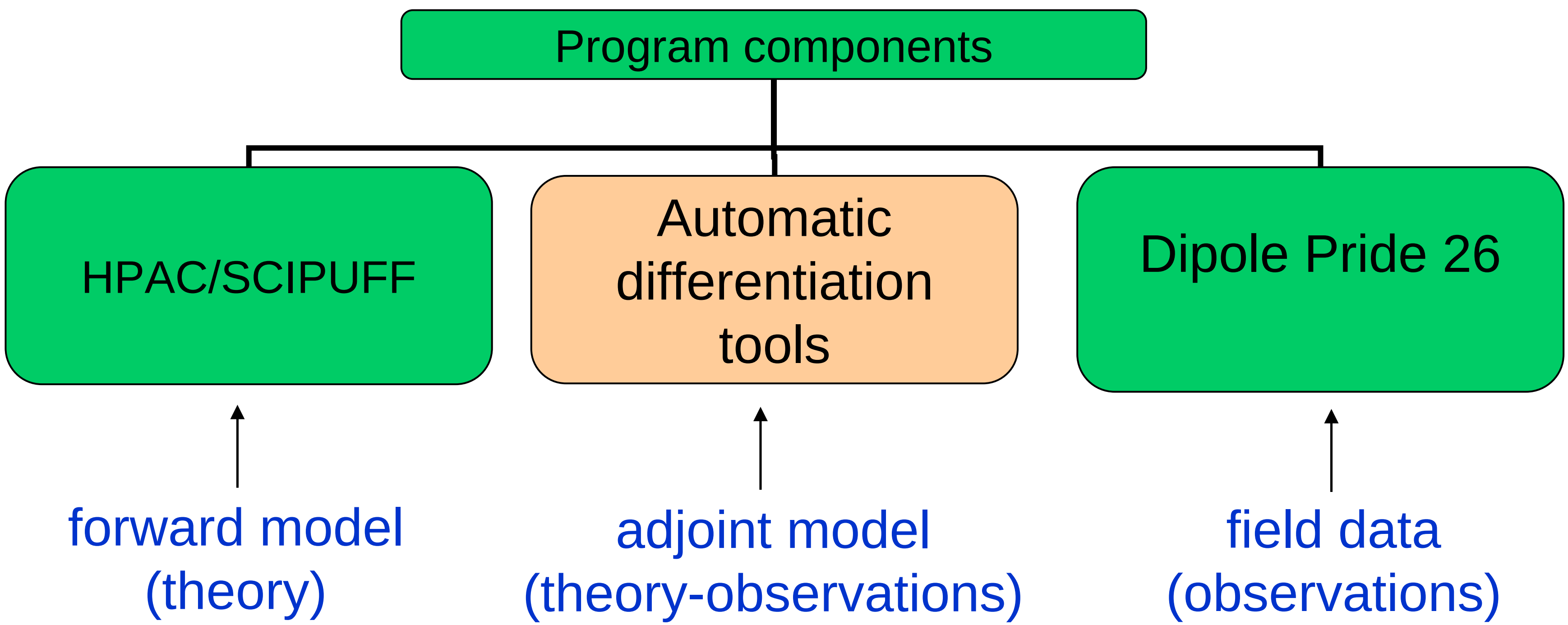
Adjoint Models

Numerical tools which provide the quantitative combination of theory and observations needed for the inverse modeling of physical systems.

- Adjoint model applications:
  - **Data assimilation: optimize model-to-data fit**
  - **Model tuning: optimize model equations**
  - **Sensitivity analysis: propagation of anomalies**

What We're Doing

Developing the adjoint model for a state-of-the-art atmospheric transport and dispersion model to characterize the source of a hazardous material release using stand-off detection data.



Automatic Differentiation

Adjoint and tangent-linear models are developed directly from the numerical code for the dynamical model.

$$\vec{\lambda}(t) = M_{\Lambda} M_{\Lambda-1} \cdots\cdots M_0 \bullet \left(\vec{\beta}\right) \qquad \delta^* \beta = M_0^T M_1^T \ldots M_{\Lambda}^T \bullet \left(\delta^* \vec{\lambda}\right)$$

Giering, Ralf and Kaminski, Thomas, Recipes for Adjoint Code Construction, ACM Trans on Math. Software, 24, 437-474, 1998.

Each line of code is view as an elementary operator M_{Λ}

$\rightarrow$ use rules for ordinary differenti ation

$\rightarrow$ code for elementary Jacobians

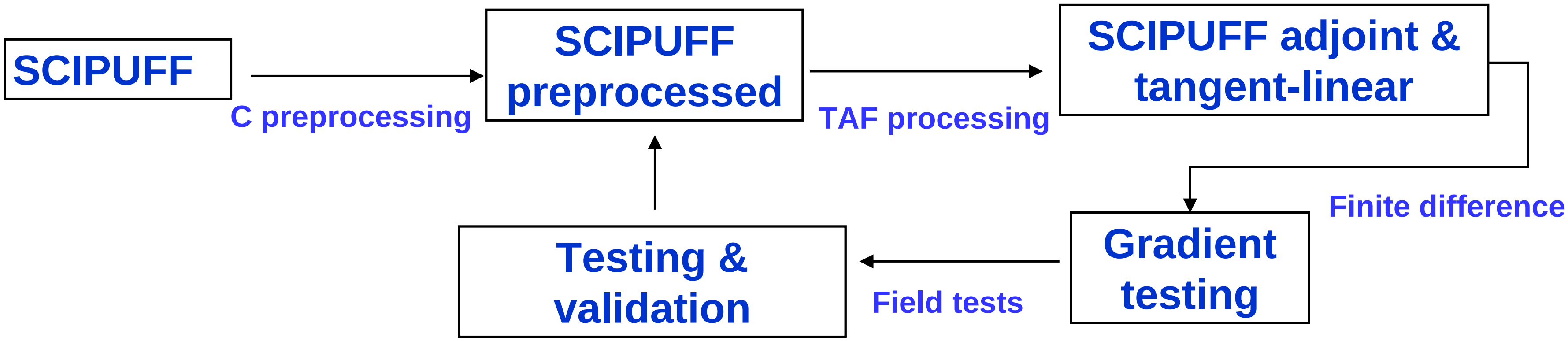
$\rightarrow$ use chain rule to compose M_{Λ}

Second-order Closure Integrated Puff (SCIPUFF)

- Features
  - Lagrangian Gaussian puff model.
  - Ensemble-average dispersion and a measure of the concentration field variability.
  - Second-order turbulence closure techniques
    - Relates dispersion rates to turbulent velocity statistics
    - Predicts statistical variance in the concentration field
  - Complete moment-tensor description
    - Wind shear distortion
    - Puff splitting algorithm and multi-grid adaptive merging algorithm
  - Adaptive time stepping scheme

Sykes, R.I., W.S. Lewellen, and S.F. Parker, "A Gaussian Plume Model of Atmospheric Dispersion Based on Second-Order Closure", J. Clim. Appl. Met., 25, 322-331, 1986.

SCIPUFF Adjoint & Tangent-Linear Models



- Incident
  - Single source, instantaneous
- Control variables
  - Single source latitude & longitude
  - Mass
  - Release time
- Dynamics
  - Single puff
  - Centroid evolution
  - Turbulent diffusion
  - Buoyancy
- Required code
  - File handling and data I/O
  - Meteorology routines
  - Materials
- Utility code
  - Drivers
  - Newton-Krylov minimization
- Not included
  - Puff splitting
  - Adaptive time stepping

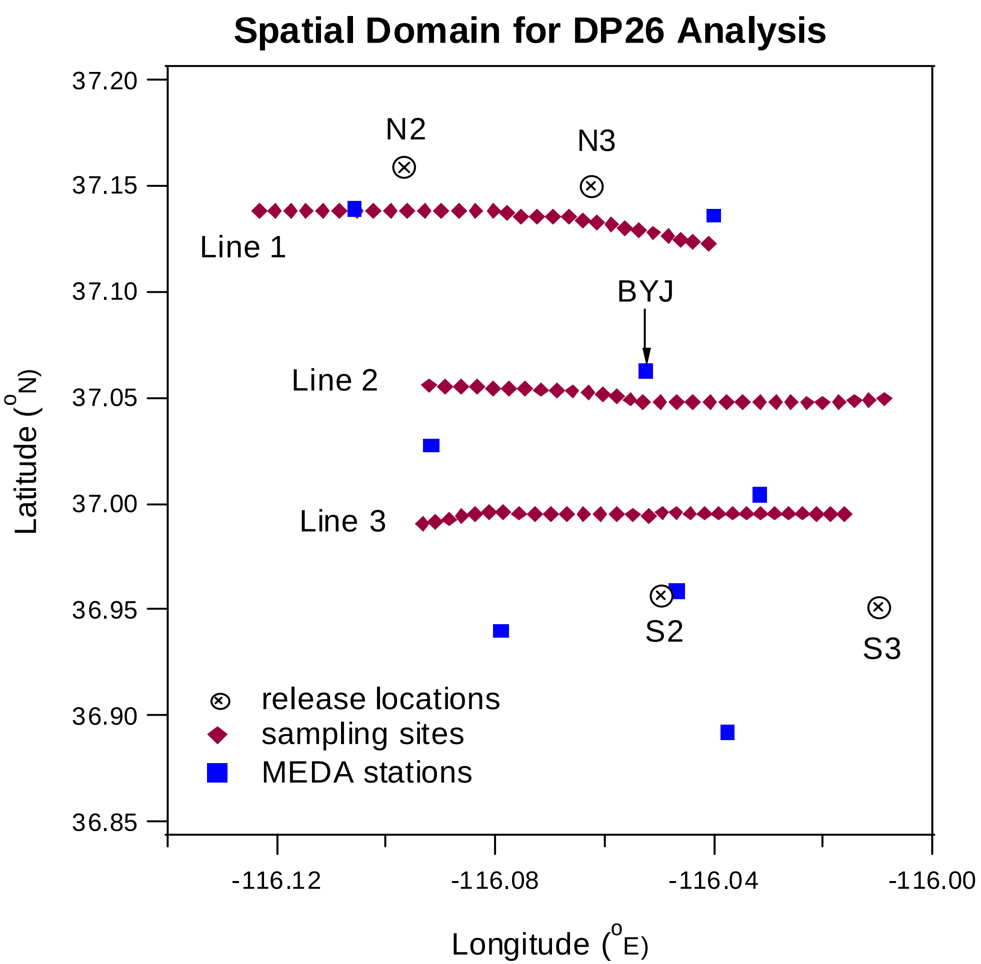
Dipole Pride 26 (DP26) Field Tests

- Defense Special Weapons Agency (DSWA) Transport and Dispersion Model Validation Program Phase II
  - To acquire data for the validation of integrated mesoscale wind field and dispersion model, in particular the HPAC model suite.
  - Conducted at Yucca Flat on the Nevada Test Site.
  - SF_6 tracer gas release with downwind tracer sampling at distances ranging to 20 km, along with extensive meteorological measurements.
  - Lateral and along-wind puff dispersion obtained from tracer concentration measurements.

C.A. Biltoft, "Dipole Pride 26: Phase II of Defense Special Weapons Agency Transport and Dispersion Model Validation," DPG-FR-97-058, Dugway Proving Ground, Dugway UT, July, 1998.

DP26 Test Site and Facilities

- Yucca Flat test site
  - North-south oriented basin
  - 30 km long and 12 km wide.
  - Yucca Lake (1195 m above mean sea level (MSL) is lowest point and the basin slopes upward to the north.
  - Basin surrounded by mountains: 1500 m (east) to 1800 m (west/north) MSL).
- Facilities
  - MEDA: network of meteorological data stations.
  - BJY: Buster-Jangle intersection.
- Whole air samplers
  - Three sampling lines; 30 samplers per line; 12 bags per sampler – 15 minute resolution.

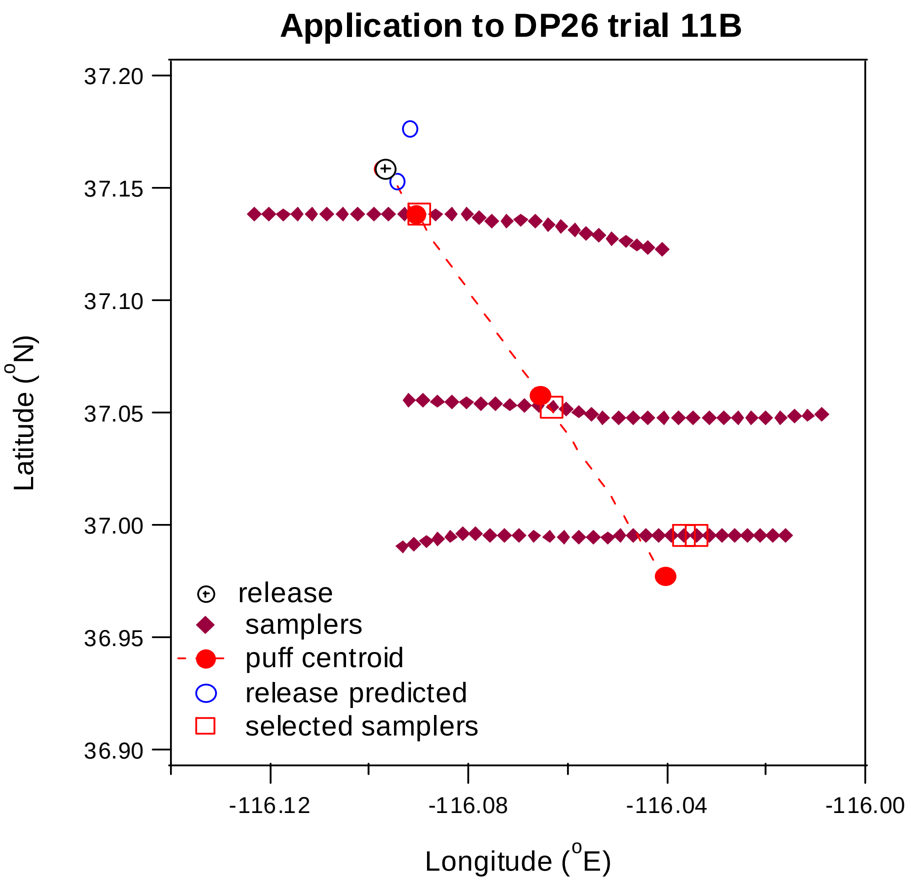


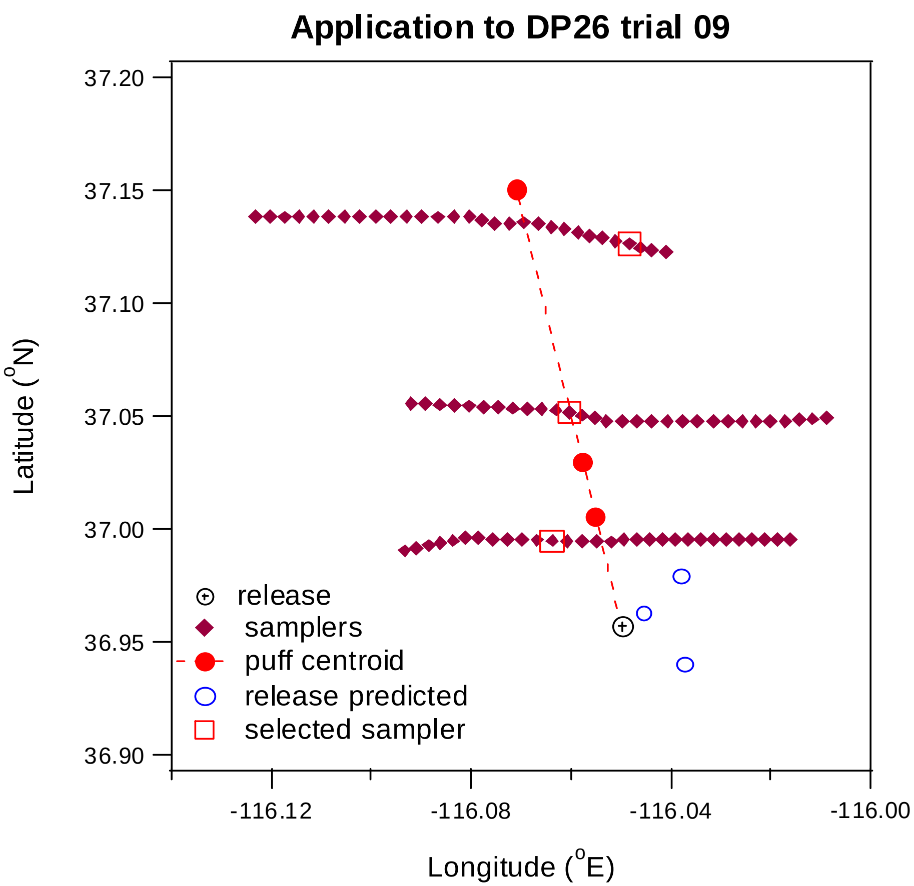
SCIPUFF Adjoint - Application to DP26

- Fixed puff width, fixed wind - not discussed
- Fixed wind
  - Controls – release latitude and longitude
  - Samplers – along a given sampling line with concentrations > 90% of the peak concentration.
- Variable wind field
  - Controls – release latitude and longitude
  - Samplers – along a given sampling line with concentrations > 10% of the peak concentration.
- Variable wind field, release time - not discussed
  - Controls – release latitude, longitude, and (manual) time.
  - Samplers – a given sampling line with conc’ns > 0.

Fixed Wind Adjoint Model

One estimated release location for each sampling line.





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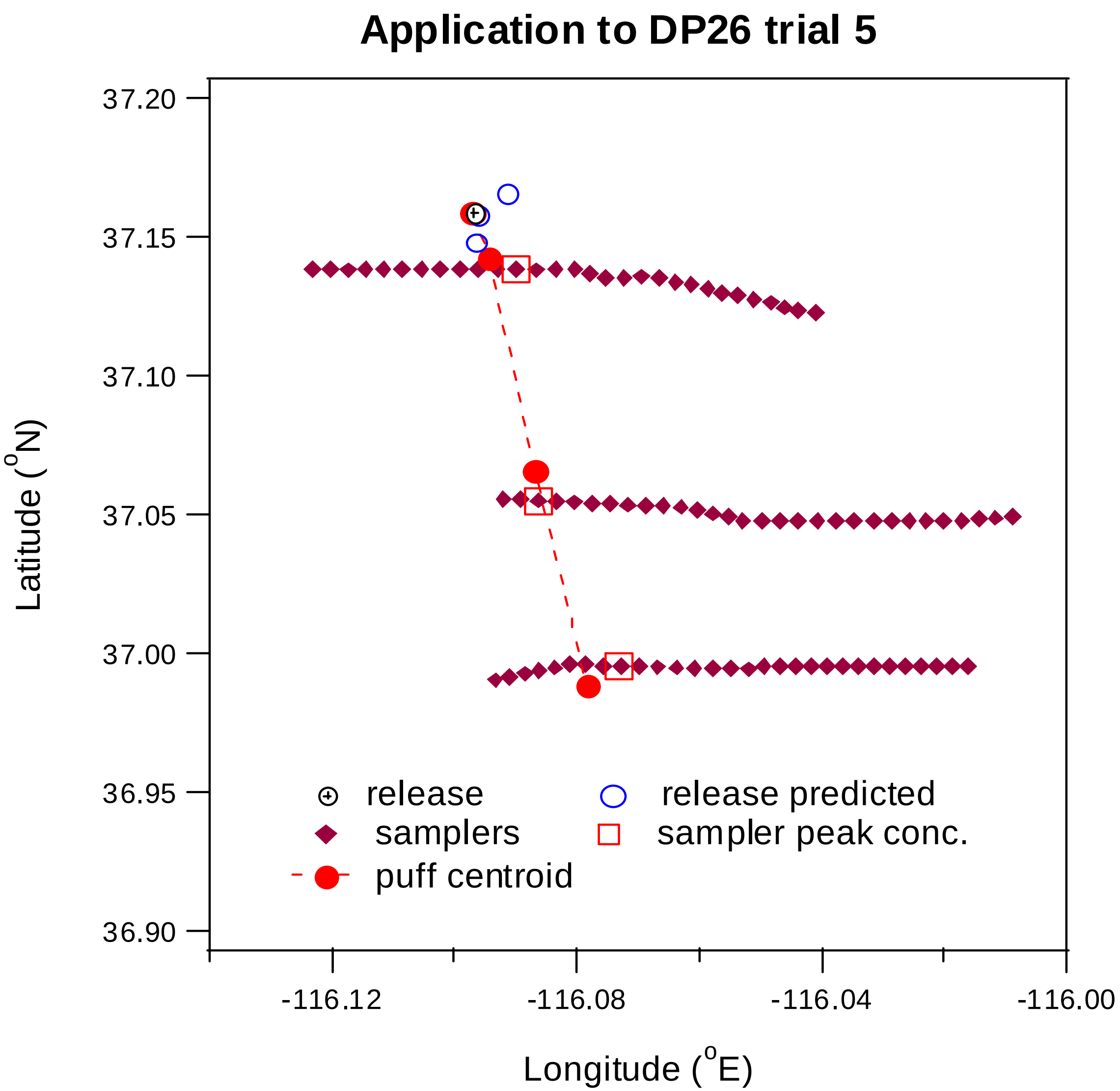
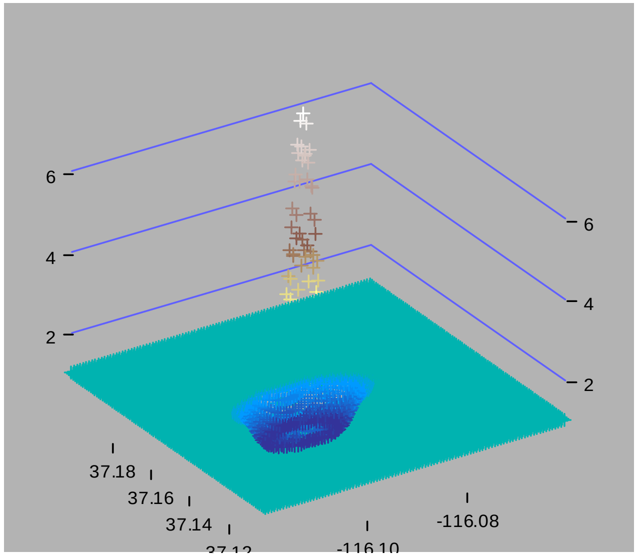
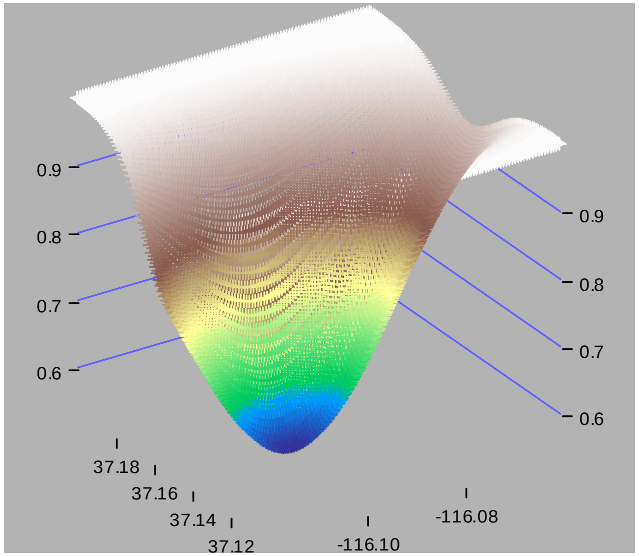
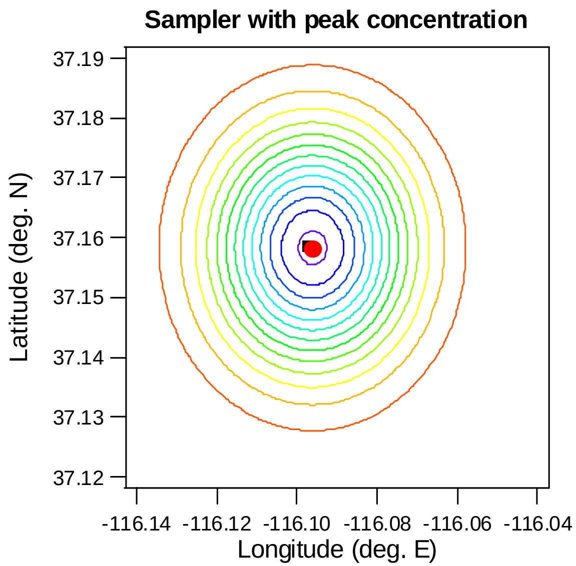
Fixed Wind Adjoint Model

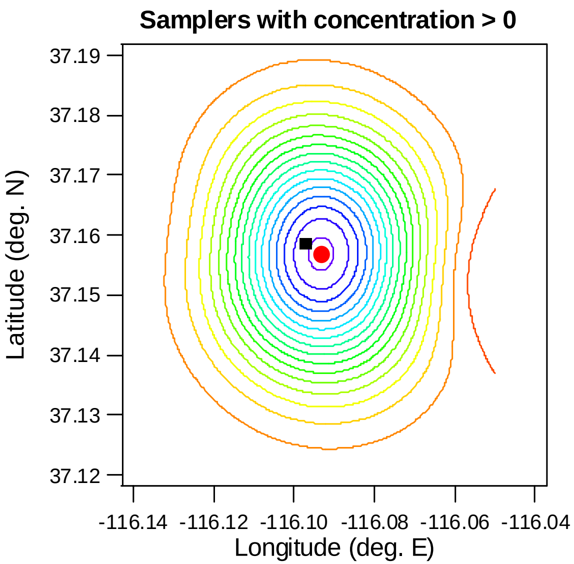


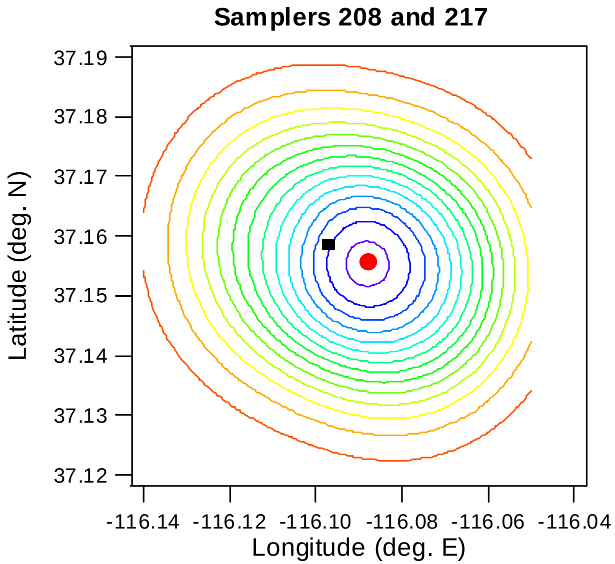


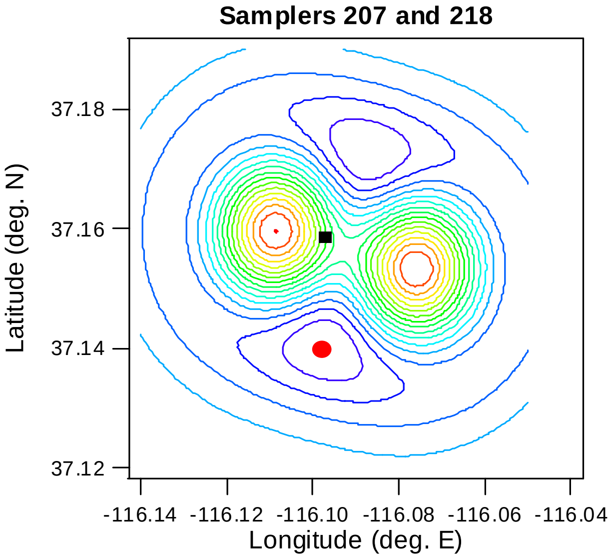


Cost Function: Fixed Wind DP26 Trial 11B – Line 2

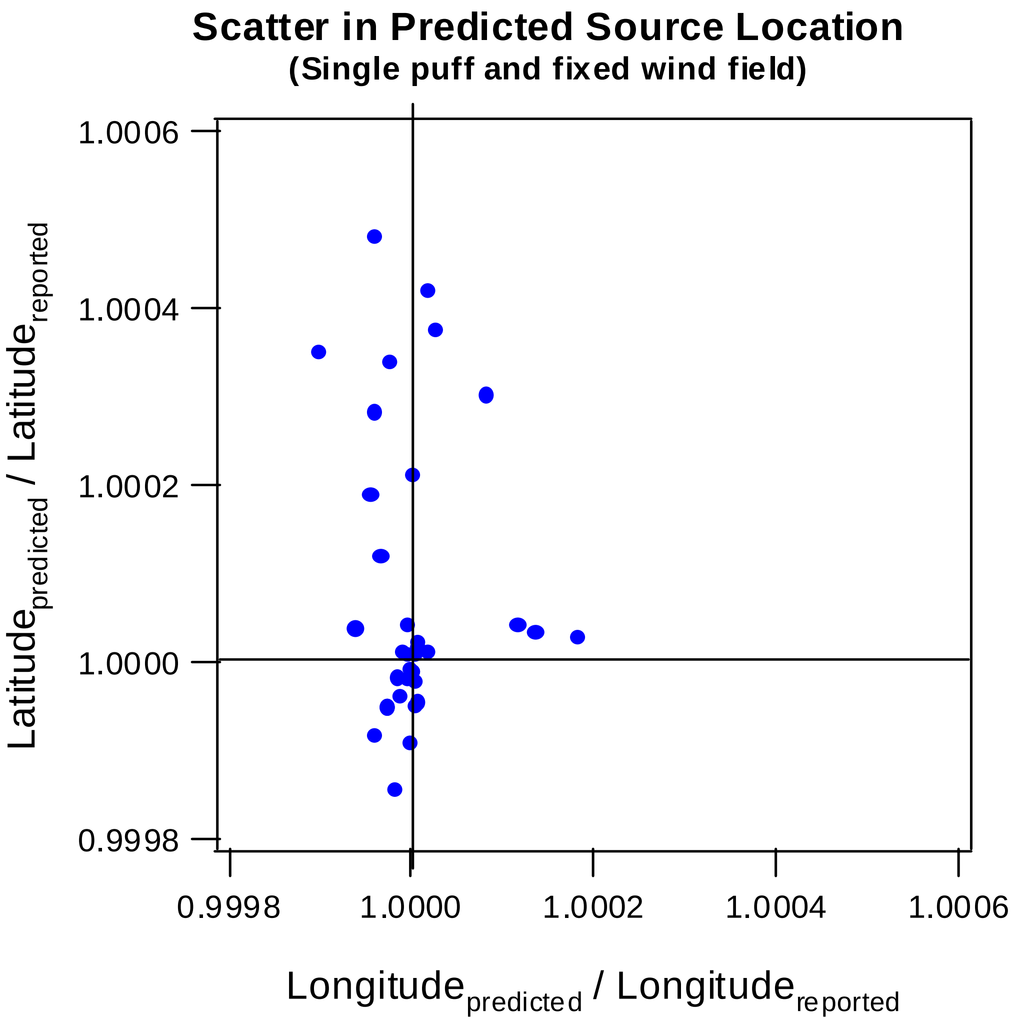




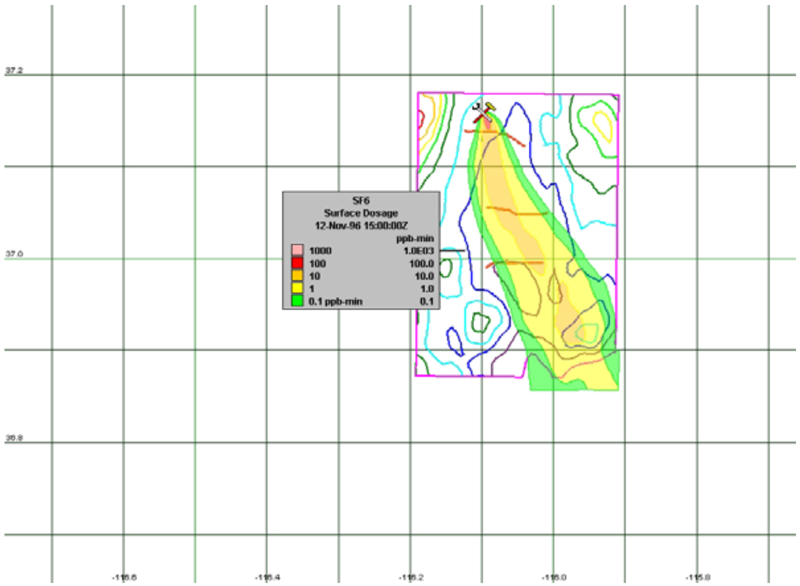




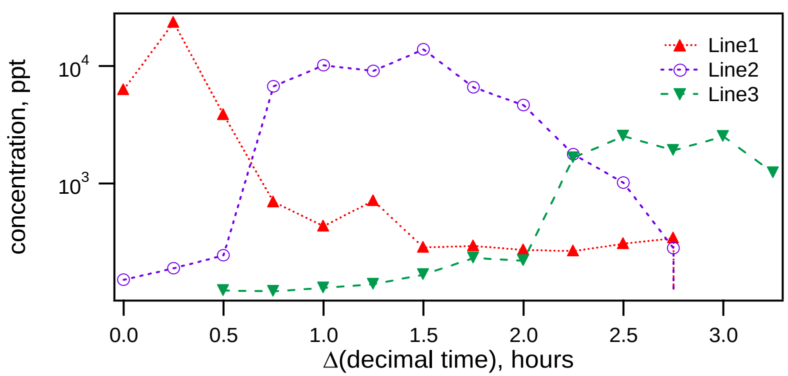
SCIPUFF (Fixed Wind) Adjoint Summary



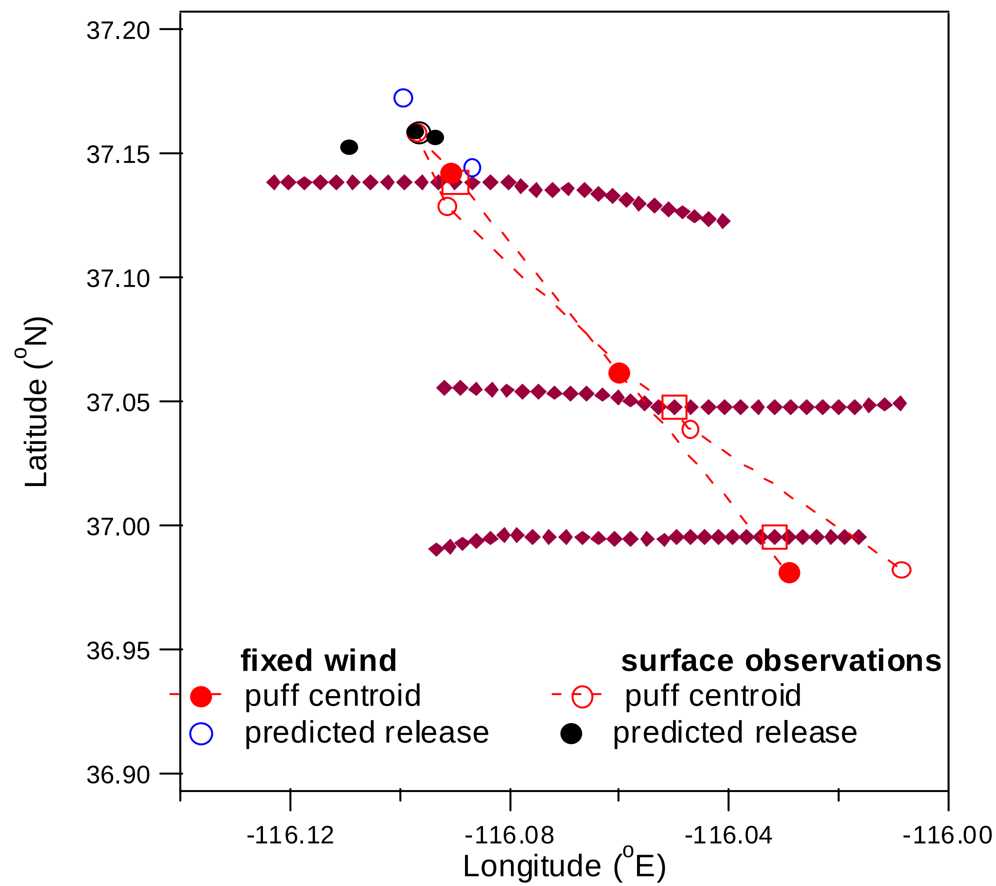
Fixed Versus Variable Wind Adjoint



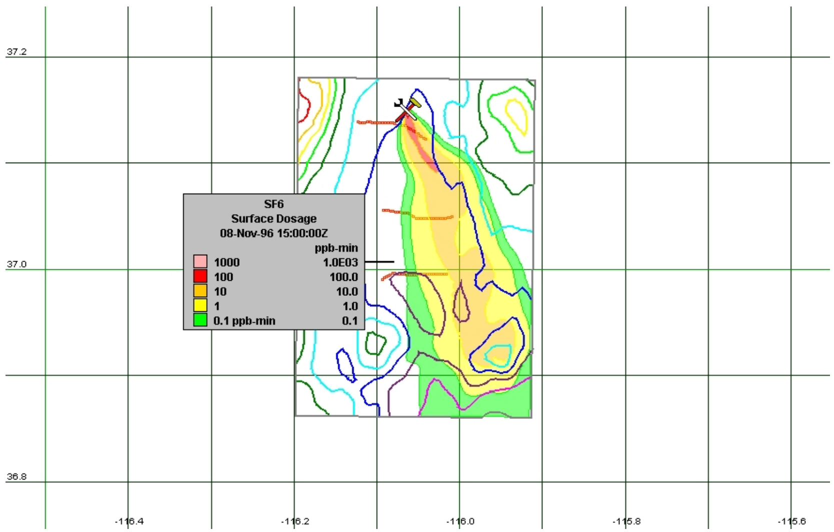
Sampling Line Integrated Tracer Concentrations

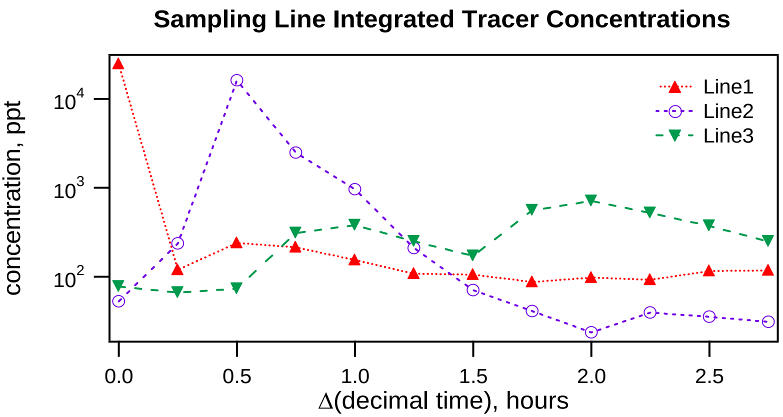


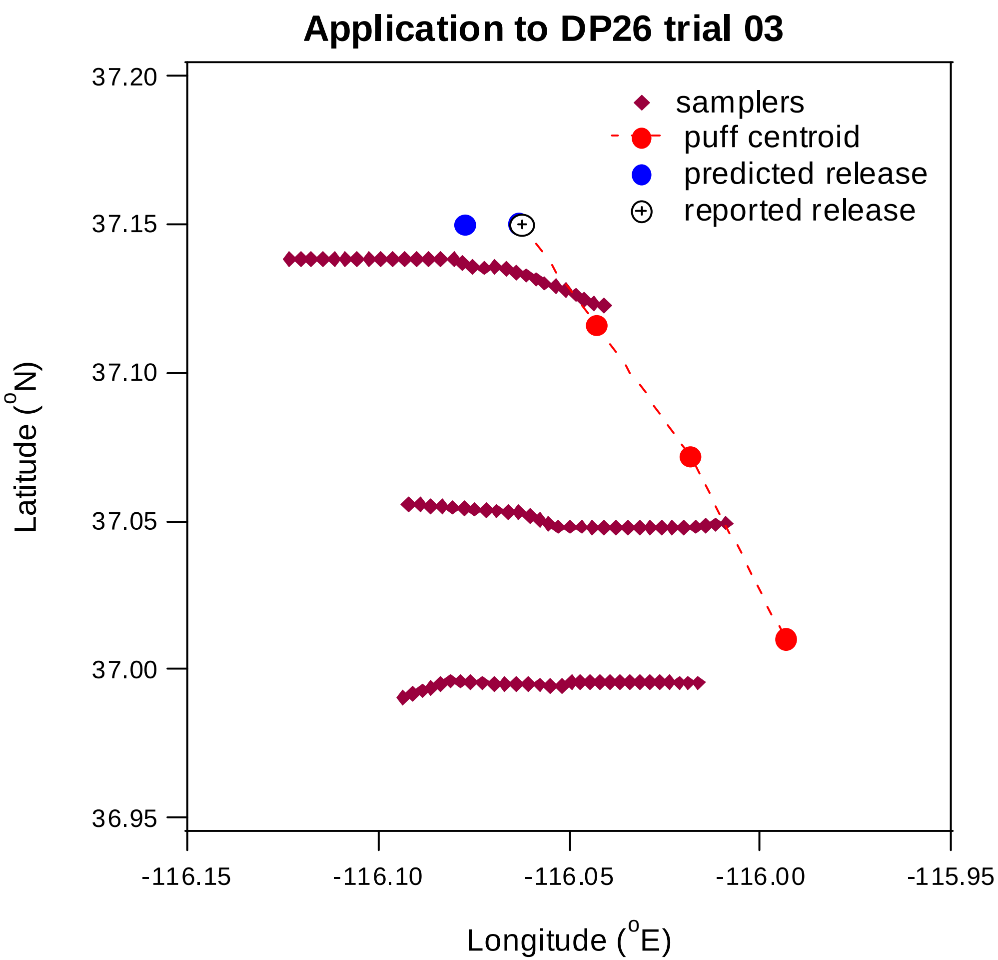
Application to DP26 trial 06



Variable Wind Adjoint







Future Work, Broad research objectives

- More fully develop theoretical and numerical foundation for source location approaches, using adjoint model with ‘ideal’ observable data
  - observational data requirements
  - sensor spatial resolution
  - the impact of faulty observational data
  - atmospheric transport and dispersion spatial range
- Incorporate measurement and model uncertainties
- Testing and validation using actual field data to ensure reliability and fully assess performance.

Future Work, Three year effort

- First year: extend SCIPUFF adjoint to enable source location using ideal observational data.
- Second year: incorporate ***measurement uncertainties***, begin testing using field data.
- Third year: treat ***model uncertainties*** and continue testing and validation using field data.
- Successful completion: numerical code, tested against field data,
  - implements adjoint-based strategies
  - locates hazardous release using observational data
  - includes estimated uncertainties in predictions

First Year Work

- Focus on adjoint model development
  - extend the SCIPUFF adjoint model for source location applications
  - use ideal or model simulated observational data
- Apply adjoint model to ‘ideal’ observable data to be address:
  - observational data requirements,
  - sensor spatial resolution,
  - the impact of faulty observational data
  - atmospheric transport and dispersion spatial range.
- Compare approaches for applying adjoint models in source location applications.

Acknowledgments

- Allan Reiter (DTRA) and Rick Fry (DTRA) – programmatic support
- Scott Bradley (DTRA) – Dipole Pride 26 data
- Jim Hurd (Northup Grumman) – technical support and coordination
- Ian Sykes and Biswanath Chowdhury (Titan) – SCIPUFF Atmospheric Transport and Dispersion Code

Transformation of Algorithms in Fortran (TAF)

- Commercial source code – to – source code translator
  - Giering, Ralf and Kaminski, Thomas, Transformation of Algorithms in Fortran, TAF Version 1.5, FastOpt, http://www.FastOpt.com, July 3, 2003.
- Features
  - Tangent-linear and adjoint models - 1st derivatives.
  - Hessian code - 2nd derivatives.
- Estimating the Circulation and Climate of the Oceans (ECCO)
  - Large data assimilation effort by MIT, SCRIPPS, NASA\JPL, and international collaborators: http://www.ecco-group.org.
  - Based on the MIT GCM (global, 3-dimensional NS solver): http://www.mitgcm.org.
  - ~100,000 lines of code; ~10^8 control variables.

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