Sensor Data Fusion Working Group
28 October 2005
Albuquerque, NM

Tracking Atmospheric Plumes Using Stand-off Sensor Data

Prepared by:

Robert C. Brown, David Dussault, and Richard C. Miake-Lye
Aerodyne Research, Inc.
45 Manning Road
Billerica, MA 01821-3976 USA

Patrick Heimbach
Department of Oceanography
Massachusetts Institute of Technology,
Cambridge, MA59717-3400 USA

The Inverse Problem

Atmospheric transport and dispersion model

Known release → **Predicted observations?**

Inverse model

Release location, magnitude, time? ← **Actual observations**

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

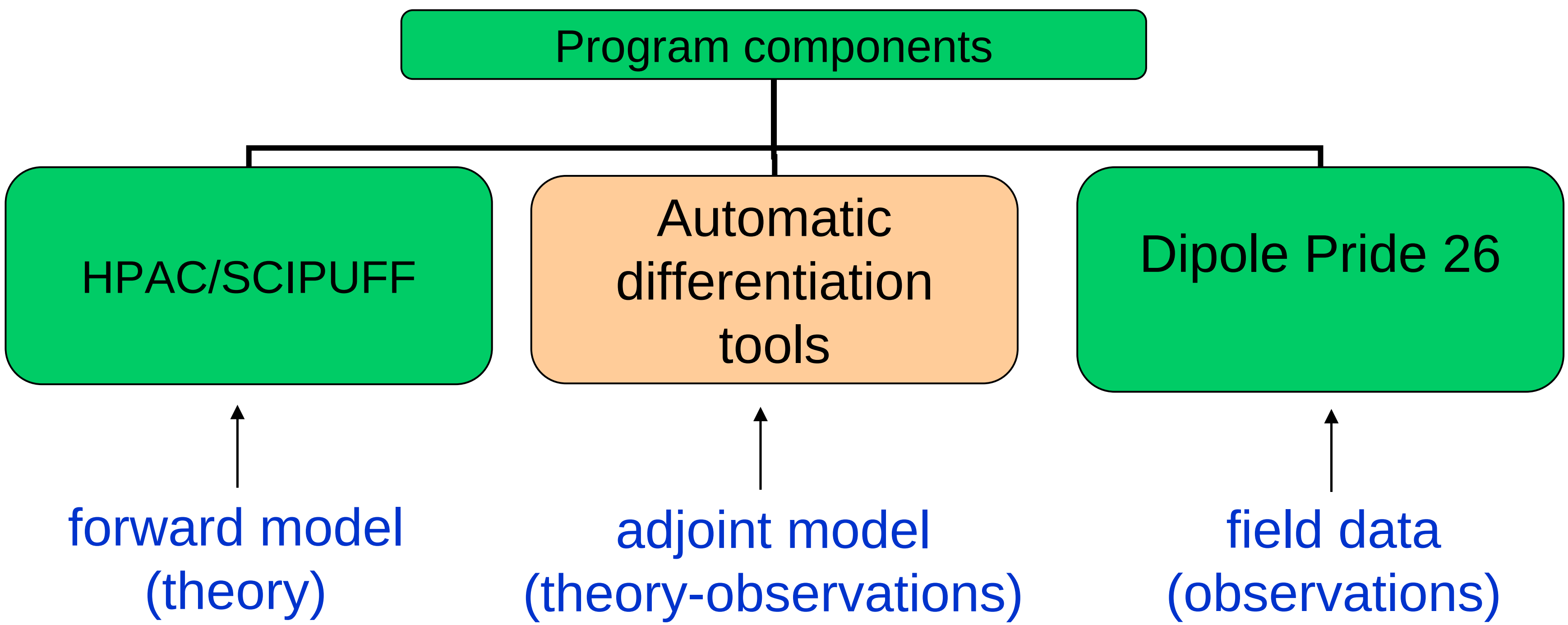
Adjoint Models

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

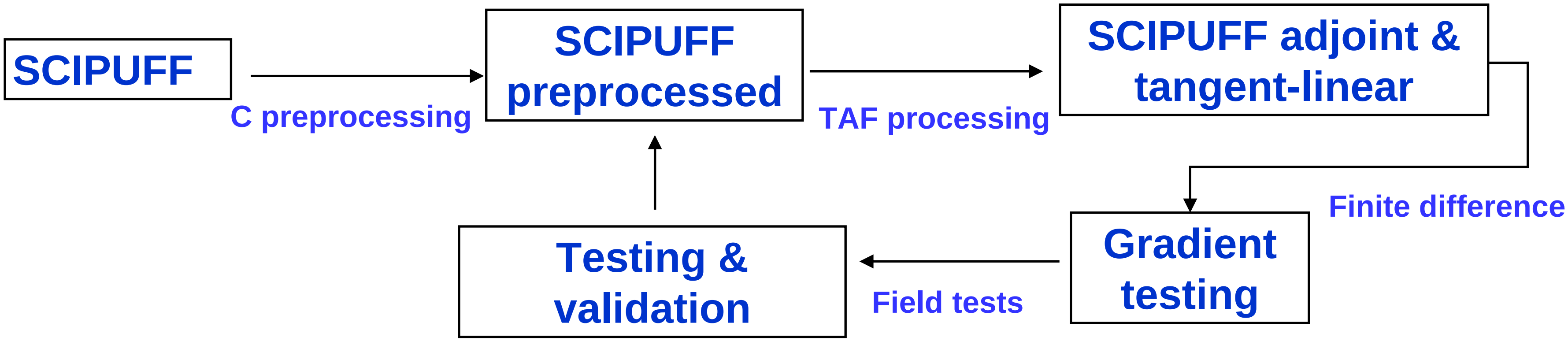
$\rightarrow$ use chain rule to compose M_Λ

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

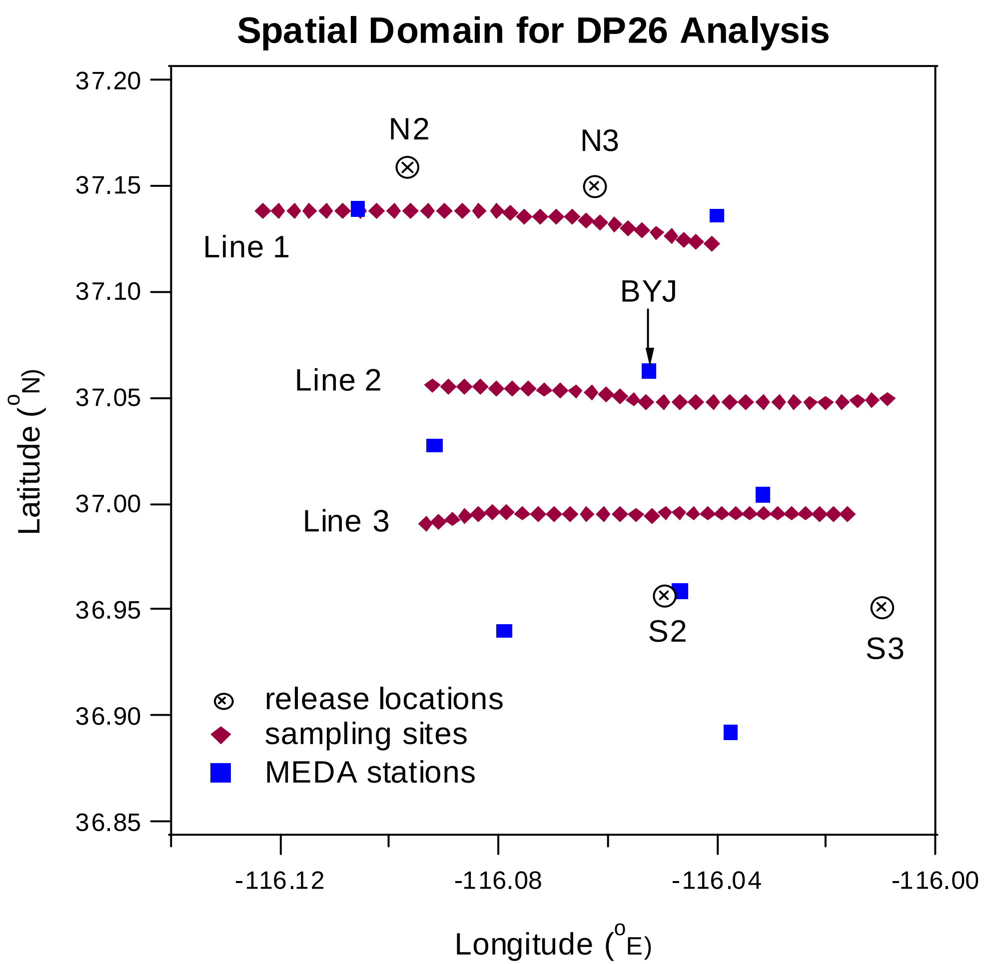
Dipole Pride 26 (DP26) Field Tests

- 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.

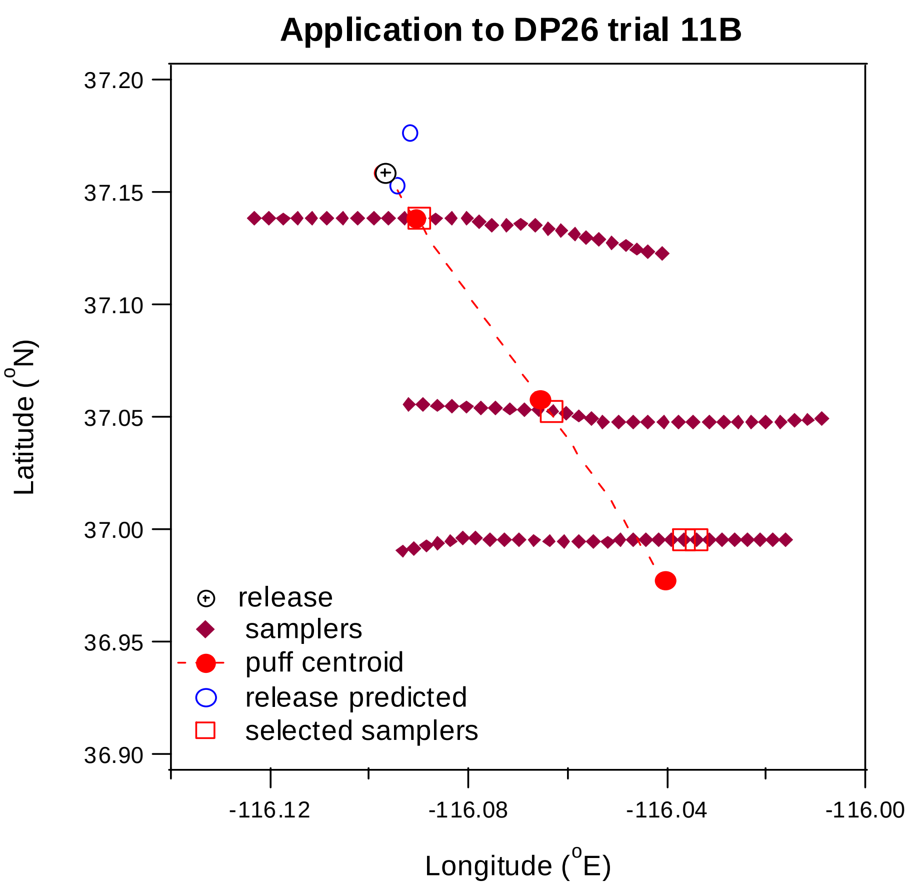


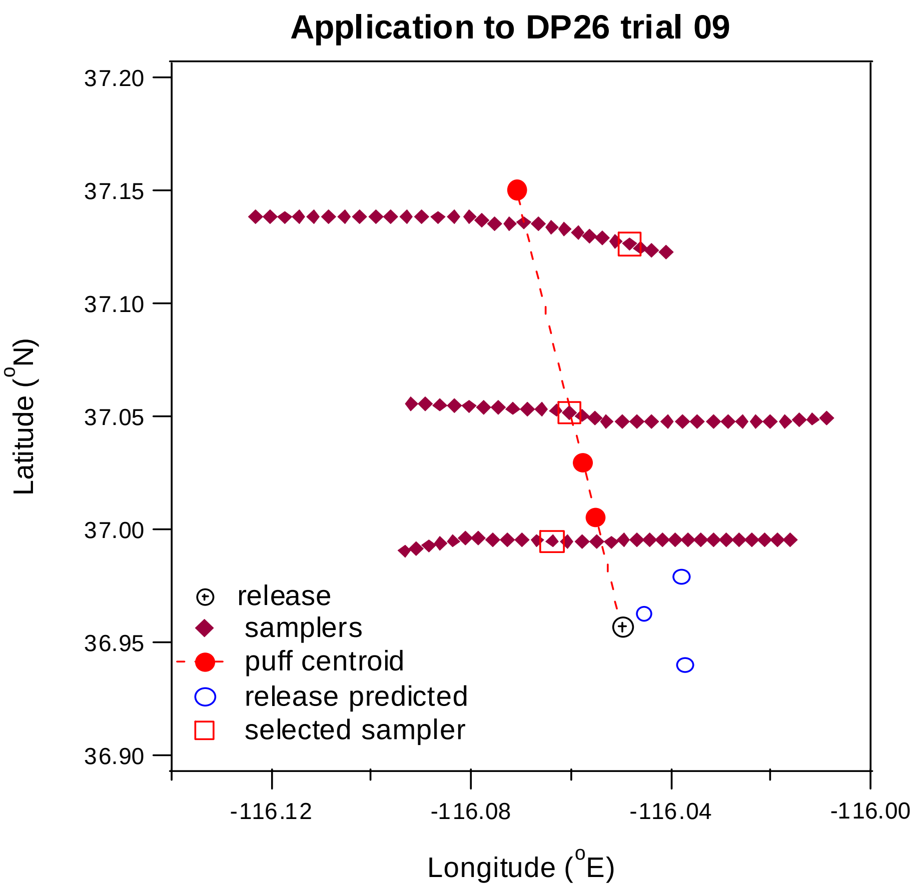
SCIPUFF Adjoint - Application to DP26

- 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.

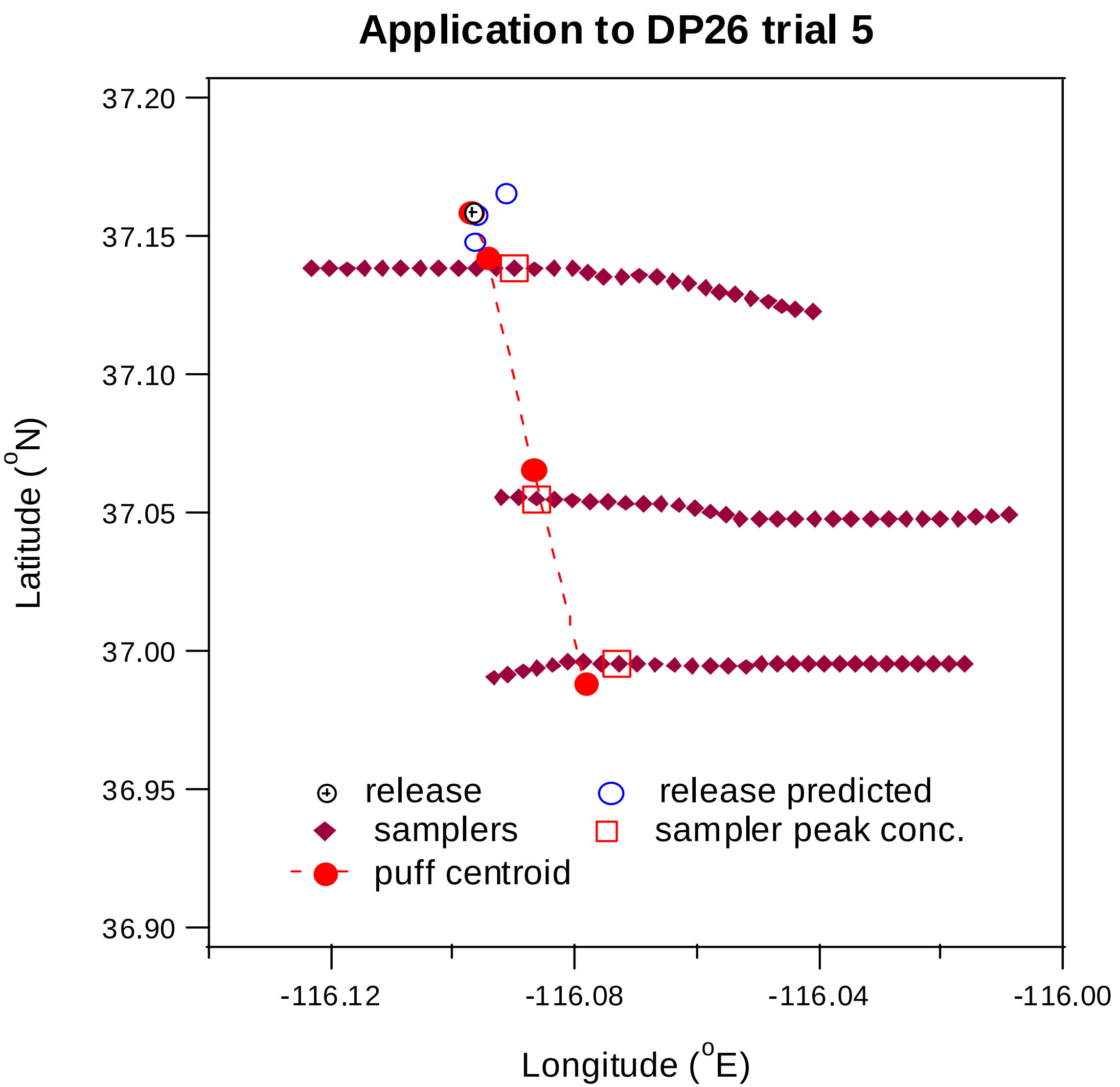
Fixed Wind Adjoint Model

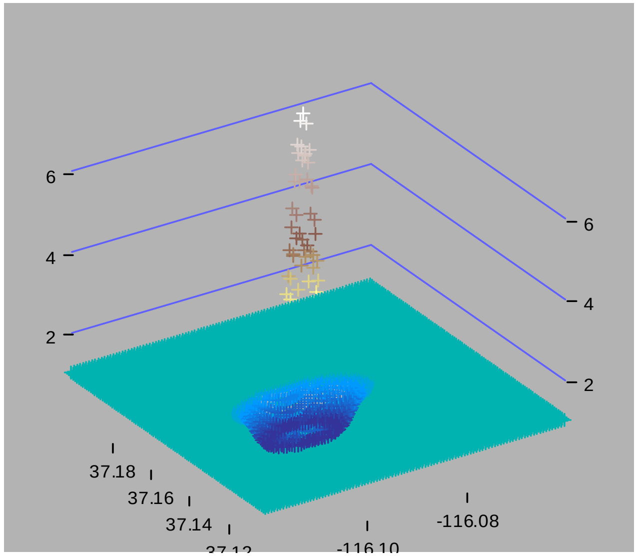
One estimated release location for each sampling line.

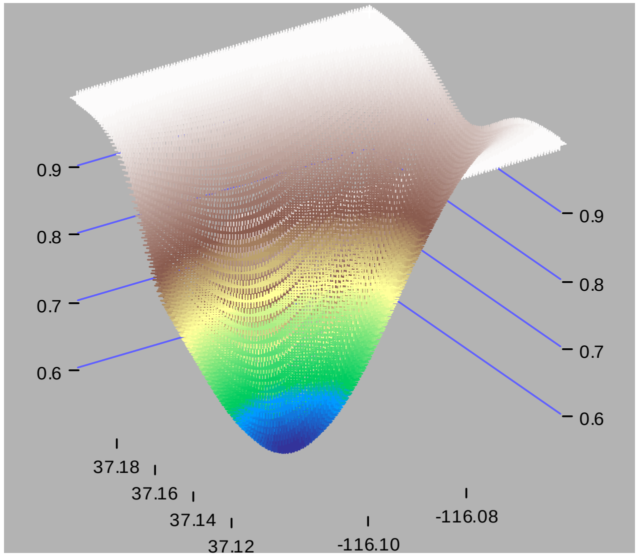




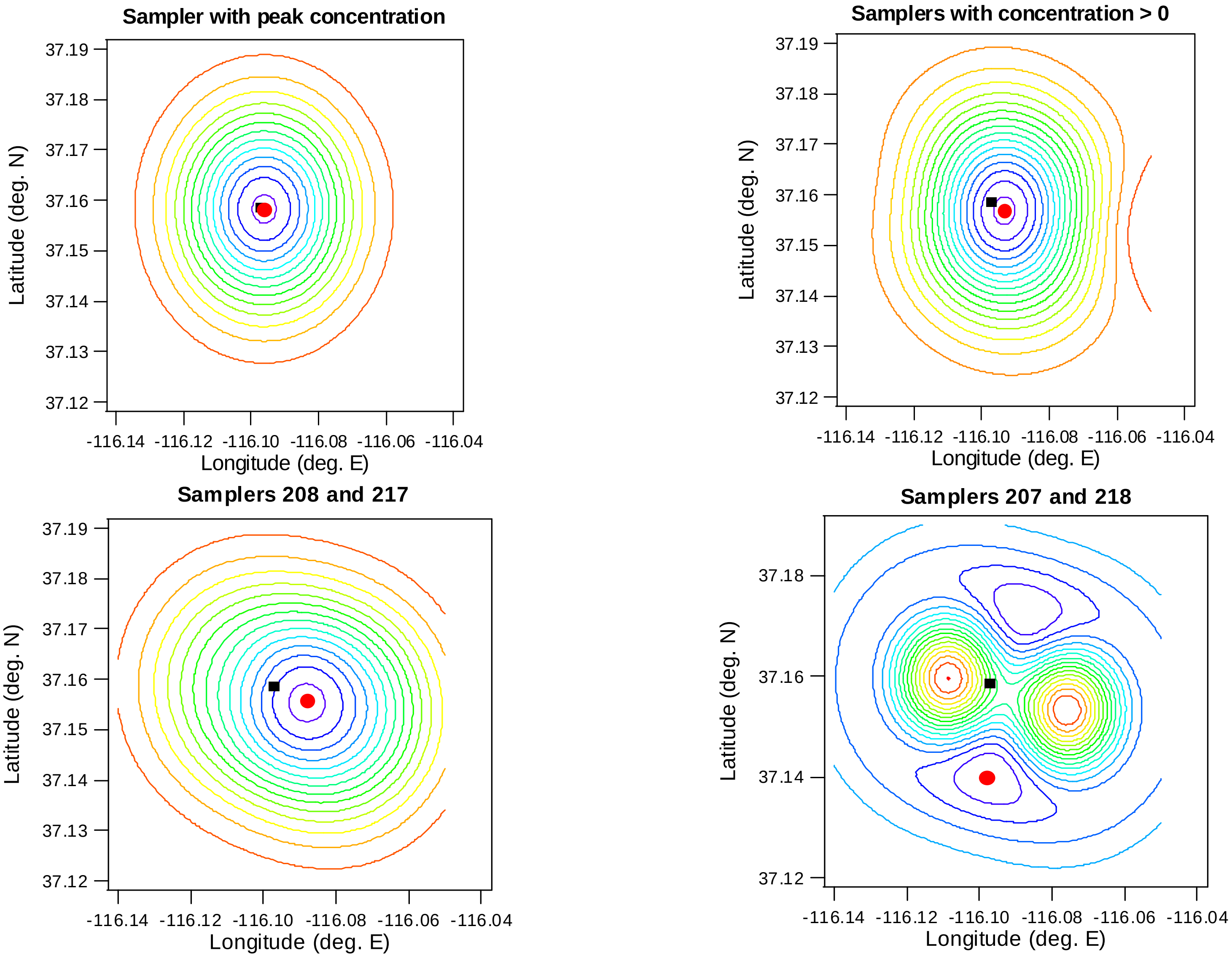
Fixed Wind Adjoint Model





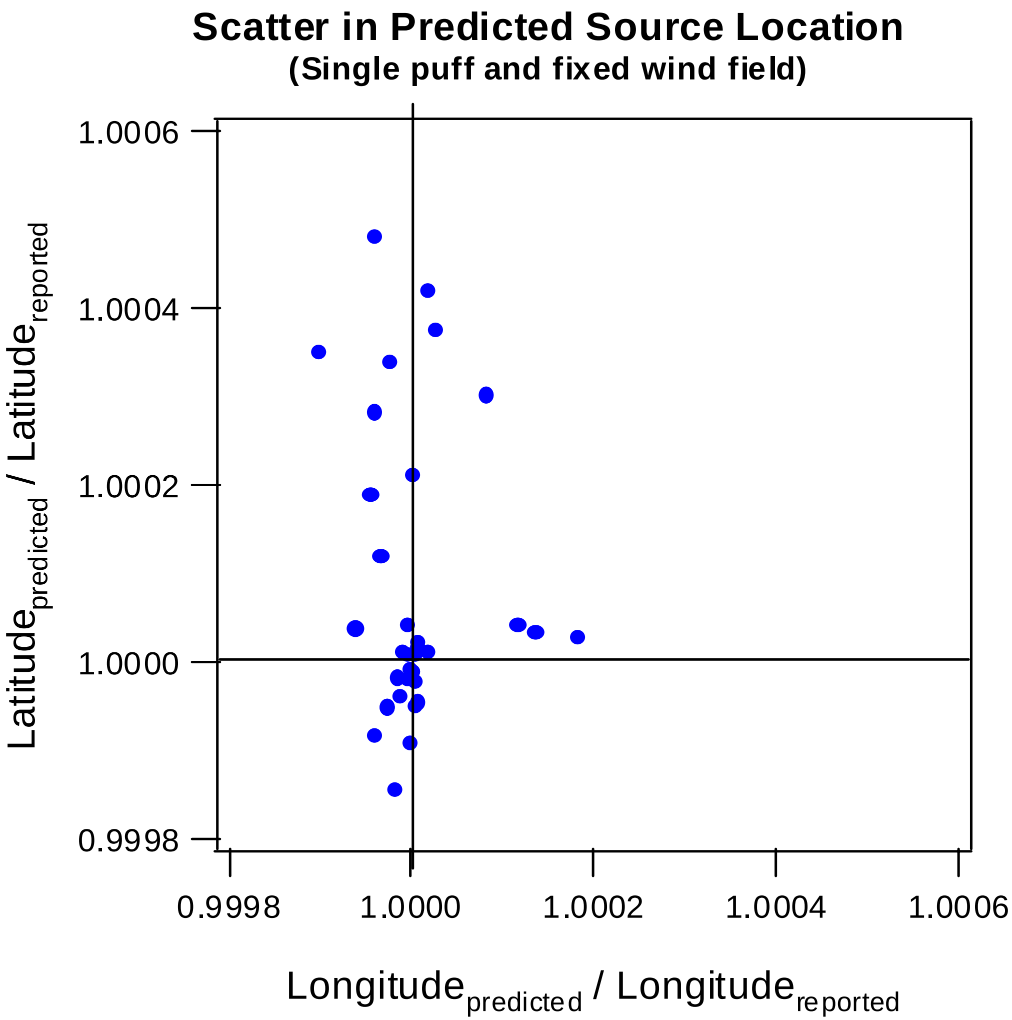


Cost Function: Fixed Wind DP26 Trial 11B – Line 2

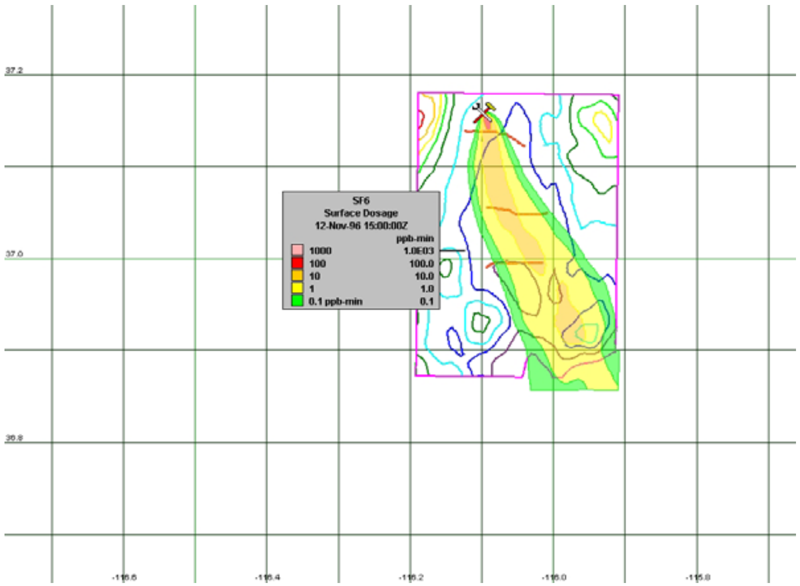


Aerodyne Research, Inc.

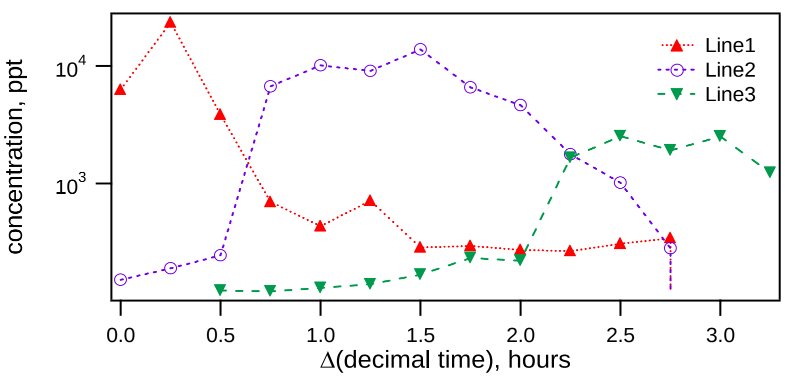
SCIPUFF (Fixed Wind) Adjoint Summary



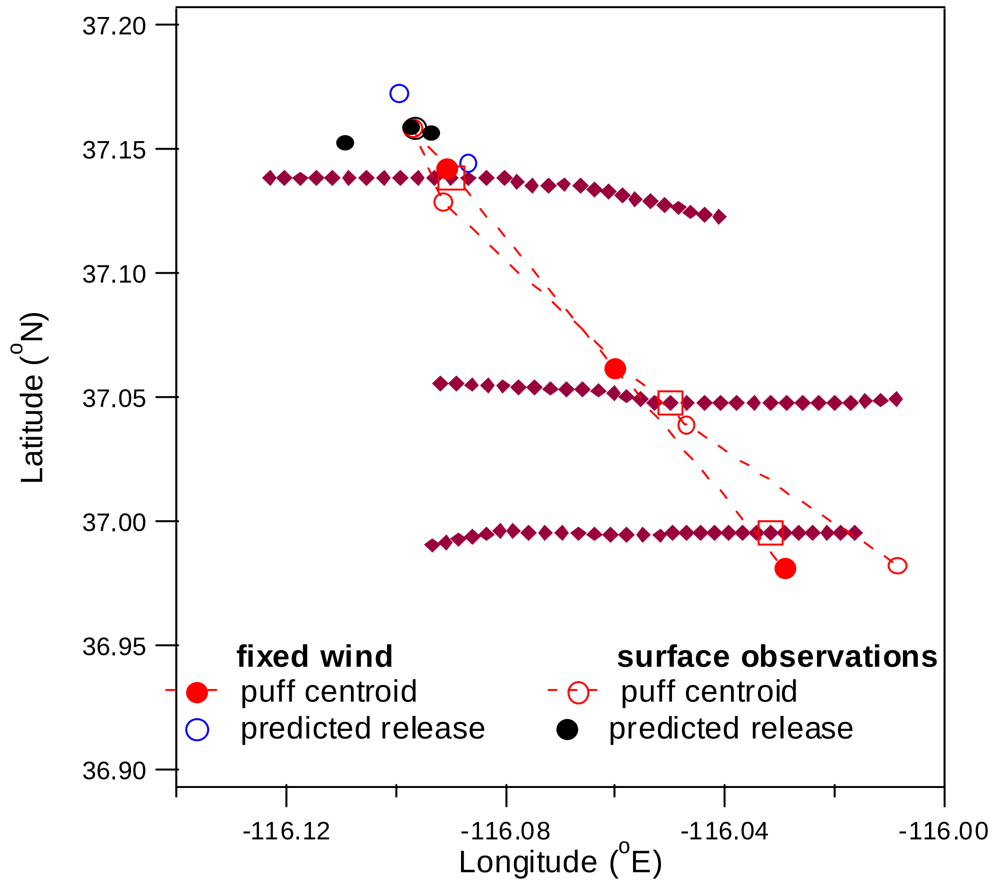
Fixed Versus Variable Wind Adjoint



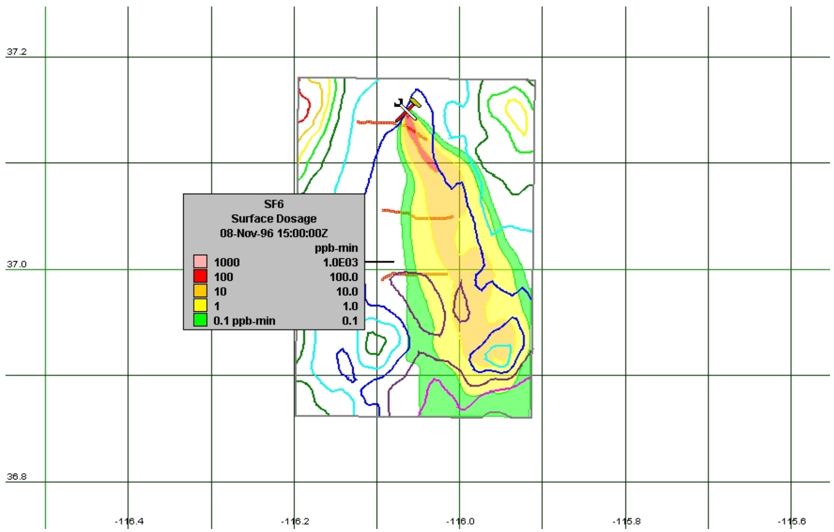
Sampling Line Integrated Tracer Concentrations



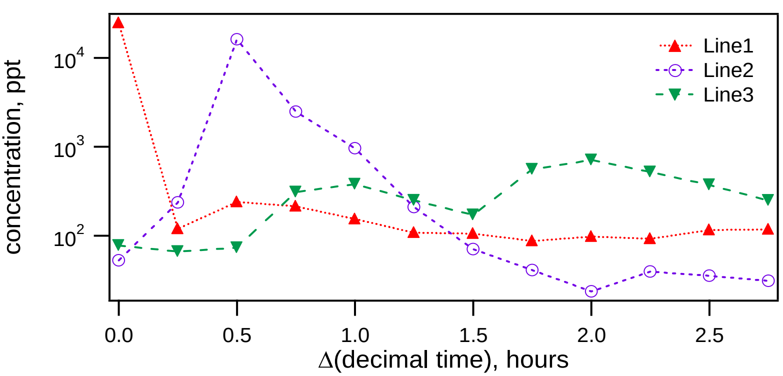
Application to DP26 trial 06



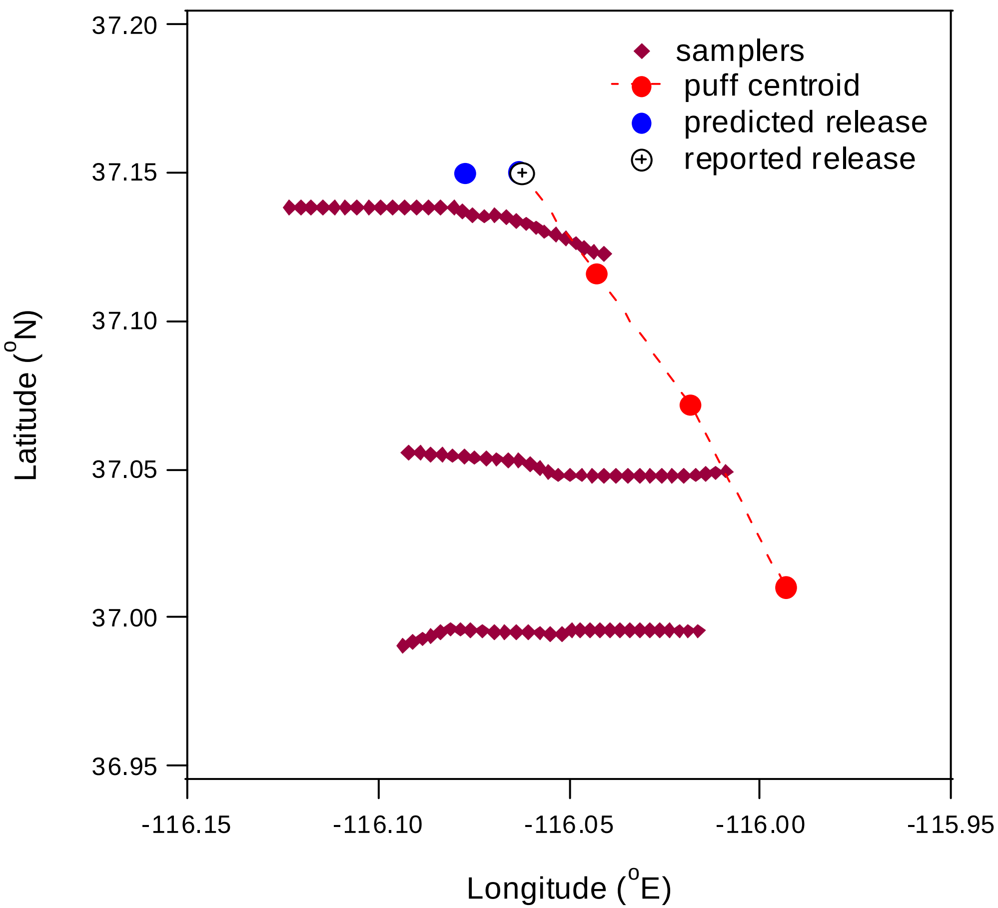
Variable Wind Adjoint



Sampling Line Integrated Tracer Concentrations



Application to DP26 trial 03



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 - 1^{st} derivatives.
  - Hessian code - 2^{nd} 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; $\sim 10^8$ control variables.

References

Biltoft, C., “Dipole Pride 26: Phase II of Defense Special Weapons Agency Transport and Dispersion Model Validation”, DPG-FR-98-001, Dugway Proving Ground, Dugway UT, January 1998.

Bradley, S. and T. Mazzola, “HPAC 3.1 Predictions Compared to Dipole Pride 26 Sampler Data”, June, 2004.

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

Giering, R. and Kaminski, T., Transformation of Algorithms in Fortran, TAF Version 1.5, FastOpt, http://www.FastOpt.com, July 3, 2003.

Science Applications International Corporation (SAIC), Hazard Prediction and Assessment Capability (HPAC), User’s Guide 4.0, Document HPAC-UGUIDE-02-U-RAC0, August 15, 2001.

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.

Sykes, R.I. and D.S. Henn, Representation of Velocity Gradient Effects in a Gaussian Puff Model, Journal of Applied Meteorology, volume 34, 2715-2723, 1995.

Sykes, R.I., C.P. Cerasoli, D.S. Henn, The representation of dynamic flow effects in a Lagrangian puff dispersion model, Journal of Hazardous Materials A:64, 223-247, 1999.

Wunsch C., The ocean circulation inverse problem, Cambridge University Press, 1996.