Introduction to Assimilation of Atmospheric Composition Observations

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WRF-Chem Tutorial
February 6–7, 2017

Overview

- Introduction to "data assimilation" terminology and methods.
- Special challenges with assimilation of observations of atmospheric composition.
- Review of chemical data assimilation efforts with WRF-Chem.
- Review of WRF-Chem/DART tutorial on localization.

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Background: Introduction to Data Assimilation Terminology and Methods

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Data Assimilation Terminology

- Analysis
- Forecast
- Objective Analysis
- Initialization
- Data Assimilation
- Prior (*a priori*)
- Posterior (*a priori*)
- Innovation
- Increment

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Data Assimilation Terminology cont.

- Deterministic Assimilation
- Probabilistic Assimilation
- Ensemble
- Ensemble mean and spread
- Spread Collapse
- Localization
- Inflation
- Analysis Fit
- Forecast Skill

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Data Assimilation Terminology cont.

- Observation
- Expected observation
- Observation Error
- Model Error
- Error Covariance (Static and Flow Dependent)

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Data Assimilation Methods

- Successive Correction (Cressman, 1959)
- Nudging (Kistler, 1974)
- Optimal Interpolation (Gandin, 1965)
- Variational Methods (3D VAR – Sasaki, 1970 and 4D VAR – Thompson, 1969; Lewis and Derber, 1985)
- OI/Var Equivalence (Lorenc, 1986)
- Ensemble Kalman Filter Methods
  - ✓ EnKF – Ensemble Kalman Filter (Houtekamer and Mitchell, 1998; 2001)
  - ✓ EAKF – Ensemble Adjustment Kalman Filter (Anderson, 2001; 2003)

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Data Assimilation Methods cont.

- Ensemble Kalman Filter Methods cont.
  - ✓ ETKF – Ensemble Transform Kalman Filter(Bishop et al., 2001)
  - ✓ LETKF – Local Ensemble Transform Kalman Filter (Ott et. al., 2002; 2004)
- Hybrid Methods
  - ✓ Weight sum (Hamill and Snyder, 2000)
  - ✓ Control variable (Lorenc, 2003)
  - ✓ EVIL – Ensemble Variational Integrated Localizaed hybrid (Aulignes et al., 2016).

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Data Assimilation Methods cont.

- Constrained Emissions (Emissions Inversion)
  - ✓ Adjoint Method
  - ✓ Variational Method
  - ✓ State Augmentation Methods

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Successive Correction Methods

$$f_i^{m+1} = f_i^m + \frac{\sum_{k=1}^{K^m} w_{ik}^m \left(O_k - f_k^m\right)}{\sum_{k=1}^{K^m} w_{ik}^m + \varepsilon^2}$$

$$w_{ik}^m = \frac{R_m^2 - r_{ik}^2}{R_m^2 + r_{ik}^2}, \ for\ r_{ik}^2 \le R_m^2$$

$$w_{ik}^m = 0, \ for\ r_{ik}^2 > R_m^2,$$

Nudging Methods

$$\frac{\partial u}{\partial t} = -\vec{V} \bullet \nabla u + fv - \frac{\partial \phi}{\partial x} + \frac{u_{obs} - u}{\tau_u}$$

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Optimal Interpolation Methods

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}\left(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b\right)$$

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

Variational Methods

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \frac{1}{2}(H(\mathbf{x}) - \mathbf{x}_o)^T \mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{x}_o)$$

$$\begin{aligned} J_j(\delta\mathbf{x}_j) &= \frac{1}{2}(\delta\mathbf{x}_j - \delta\mathbf{x}_j^b)^T\mathbf{B}^{-1}(\delta\mathbf{x}_j - \delta\mathbf{x}_j^b) \\ &+ \frac{1}{2}\sum_{k=0}^{K}(\mathbf{H}_{j,k}\mathbf{M}_{j,k}\delta\mathbf{x}_j - \mathbf{d}_{j,k})^T\mathbf{R}^{-1}(\mathbf{H}_{j,k}\mathbf{M}_{j,k}\delta\mathbf{x}_j - \mathbf{d}_{j,k}) \end{aligned}$$

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Ensemble Kalman Filter Methods

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{K}\left(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b\right)$$

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

$$\mathbf{K} = \mathbf{P}^b\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

Hybrid Variational Methods

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x}_b)^T\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \frac{1}{2}(H(\mathbf{x}) - \mathbf{x}_o)^T\mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{x}_o)$$

$$\mathrm{B} = \alpha_1\mathrm{B}_1 + \alpha_2\mathrm{B}_2,\ \alpha_1 = 1 - \alpha_2$$

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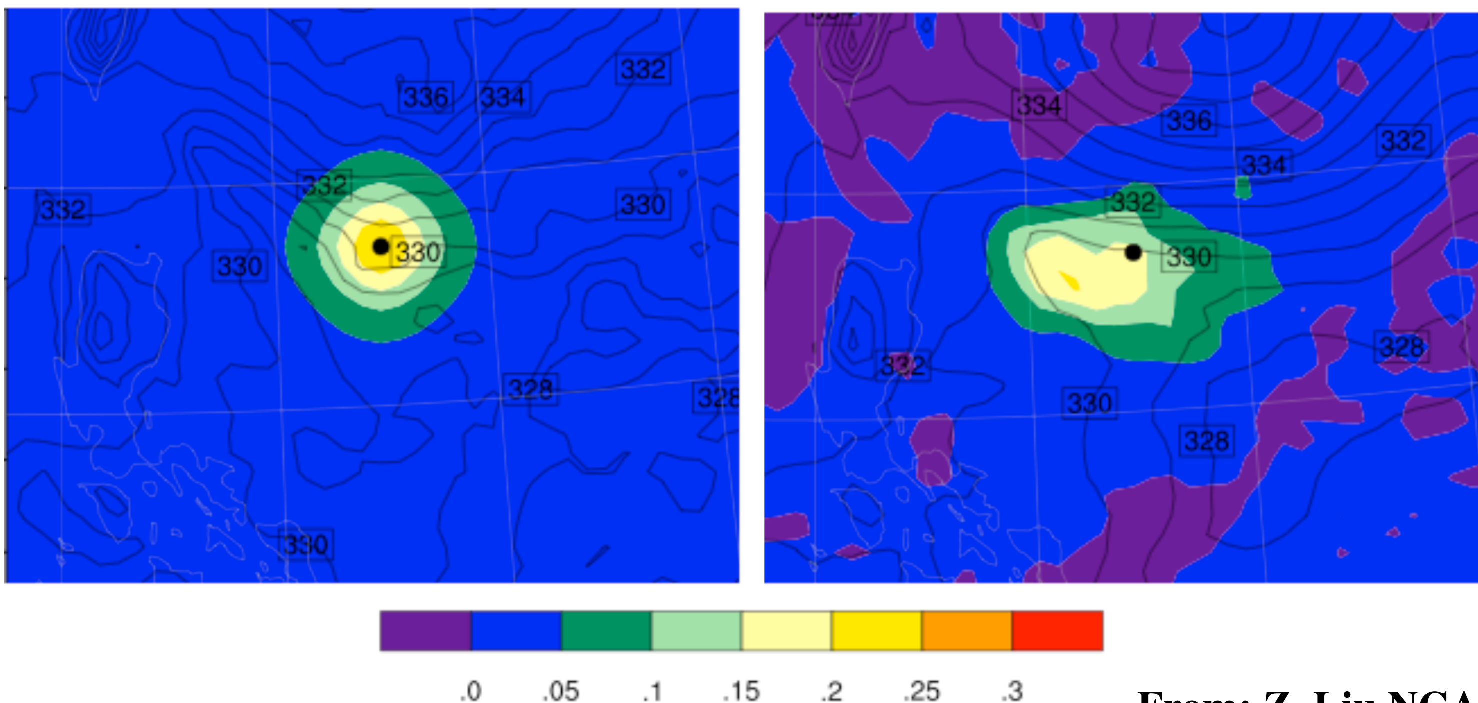
Hybrid: Single Obs Experiment

T Analysis increments from a single T obs

1K difference, 1K error

3DVAR | **Hybrid (64 members)**



From: Z. Liu NCAR/MMM

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Special Challenges with Assimilation of Observations of Atmospheric Composition

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Chemical Data Assimilation Challenges

- Sparse observations, mostly surface observations collected for regulatory purposes.
- Upper atmosphere/profile observations are primarily satellite-based retrievals (indirect observations, large data volume, low information density, large storage and assimilation computational requirements).
- Retrievals contain redundant information and influence of retrieval prior through the retrieval equation.
- Interaction of meteorology and chemistry observations on state variables during assimilation can disrupt chemistry (requires state-variable localization).

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Chemical Data Assimilation Challenges cont.

- Under-sampling and spread collapse issues require radius-of-influence localization and inflation but appropriate localization radius and spread uncertain.
- Forecast results are sensitive to correct emissions but large uncertainty in emissions and emissions error covariance is unknown.
- Retrieval error covariance products generally contain error cross-correlations.
- Chemical transformations occur on time-scales ranging from hours to months.

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Review of Chemical Data Assimilation Efforts with WRF-Chem

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WRF-Chem/Chem DA Efforts

- WRF-Chem/GSI
  - ✓ Liu et al., NCAR/MMM – Assimilate MODIS AOD, $PM_{2.5}$, and PM_{10} surface observations.
  - ✓ Pagowski and Grell, NOAA – Assimilate O_3 and $PM_{2.5}$.
  - ✓ Saide et al ., Univ. of Iowa and NCAR/ACOM – Assimilate MODIS AOD with constrained emissions.
- WRF-Chem/EnKF
  - ✓ Pagowski and Grell, NOAA – Assimilate $PM_{2.5}$ surface observations.
- WRF-Chem/DART (EAKF)
  - ✓ Mizzi and Edwards, NCAR/ACOM; Anderson, NCAR/IMAGe; and Arellano, Univ. of Arizona – Assimilate MOPITT and IASI CO profiles and MODIS AOD with constrained emissions.

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WRF-Chem/Chem DA Efforts cont.

- WRF-Chem/DART (EAKF) cont.
  - ✓ Mizzi, NCAR/ACOM; and Cohen and Liu, Univ. of California, Berkeley – Assimilate OMI total column NO_2 with constrained emissions.
  - ✓ Mizzi, NCAR/ACOM; and Chen, Miao, and Liang, York University – Assimilate MOPITT total column CO with constrained emissions and MODIS AOD.
  - ✓ Mizzi, Pfister, and Edwards, NCAR/ACOM – Application of WRF-Chem/DART to quasi-real time dual-resolution air quality forecasting/cycling in FRAPPE/DiscoverAQ.
  - ✓ Mizzi, NCAR/ACOM; and Mirzargar, Univ. of Miami – Using data-depth algorithms to identify the most representative ensemble member for quasi-real, time dual-resolution air quality forecasting/assimilation.

WRF-Chem/Chem DA Efforts cont.

- WRF-Chem/DART (EAKF) cont.
  - ✓ Mizzi, NCAR/ACOM; and Brasseur and Bouarar, Max Plank Inst. for Meteorology – Application of WRF-Chem/DART to quasi-real time, dual-resolution air quality forecasting/cycling for eastern China in connection with PANDA.
  - ✓ Mizzi, NCAR/ACOM; and Wang, Nanjing University – Application of WRF-Chem/DART to quasi-real, time dual-resolution air quality forecasting/cycling for eastern China.

WRF-Chem/GSI – Liu et al., NCAR/MMM

- Directly analyze 3D aerosol mass concentration with a one-step procedure of variational minimization within the GSI
  - Do NOT apply any assumption about vertical shape and relative weight of individual species.

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}[y - H(x)]^T R^{-1}[y - H(x)]$$

- 14 WRF/Chem-GOCART 3D aerosol mass concentration as analysis variables
  - need background error covariance statistics for each aerosol species

- Use CRTM as AOD observation operator, including both forward and Jacobian models
  - Dr. Quanhua (Mark) Liu at the JCSDA developed the CRTM-AOD operator.
  - We (NCAR) made CRTM-AOD operator interface to GSI.

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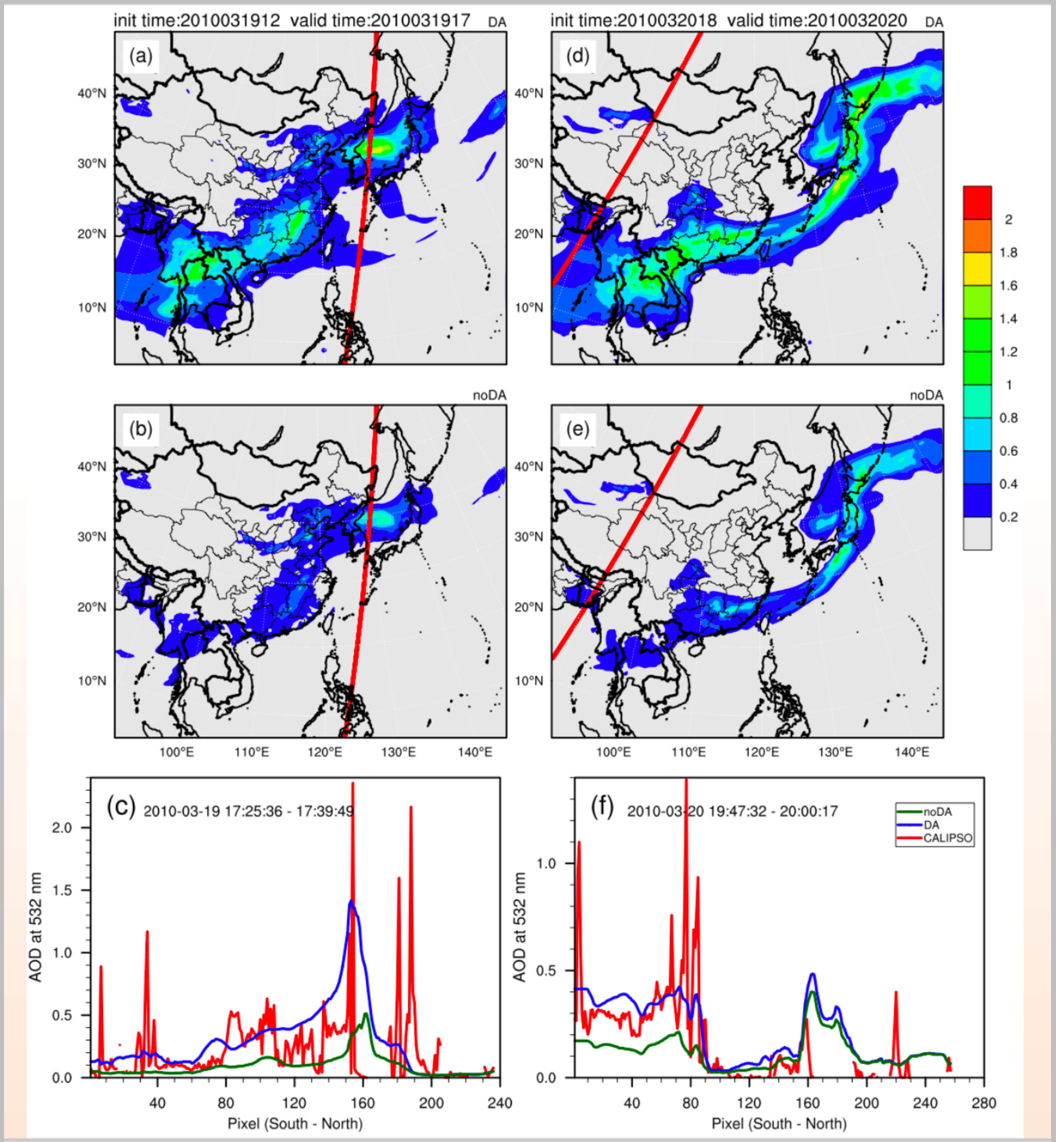
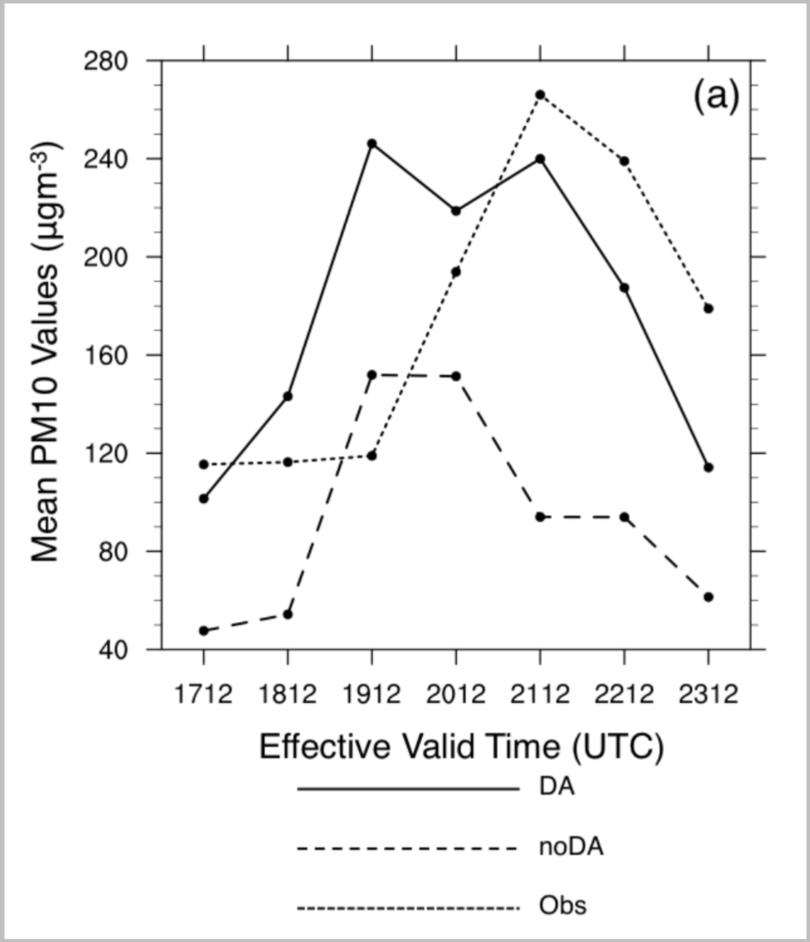
WRF-Chem/GSI – Liu et al., NCAR/MMM

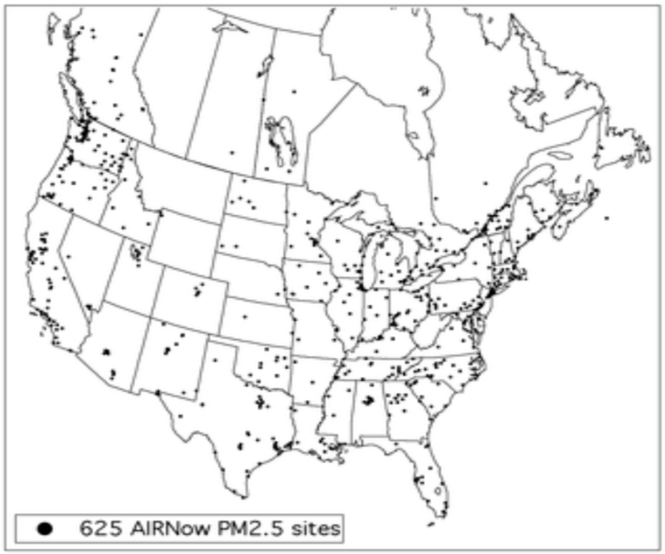




WRF-Chem/GSI – Pagowski and Grell, NOAA

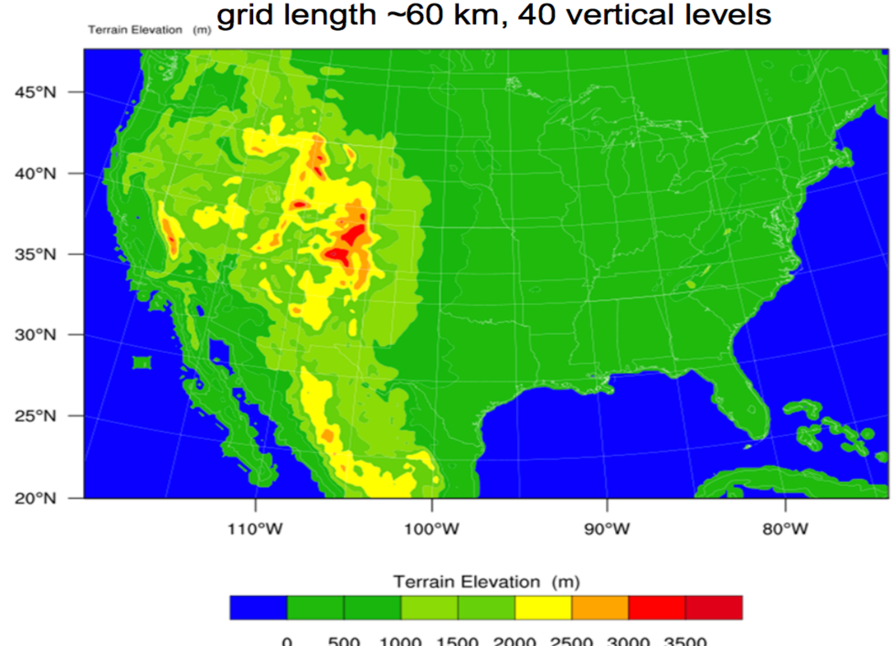
Observations and Model

Real-time PM2.5 measurements network AIRNow



ARW WRF-Chem updated version 3.2.1

grid length ~60 km, 40 vertical levels



GOCART aerosol for computational reasons, assimilate standard meteorological observations (prepbufr) and AIRNow PM2.5 in 6-hr cycle with 1-hr window, NMM lateral boundary conditions;

GSI: Background Error Statistics derived from continuous forecasts in summer 2006 using NMC method;

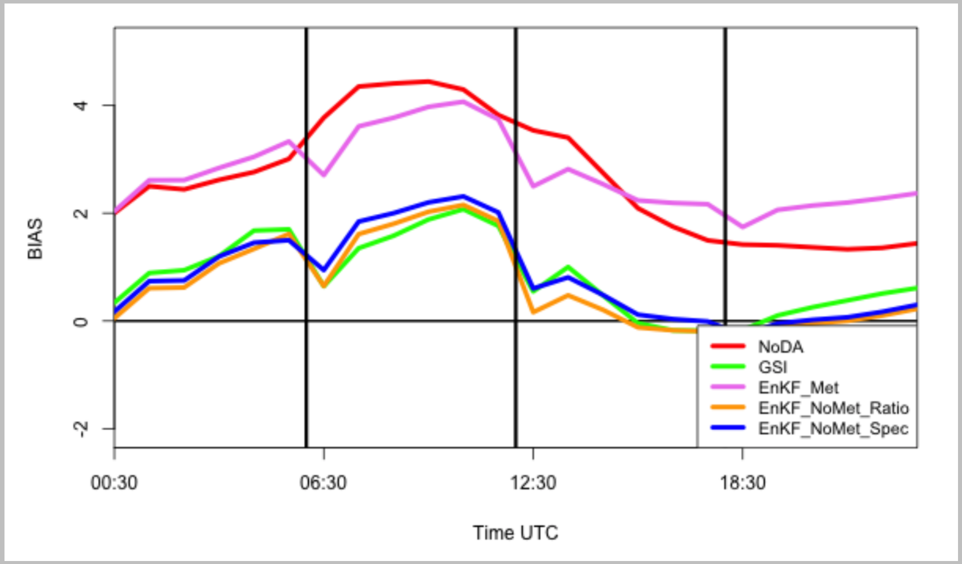
EnKF: 50 ensembles initialized from NMM using background error statistics and perturbing emissions.

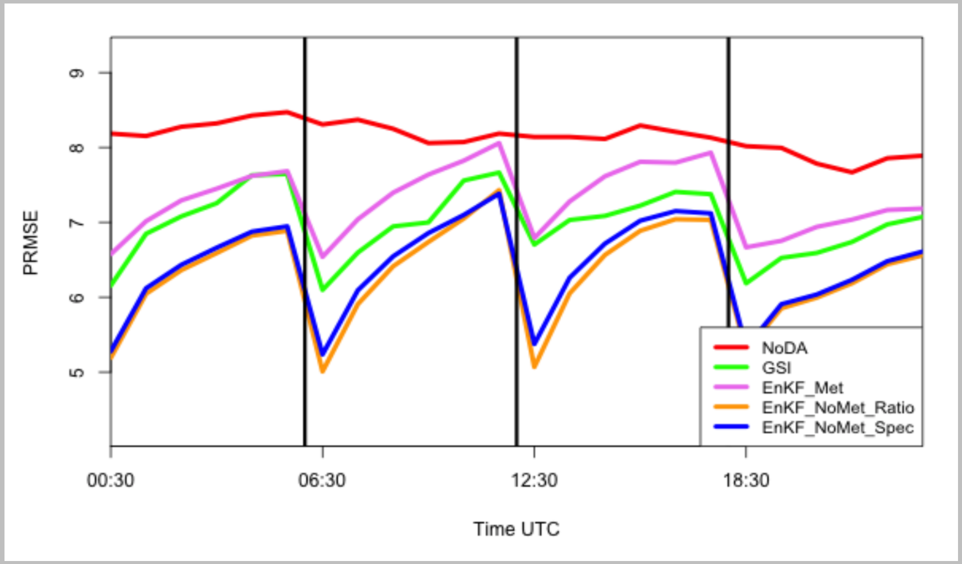
Total aerosol mass;

1-hr average available round the clock;

urban, suburban, rural sites.

WRF-Chem/GSI – Pagowski and Grell, NOAA

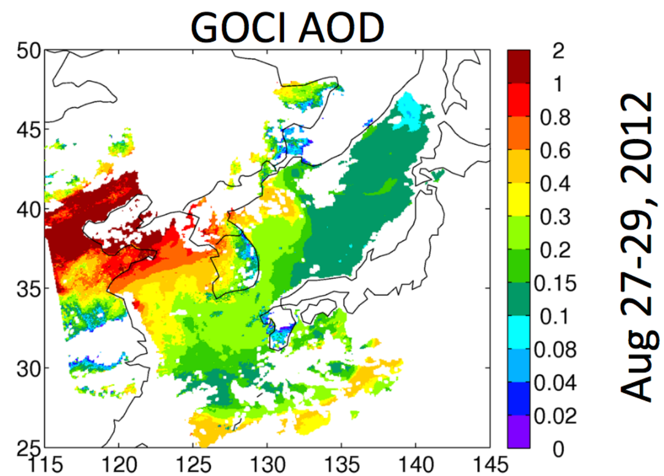


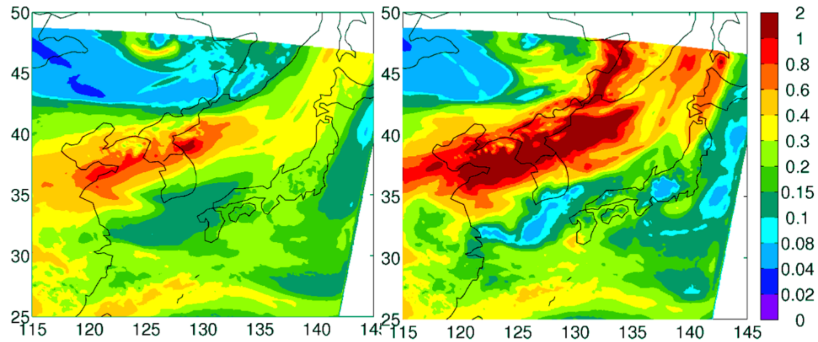


WRF-Chem/GSI – Saide et al., Univ. of Iowa and NCAR/ACOM

Assimilation experiments

- Objectives: Assess performance of assimilating GOCI AOD into a system already assimilating MODIS AOD
- System: WRF-Chem - GSI for MOSAIC sectional aerosol model (Saide et al., ACP 2013) allows assimilation of multiple data
- GSI AOD assimilation every 3 hours, MODIS only, MODIS+GOCI.
- GOCI assimilated is only over ocean





WRF-Chem NO Assim

WRF-Chem MODIS+GOCI Assim

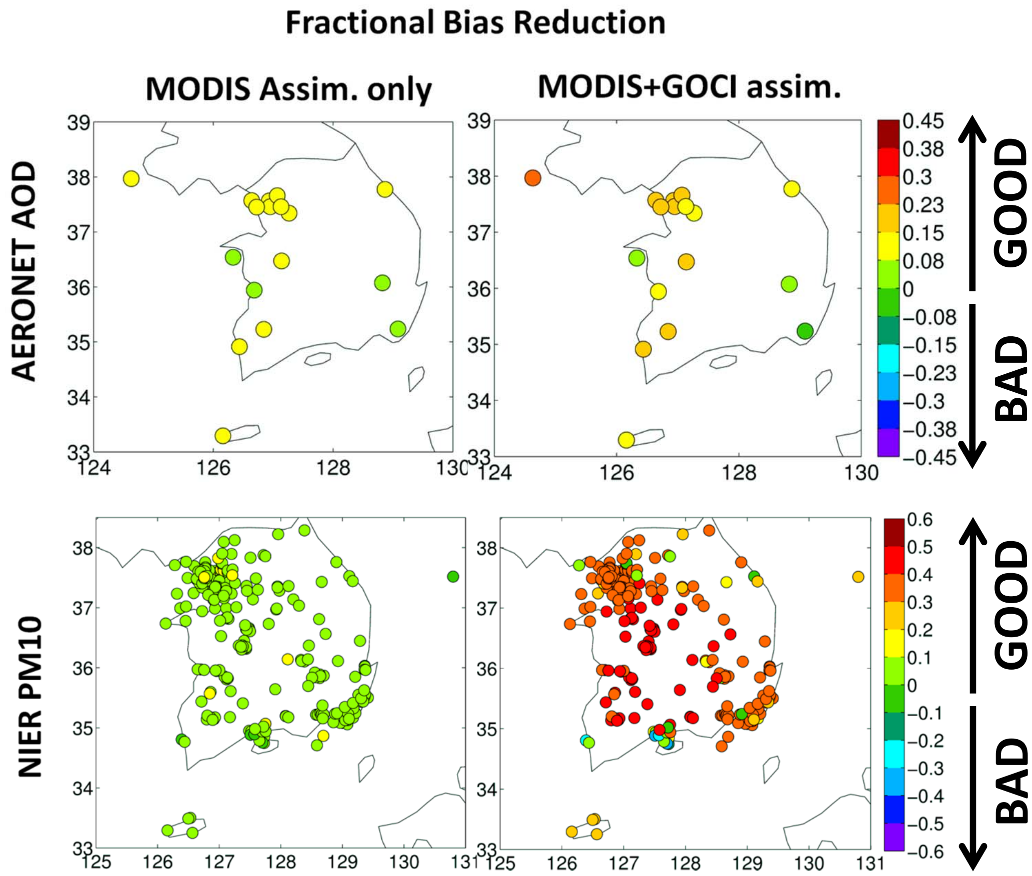
Lee et al., RSE 2010, Park et al., ACP 2014

4

WRF-Chem/GSI – Saide et al., Univ. of Iowa and NCAR/ACOM

Statistics per station

- AERONET DRAGON network available
- Substantial Error and bias reduction when including GOCI
- Reasons: GOCI fills gaps of MODIS (clouds, ocean glint)



5

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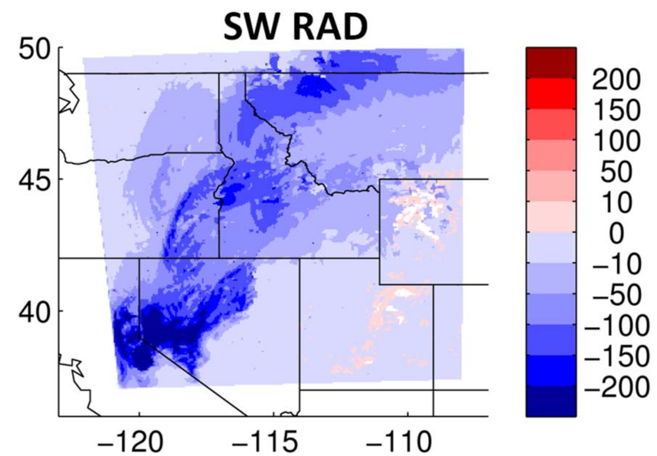
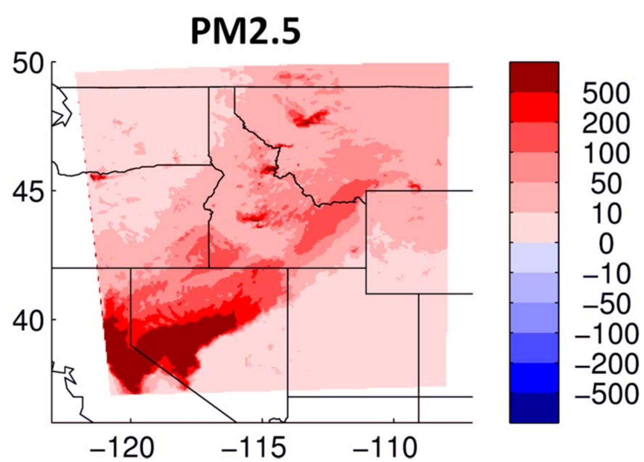
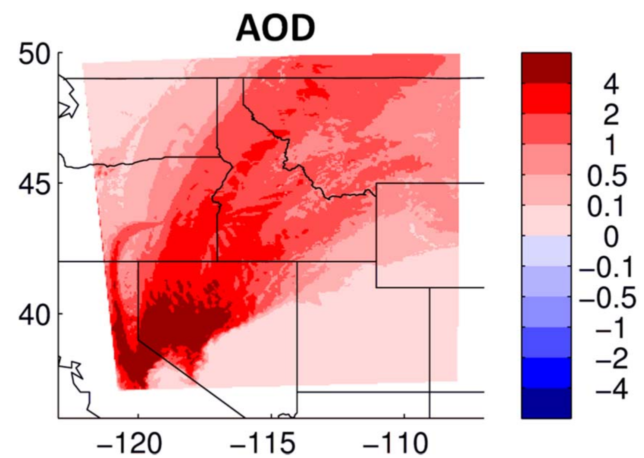
WRF-Chem/GSI – Saide et al., Univ. of Iowa and NCAR/ACOM

Impacts of constrained emissions

- Maximum changes shown comparing simulation with initial and constrained emissions
- Impacts can be substantial







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WRF-Chem/DART

- WRF-Chem – the Weather Research and Forecasting (WRF) model with online chemistry.
- DART – the Data Assimilation Research Testbed modified for assimilation of atmospheric composition observations.
  - MOPITT and IASI partial and total column CO
  - IASI partial and total column O3 (under development)
  - MODIS AOD and OMI total column NO2
  - AirNOW in situ observations (under testing)
  - Emission constraints – State augmentation method
  - Assimilate as RETRs, QORs), and CPSRs
  - State variable localization (joint or independent assimilation)
  - Quasi-Realtime and dual-resolution cycling.

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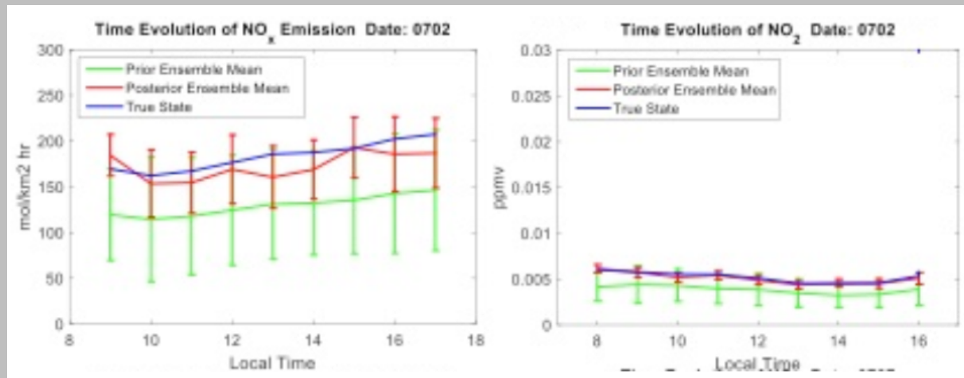
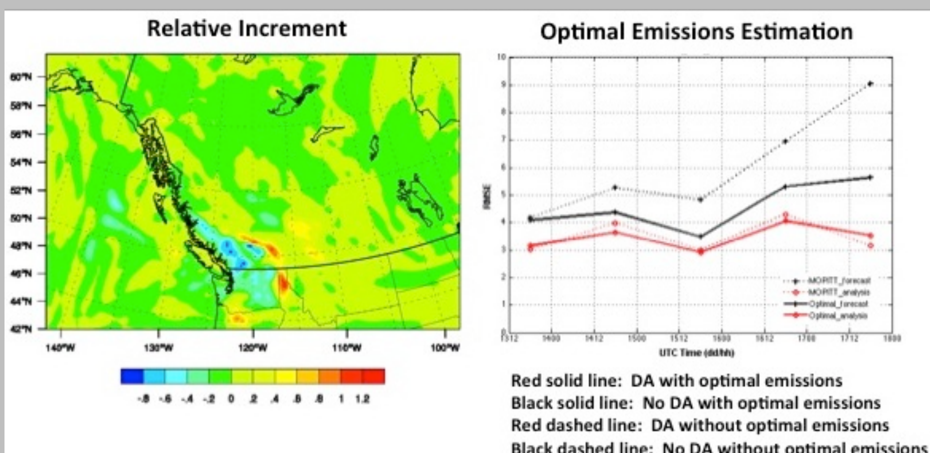
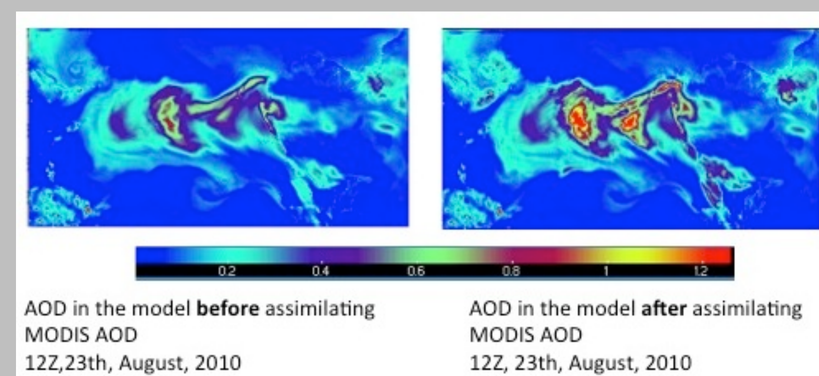
WRF-Chem/DART: NCAR/Univ. Collaborations



Berkeley: Liu and Cohen
OMI NO2 and emission estimation



York Univ.: Miao and Chen
MOPITT total column CO and emission estimation



York Univ.: Liang and Chen
MODIS AOD

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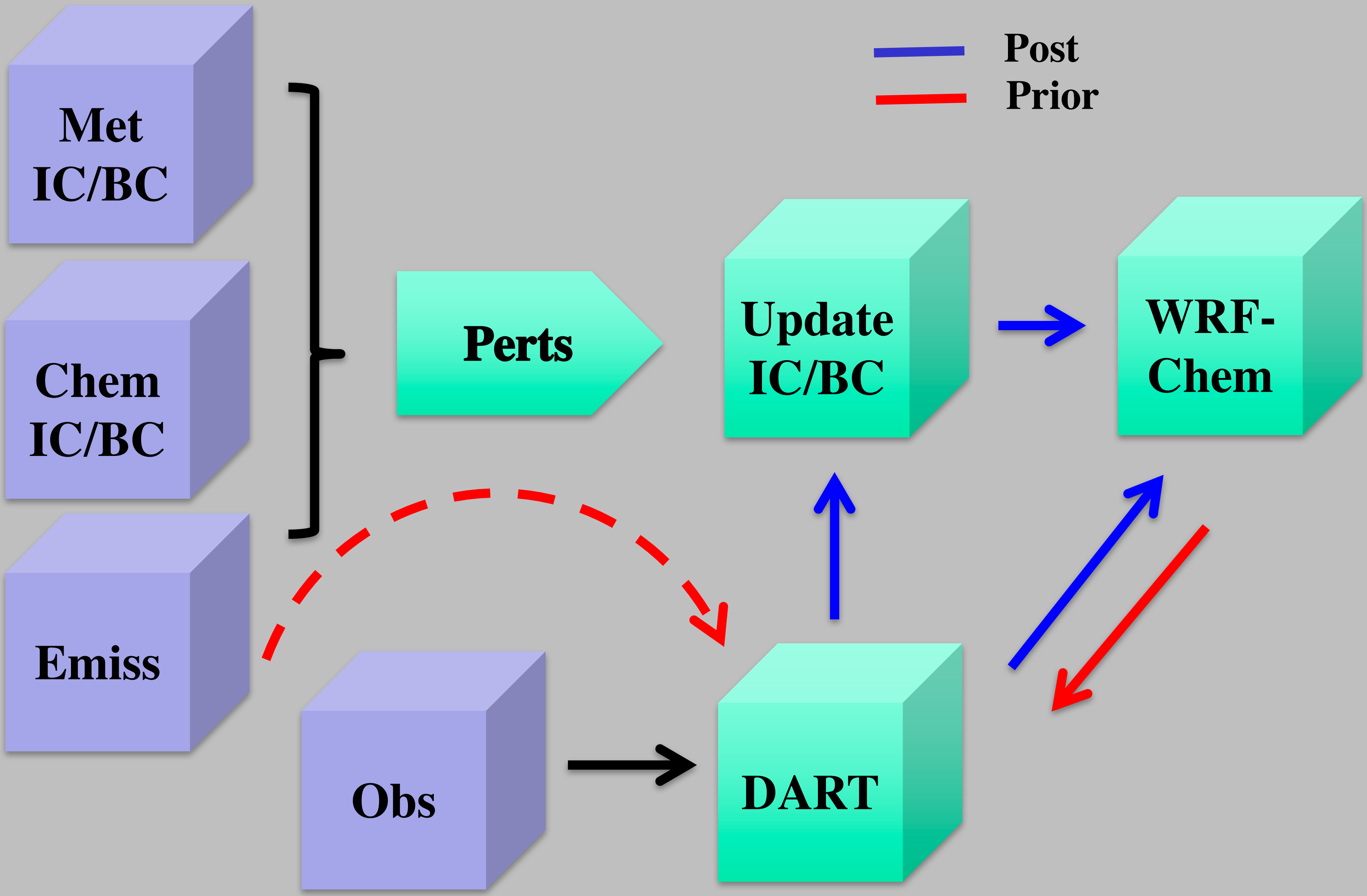
Real-Time WRF-Chem/DART Flow



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CPSR: Full Retrieval Profiles

- $y_r = Ay_t + (I - A)y_a + \varepsilon \Longrightarrow y_r - (I - A)y_a - \varepsilon = Ay_t$ where A is singular and its leading left singular vectors span its range.
- Project the quasi-optimal retrieval onto the leading left singular vectors of A: data compression step.
- That transform reduces the number of observations from the dimension of the retrieval profile to the number of non-zero singular values.
- The transformed E_m^2 is non-diagonal: use an SVD diagonalization (Anderson, 2003; Migliorini et al., 2008): diagonalization step.
- 1st SVD: $A = \Omega\Sigma\Psi^T = \Omega_0\Sigma_0\Psi_0^T$ - Compression Transform;

  2nd SVD: $\Omega_0^T E_m^2 \Omega_0 = \Pi\Lambda\Theta^T$ - Diagonalization Transform;

  Assimilate CPSRs:

$$\Pi^T\Lambda^{-1/2}\Omega_0^T(y_r - (I - A)y_a - \varepsilon) = \Pi^T\Lambda^{-1/2}\Sigma_0\Psi_0^T y_t.$$

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CPSRs: Extension to Truncated Retrieval Profiles

- Mizzi et al. (2017a):

$$\boldsymbol{y_r} - (\boldsymbol{I} - \boldsymbol{A})\boldsymbol{y_a} - \boldsymbol{\epsilon} = \boldsymbol{A}\boldsymbol{y_t}$$

  - ✓ Discard $\boldsymbol{m}$ elements of $\boldsymbol{y}_r$. The resulting dimension is $\boldsymbol{n}-\boldsymbol{m}$.
  - ✓ Discard the corresponding rows of $\boldsymbol{A}$, and the corresponding rows and columns of $\boldsymbol{E}_m$ (resulting dimension $(\boldsymbol{n}-\boldsymbol{m})\times(\boldsymbol{n}-\boldsymbol{m})$).
  - ✓ $\boldsymbol{A}$ was a square $\boldsymbol{n}\times\boldsymbol{n}$ matrix. It is now a rectangular $(\boldsymbol{n}-\boldsymbol{m})\times\boldsymbol{n}$ matrix. Thus, assimilation of retrieval partial profiles is called "CPSRs applied to rectangular systems."
  - ✓ The rest of the derivation follows Mizzi et al. (2016) due to their use of SVDs for the "compression" and "diagonalization" transformations.

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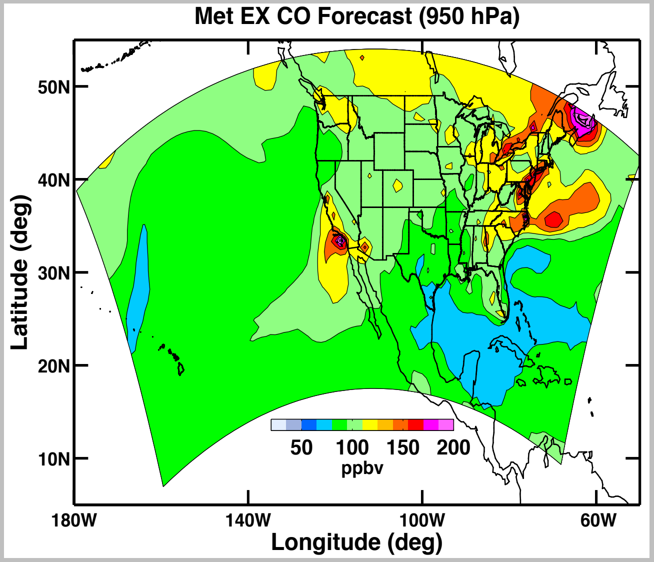
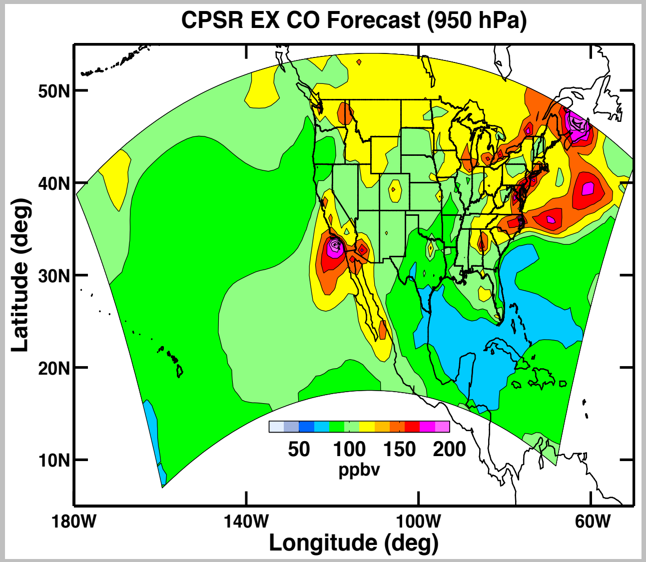
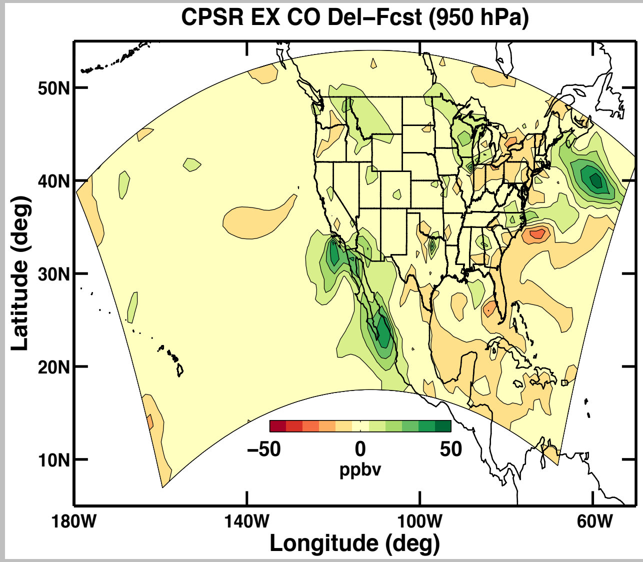
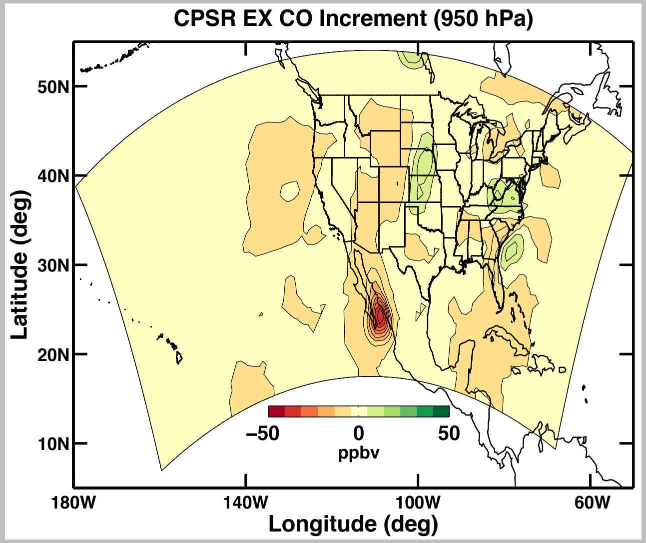
2008 Case Study: (June 19, 2008 18 UTC)









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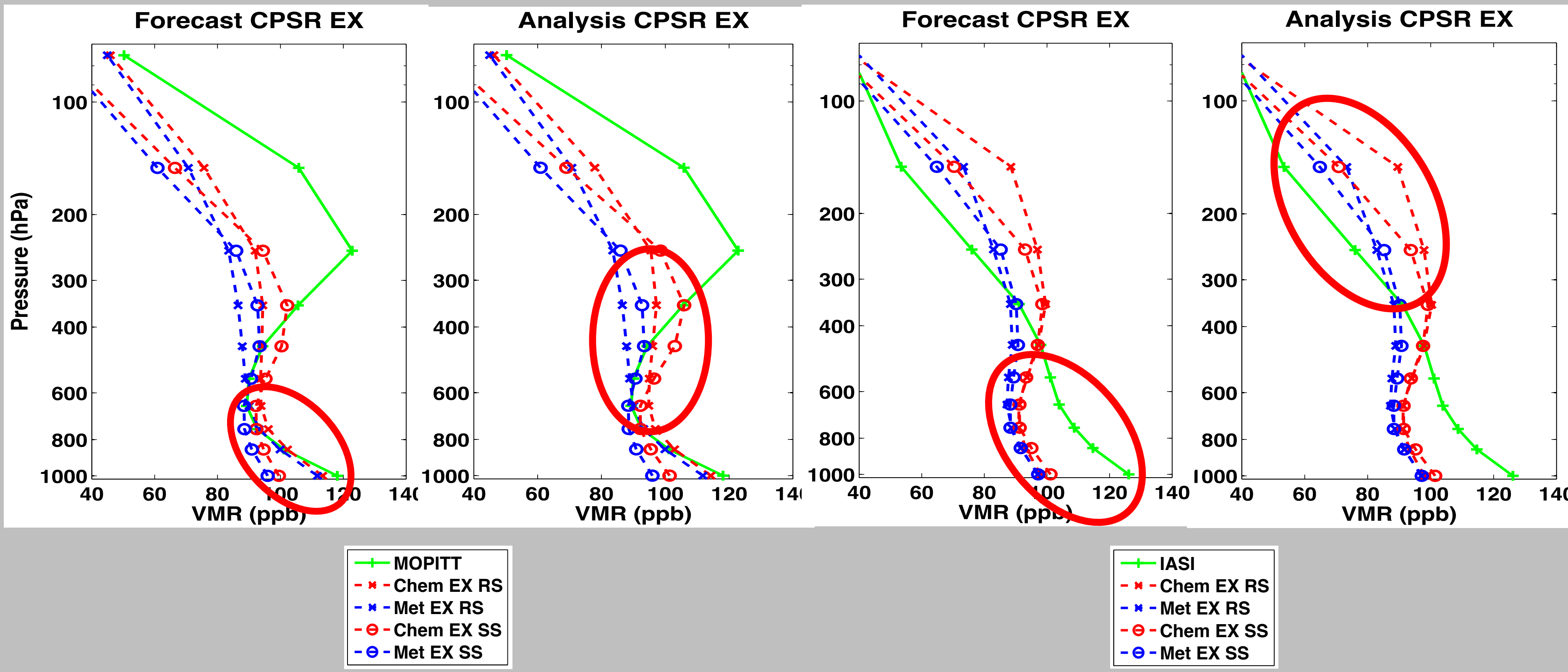
Vertical Profiles (Full Retrieval Profiles)



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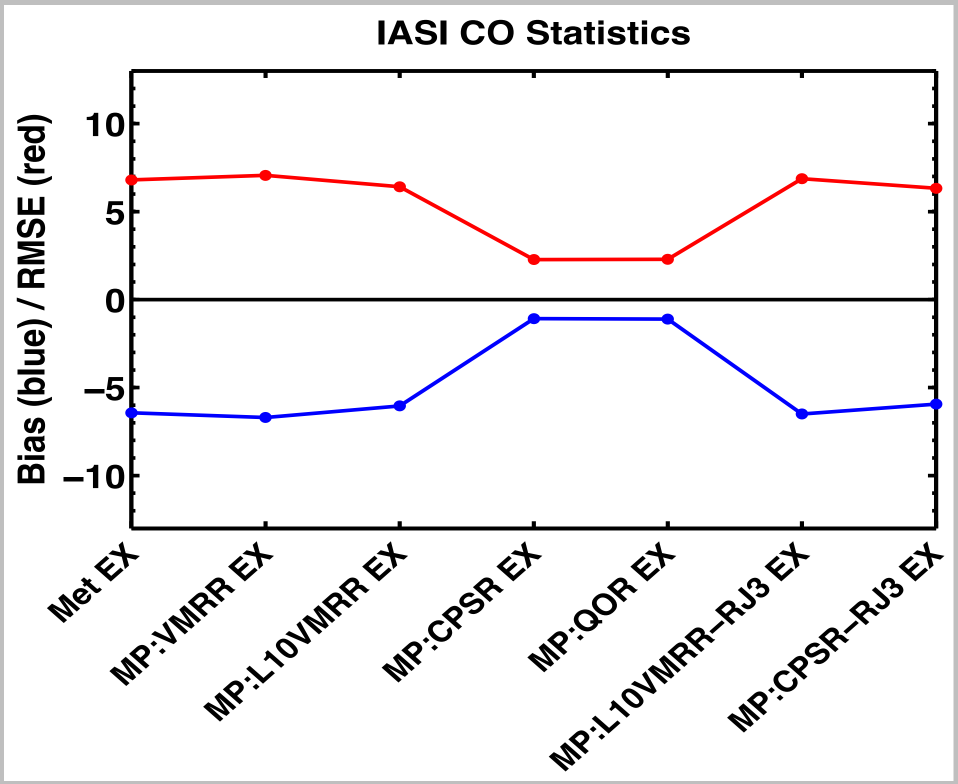
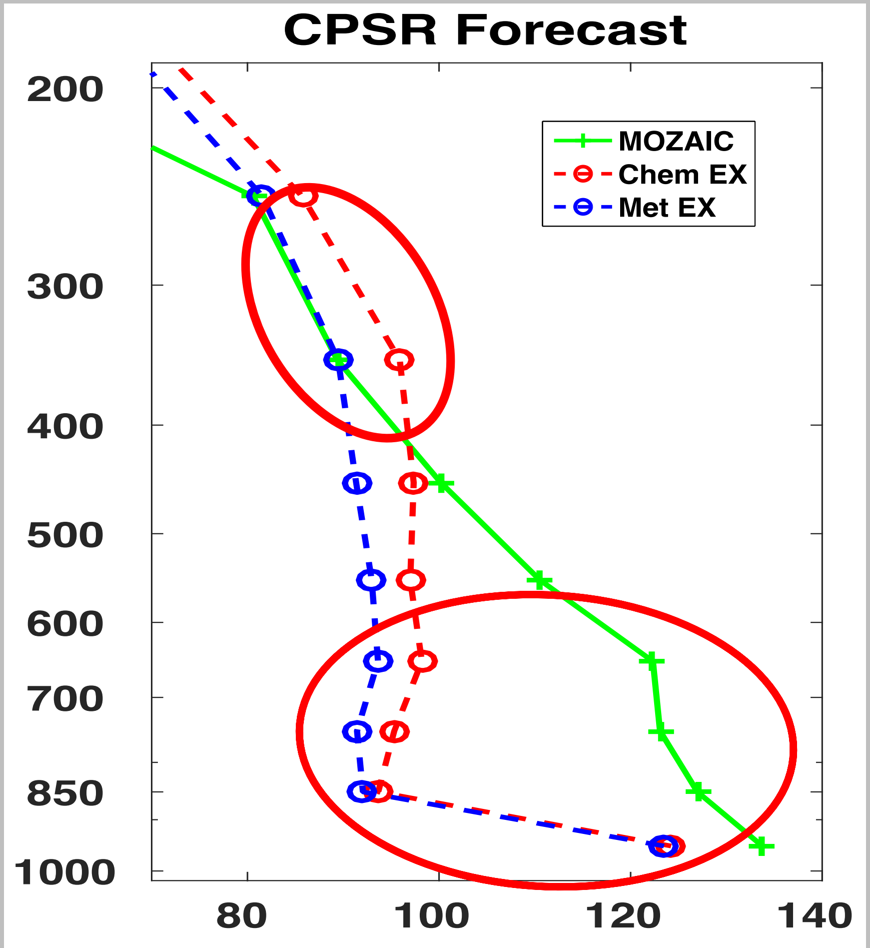
2008 Case Study: Forecast Verification





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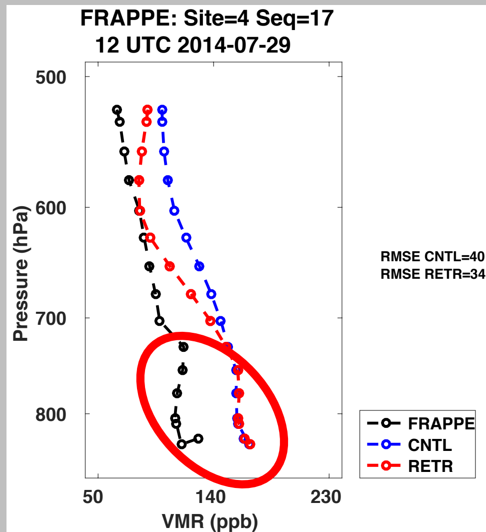
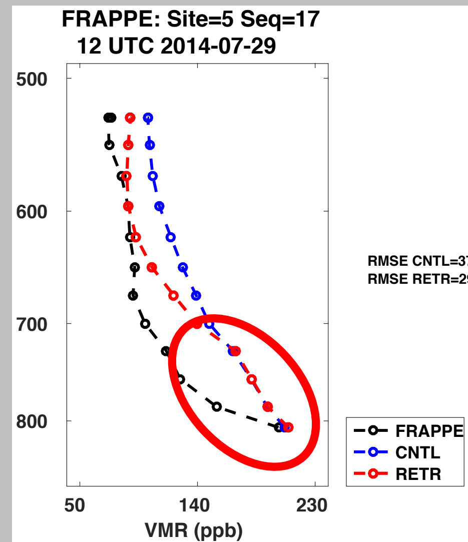
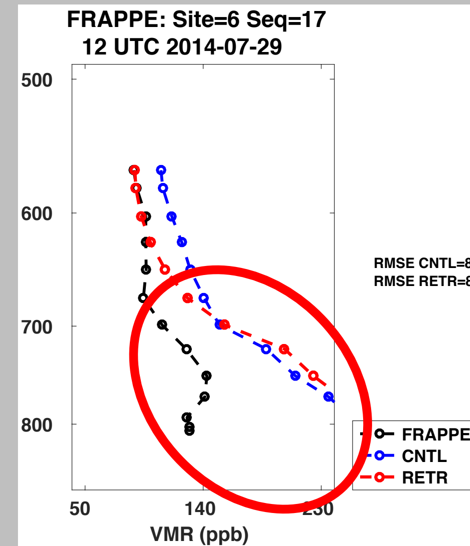
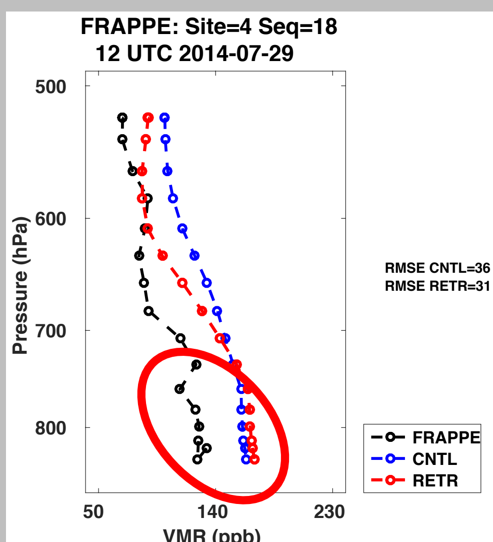
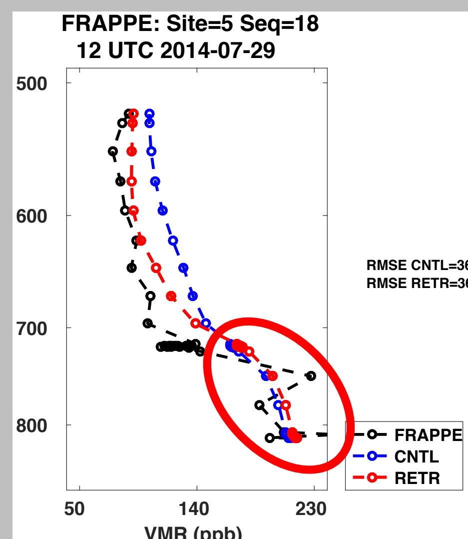
FRAPPE Results (July 29, 2014)

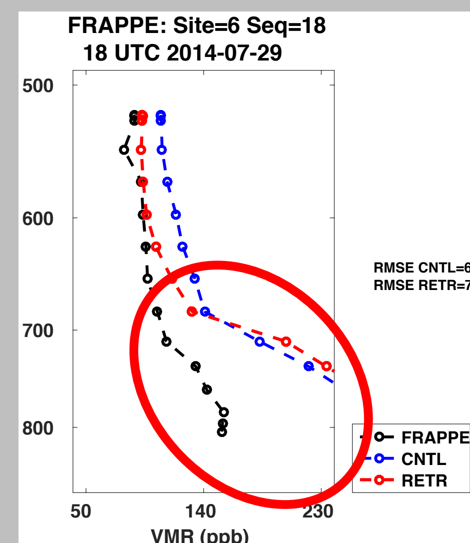












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Review of WRF-Chem/DART Tutorial Exercise on Localization

Ensemble Kalman Filter

- Mitchell and Houtekamer (2001):

$$\boldsymbol{x^a} = \boldsymbol{x^b} + \boldsymbol{K}\left(\boldsymbol{y^o} - \boldsymbol{Hx^b}\right)$$

  where $\boldsymbol{K} = \boldsymbol{PH^T}(\boldsymbol{HPH^T} + \boldsymbol{R})^{-1}$ - $\boldsymbol{P}$ is the ensemble error covariance, $\boldsymbol{R}$ is the observation error covariance, and $\boldsymbol{H}$ is the forward operator mapping state variable $\boldsymbol{x}$ to observation $\boldsymbol{y}$.
- **Problem:** undersampling can lead to spurious correlations in $\boldsymbol{P}$.
- **Problem:** overfitting and cycling can lead to degeneracy/spread collapse.
- **Solution:** Localization – limit the spatial extent and/or state variable/observation correlations (reduce or set them to zero).
- **Solution:** Increase observation error to avoid overfitting
- **Solution:** Use prior or posterior covariance inflation.

Ensemble Kalman Filter Least Squares Framework - Spread Collapse

$$\Delta \boldsymbol{x} = \left(\frac{\boldsymbol{cov}(\boldsymbol{x}, \boldsymbol{y})}{\boldsymbol{var}(\boldsymbol{y})}\right)^{1/2} \times \Delta \boldsymbol{y}$$

$\boldsymbol{x}$ **-** the ensemble of state variables at a grid locations

$\boldsymbol{y}$ **-** the ensemble of expected observations at an observation location

$\boldsymbol{y} = \boldsymbol{H}(\boldsymbol{x})$ where $\boldsymbol{H}$ is the forward operator

$\Delta \boldsymbol{y}$ - the ensemble of expected observation increments

$\Delta \boldsymbol{x}$ - the ensemble of state variable increments

With spread collapse ***var(y)*** $\rightarrow 0$

Anderson (2003)

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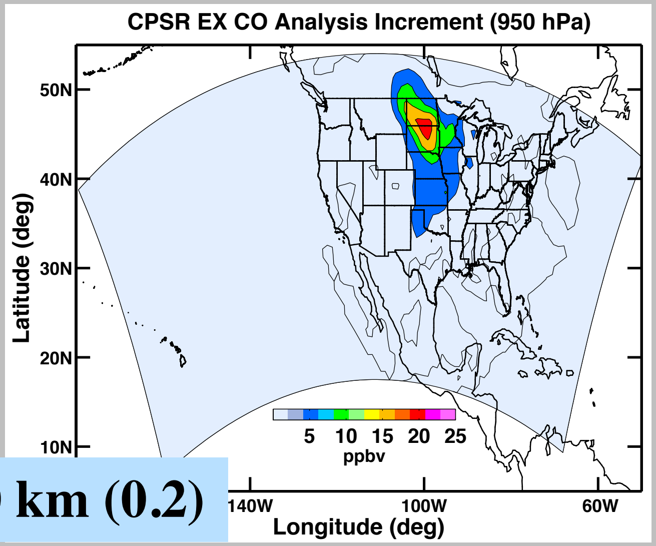
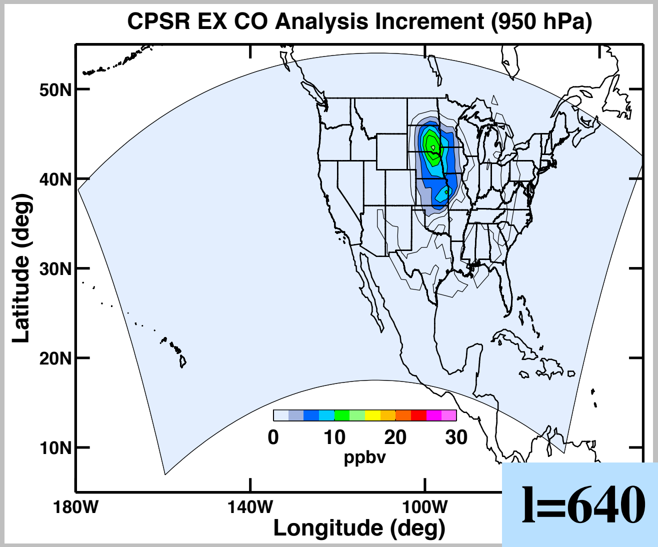
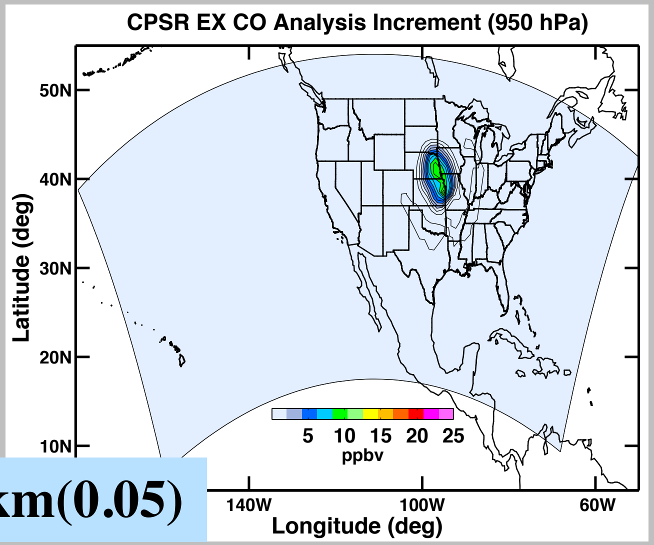
WRF-Chem/DART: Localization Examples



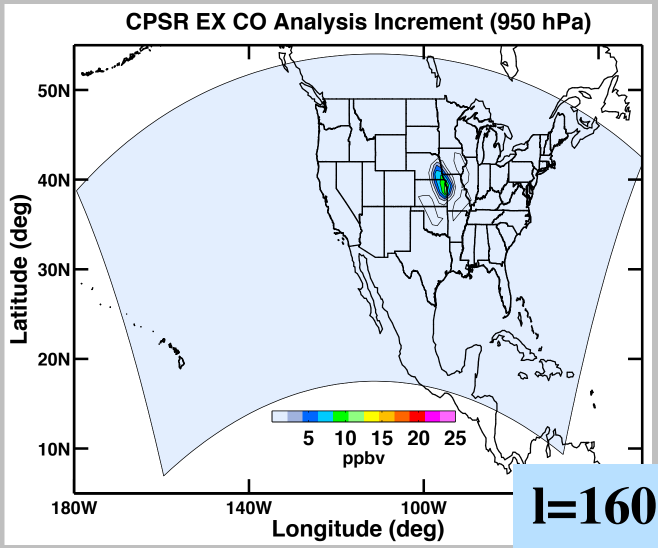
l=1300 km (0.2)



l=640 km (0.1)



l=320 km(0.05)



l=160 km (0.025)

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References:

- Mizzi, A. P., A. F. Arellano, D. P. Edwards, J. L. Anderson, and G. G. Pfister (2016): Assimilating compact retrievals of atmospheric composition with WRF-Chem/DART: A regional chemical transport/ensemble Kalman filter data assimilation system. *Geosci. Model Dev*., 9, 1-14.
- Mizzi, A. P., D. P. Edwards, and J. L. Anderson (2017a): Assimilating compact phase space retrievals (CPSRs): Comparison with independent observations (MOZAIC in situ and IASI retrievals) and extension to assimilation of retrieval partial profiles. [*under internal review*].
- Mizzi, A. P., X. Liu, A. F. Arellano, J. Liang, R. C. Cohen, Y. Chen, D. P. Edwards, and J.L. Anderson (2017b): Assimilating compact phase space retrievals (CPSRs): Joint assimilation of MOPITT and IASI CO CPSRs and MODIS AOD retrievals with constrained emissions. [*in preparation*].

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