WRFDA-Chem 4D-Var: Implementation and application to inverse modeling of black carbon emissions

Jonathan (JJ) Guerrette
Daven Henze
University of Colorado at Boulder
Department of Mechanical Engineering

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Outline

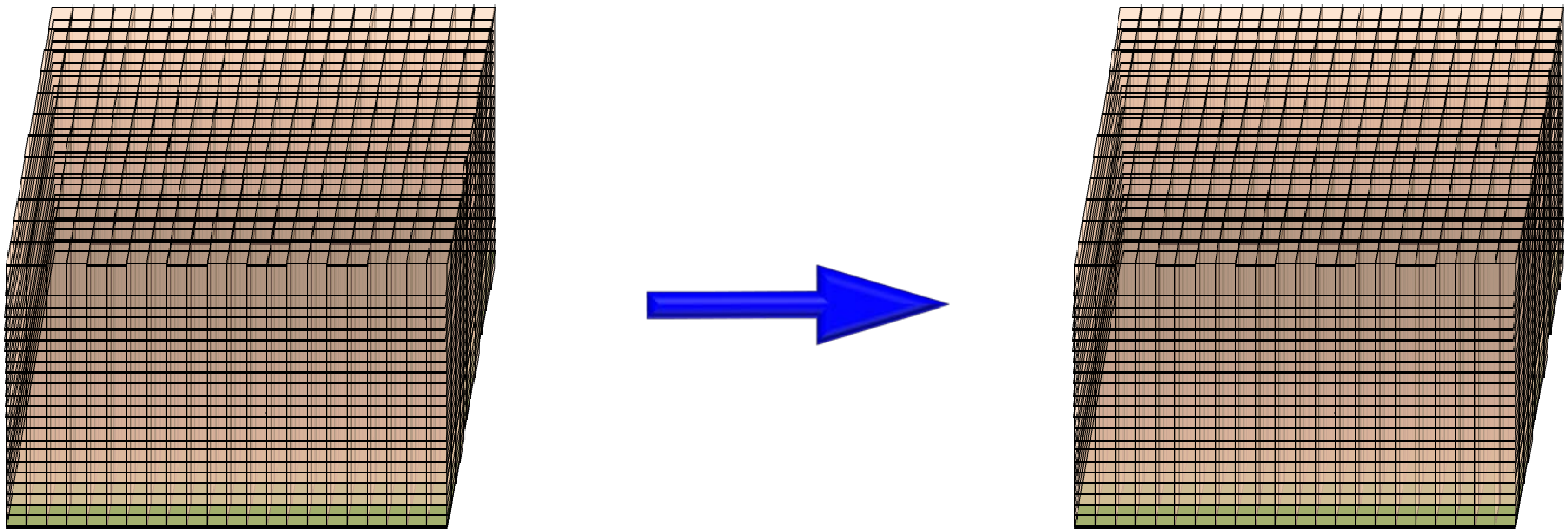
I. Short WRF-Chem primer

II. WRFPLUS-Chem and WRFDA-Chem developments

III. Black carbon emission problem and results

WRF-Chem Primer

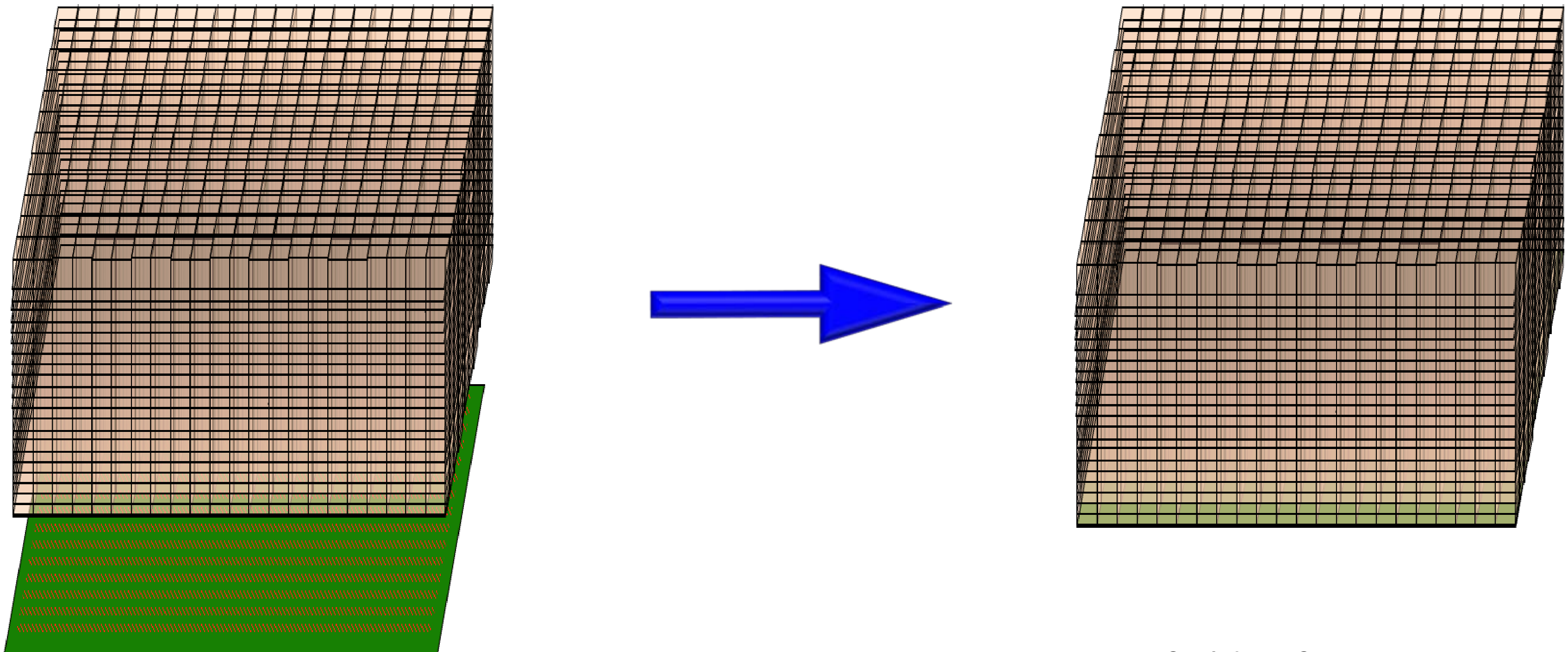
WRF Simulation



3D fields of T, p, q, u, v

3D fields of T, p, q, u, v

WRF-Chem Simulation



3D fields of T, p, q, u, v, **C**

3D fields of T, p, q, u, v, **C** (chemical concentrations)
2D (spatial) + 1D (temporal) fields of **E** (chemical emission rates/fluxes)

Column Processes*

Lower Troposphere

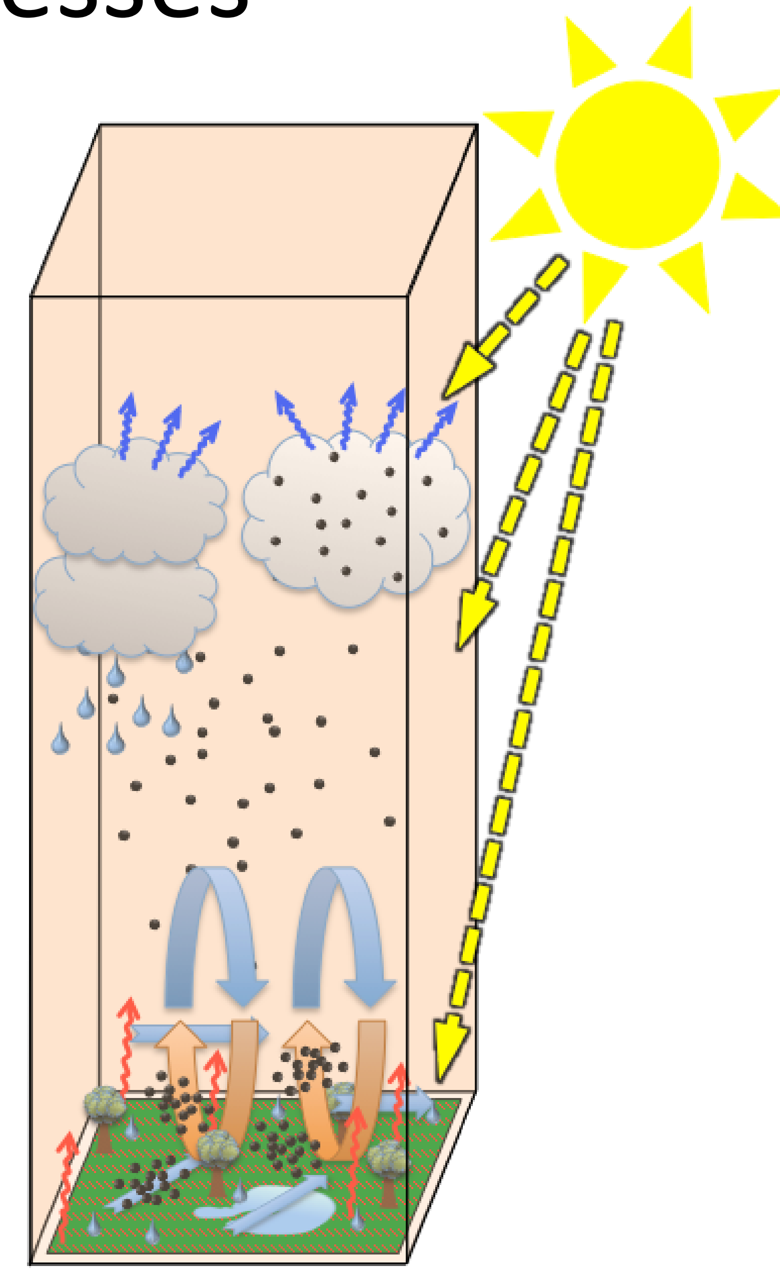
- Surface-air interactions (LSM)
- Turbulent Mixing (PBL)
- **Emissions and Deposition**

All Trop.

- Radiation
- **Chemical Transformation**
- Microphysics

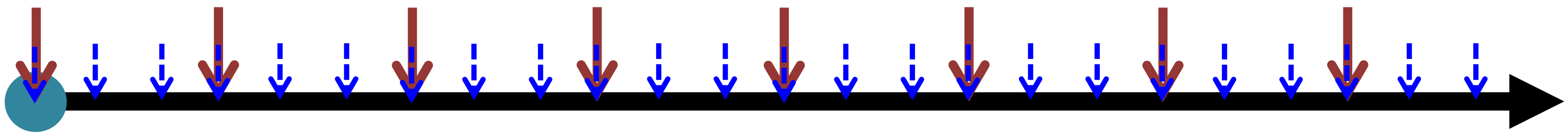
Mid to Upper Trop.

- Cumulus Convection



*Disclaimer: Not illustrated by a meteorologist

WRF-Chem Forward Integration



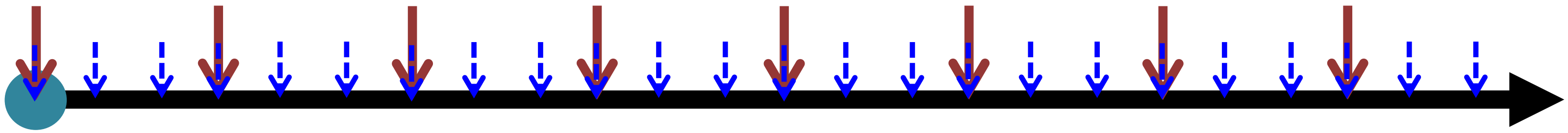
$$\Delta t_{emiss} = 1hr;\ \Delta t_{bound} = 3hr$$

Initial and predicted 3D fields of T, p, q, u, v, **C**
(wrfinput_d01)

Lower boundary surface: **E**
(wrfchemi_d01, wrffirechemi_d01, wrfbiochemi_d01)
anthropogenic biomass burning biogenic

Lateral boundary surfaces: T, p, q, u, v, **C**
(wrfbdy_d01)

WRF-Chem Forward Integration



$$\Delta t_{emiss} = 1hr;\ \Delta t_{bound} = 3hr$$

Initial and predicted 3D fields of T, p, q, u, v, **C**
(wrfinput_d01)

Lower boundary surface: **E**
(wrfchemi_d01, wrffirechemi_d
anthropogenic biomass burni

Lateral boundary surfaces: T, p, q, u, v, **C**
(wrfbdy_d01)

WRFDA-Chem aims to improve these variables through Bayesian statistical analysis (only emissions so far)

WRFPLUS-Chem and WRFDA-Chem Implementation

WRF(-Chem) Model Family

WRF: Non-hydrostatic moist dynamics, diffusion; subgrid PBL mixing, Cumulus Convection, Microphysics, Radiation

[Skamarock et al. (2008)]

-Chem: Chemical transformation, advection, emission, fire plume rise, 1st-order decay, dry/wet deposition losses, PBL and convective transport of aerosols and trace gases

[Grell et al. (2005)]

WRFPLUS: Adjoint **(AD)** and Tangent Linear **(TL)** models for dynamics, diffusion, and select physics packages

[Zhang et al. (2013)]

-Chem: AD/TL of PBL transport, emissions, and dry deposition of GOCART aerosols

[Guerrette and Henze (*GMD*, 2015)]

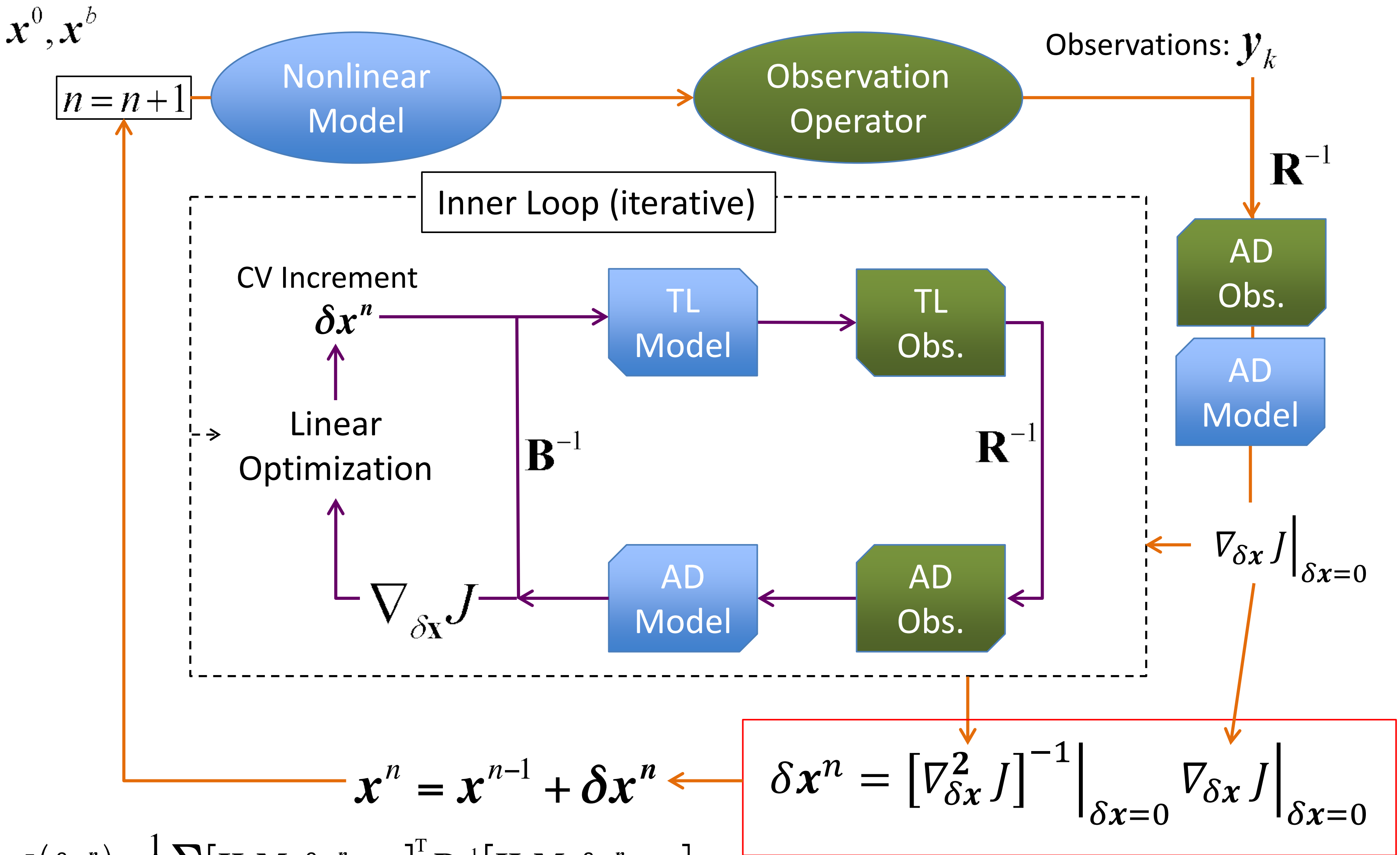
WRFDA: 3D-Var, 4D-Var, and hybrid methods for MET control variables using many in-situ and remote obs. types

[Barker et al. (2005); Huang et al. (2009); Zhang et al. (2014)]

-Chem: 4D-Var for chemical emission control variables using surface and aircraft obs.

[Guerrette and Henze, submitted to *ACP*]

Incremental 4D-Var minimization



$$J\left(\delta x^n\right) = \frac{1}{2}\sum_k \left[\mathbf{H}_k \mathbf{M}_k \delta x^n + r_k\right]^{\mathrm{T}} \mathbf{R}_k^{-1} \left[\mathbf{H}_k \mathbf{M}_k \delta x^n + r_k\right]$$

$$+\frac{1}{2}\left[\delta x^n + x^{n-1} - x^b\right]^{\mathrm{T}} \mathbf{B}^{-1} \left[\delta x^n + x^{n-1} - x^b\right]$$

Courtier et al., 1994

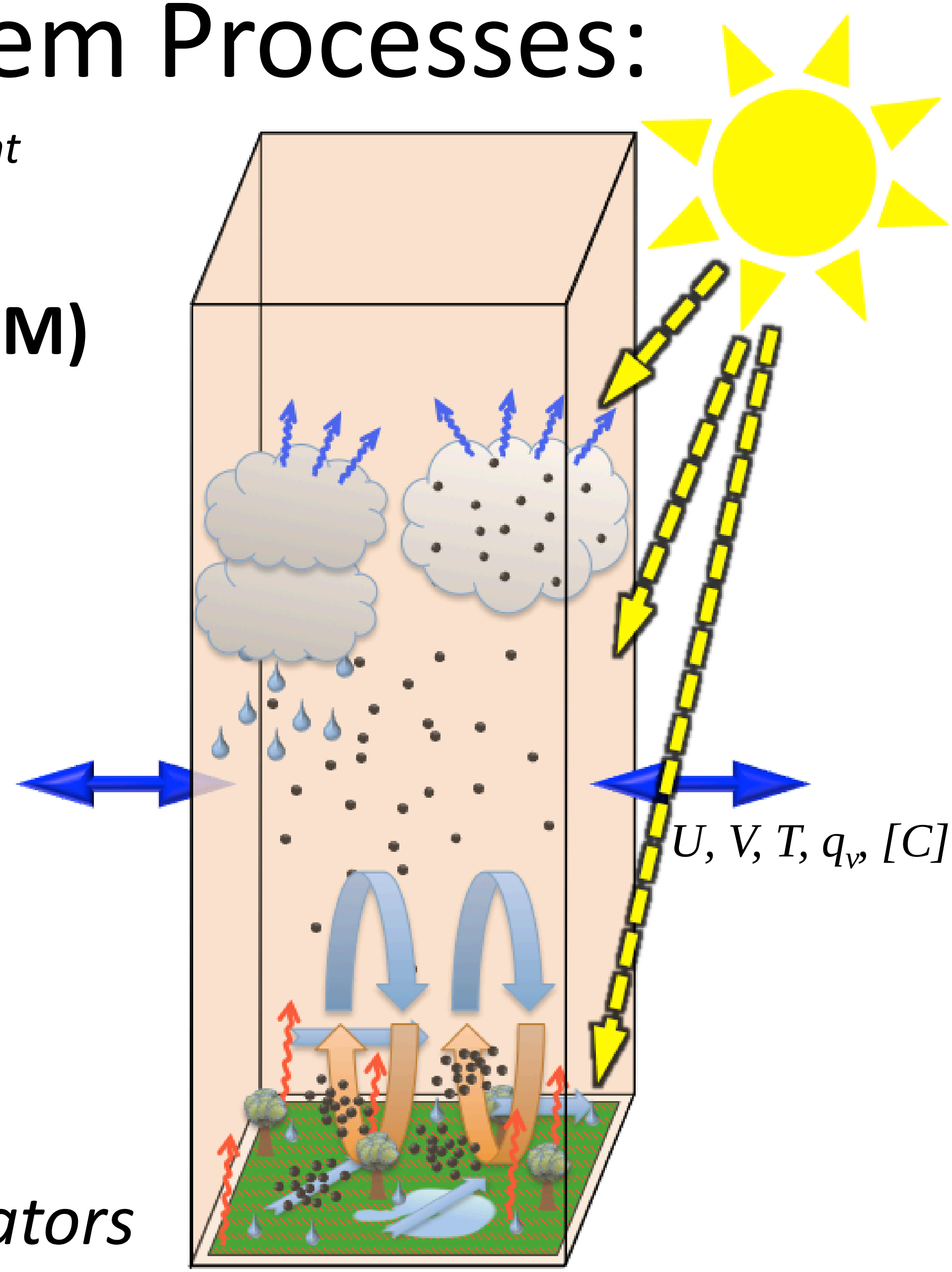
Pieces Needed for -Chem

- Adjoint and tangent linear models
- $\geq$24 hour assimilation window
- Control variable to state variable conversion
- Applicable optimization algorithm
- **B**, background covariance
- **R**, model-observation covariance

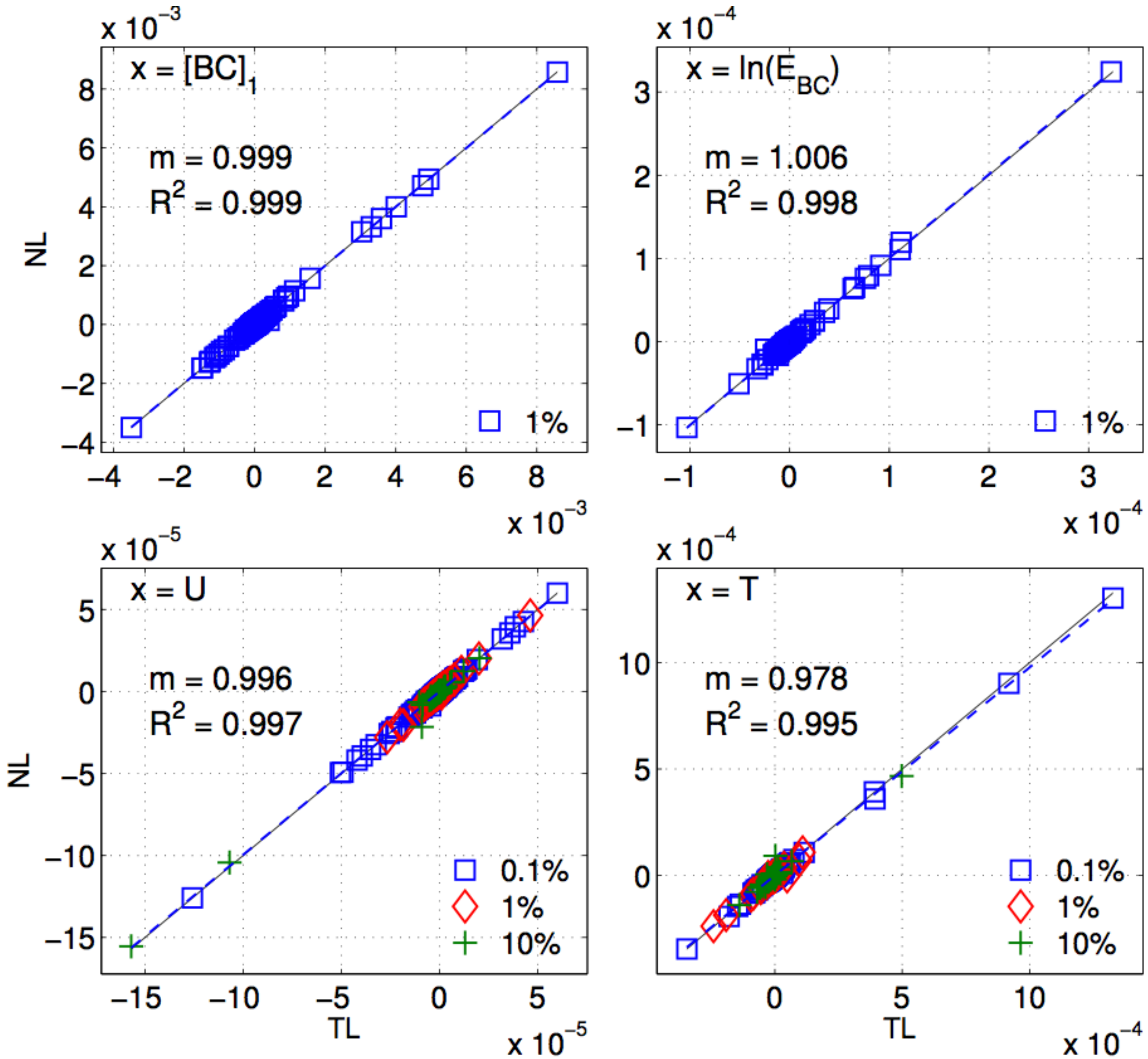
WRFPLUS-Chem Processes:

Functional AD/TL *Future Development*

- **Advection and Diffusion**
- **Surface-air interactions (LSM)**
- **Turbulent Mixing (PBL)**
- * *Cumulus Convection*
- **Emissions**
- * *Wet* and **Dry Deposition**
- **GOCART Aerosols**
- * *CCN activation of aerosols*
- *Radiation*
- Microphysics
- **In-situ obs. operator**
- * *Remote sensing obs. operators*



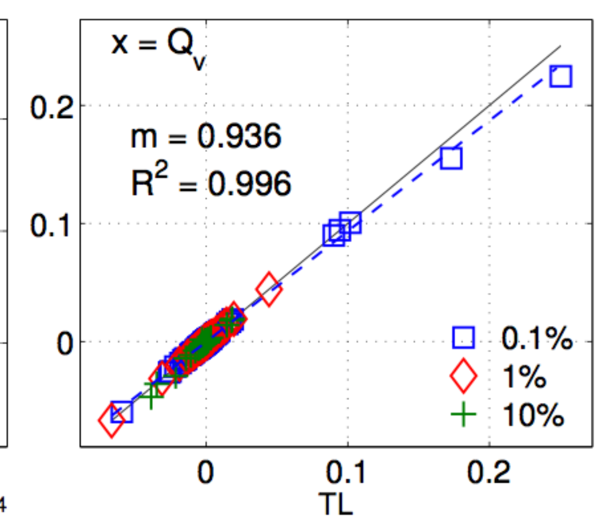
Finite Difference Test



$$\frac{\partial[\mathrm{BC}_{1,2}]}{\partial \mathbf{x}}$$

TL and AD agree to 8+ digits

Note: results are from a 3 hr simulation



Guerrette and Henze (2015)

Pieces Needed for -Chem

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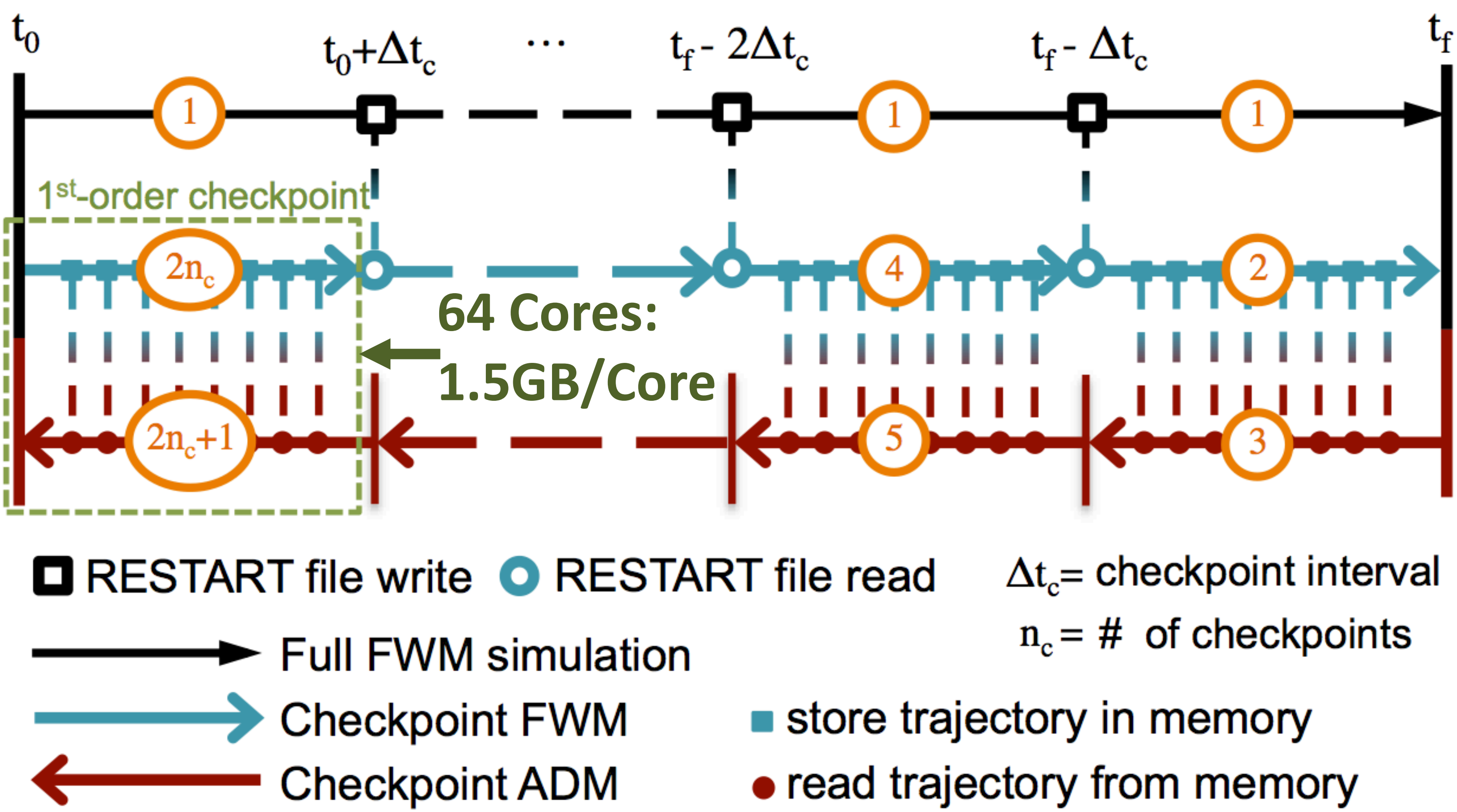
2^{nd} Order Checkpointing

Restrepo et al. (1998)

- Necessary for accumulating sensitivities with respect to time-varying emissions over days to weeks
- Trade off between memory storage requirement and wall-clock time (for extra disk I/O and computations)
- In WRFPLUS-Chem, reduces memory requirement of simulations longer than 3 hours

2^{nd} Order Checkpointing

def. **Trajectory**: Stored values of all state variables at all time steps during a simulation.
(e.g., u, v, T, Φ, Q_v, Q_r, [BC], [SO_2], [NO_2]; configuration dependent)



Pieces Needed for -Chem

- Adjoint and tangent linear models
- $\geq$24 hour assimilation window
- Control variable to state variable conversion
- Applicable optimization algorithm
- **B**, background covariance
- **R**, model-observation covariance

Special Inversion Framework

1. Exponential scaling factors: $E_i^n = E_i^0 e^{x_i^n}$
   - Log-normally distributed emission errors (positive definite emissions), Gaussian x
   - Gaussian modeled/observed concentration errors

$$J(\delta \boldsymbol{x}^n) = \frac{1}{2}\sum_k \left[\mathbf{H}_k \mathbf{M}_k \delta \boldsymbol{x}^n + \boldsymbol{r}_k\right]^{\mathrm{T}} \mathbf{R}_k^{-1} \left[\mathbf{H}_k \mathbf{M}_k \delta \boldsymbol{x}^n + \boldsymbol{r}_k\right]$$

$$+ \frac{1}{2}\left[\delta \boldsymbol{x}^n + \boldsymbol{x}^{n-1} - \boldsymbol{x}^b\right]^{\mathrm{T}} \mathbf{B}^{-1} \left[\delta \boldsymbol{x}^n + \boldsymbol{x}^{n-1} - \boldsymbol{x}^b\right]$$

$$\delta \boldsymbol{x}^n \in \mathcal{R}^{n_x \times n_y \times n_t}$$

2. Damped Gauss Newton increment for nonlinear control variables

e.g., Kelley (1999)

$$\delta \boldsymbol{x}^n = \eta^n \left[\nabla^2_{\delta \boldsymbol{x}} J\right]^{-1}\Big|_{\delta \boldsymbol{x}=0} \nabla_{\delta \boldsymbol{x}} J\Big|_{\delta \boldsymbol{x}=0} ; 0 < \eta^n \le 1$$

Pieces Needed for -Chem

- Adjoint and tangent linear models
- $\geq$24 hour assimilation window
- Control variable to state variable conversion
- Applicable optimization algorithm
- **B**, background covariance
- **R**, model-observation covariance

Background Covariance, $\mathbf{B}$

- Square root preconditioning (same as for MET variables)
- Horizontal and temporal correlation decay across characteristic scales

  (cv_option = 10)

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^b)^{\mathrm{T}} \boxed{\mathbf{B}}^{-\mathbf{1}}(\boldsymbol{x} - \boldsymbol{x}^b) + \frac{1}{2}[H(\boldsymbol{x}) - \boldsymbol{y}^{\boldsymbol{o}}]^{\mathrm{T}} \mathbf{R}^{-\mathbf{1}} [H(\boldsymbol{x}) - \boldsymbol{y}^{\boldsymbol{o}}]$$

$$\mathbf{B} = \mathbf{U}\mathbf{U}^T$$

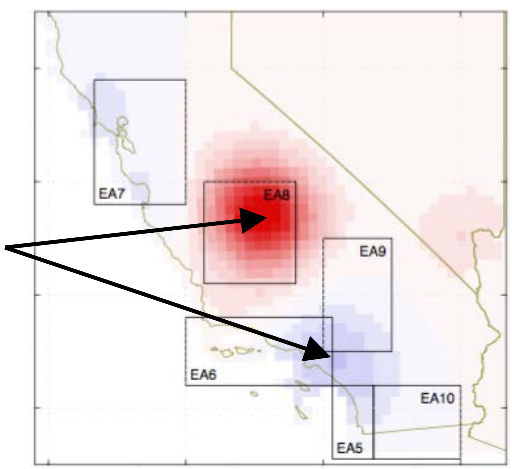
$L_t \sim hours$

$$\mathbf{U} = \mathbf{U}_t \mathbf{U}_x$$

$L_x \sim$grid scale

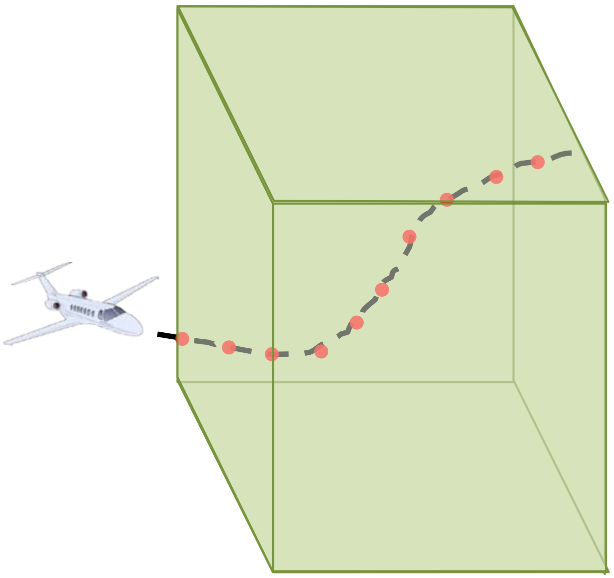
(similar to $\mathbf{U}_v$ for MET variables)

(similar to $\mathbf{U}_x$ for MET variables)



In-situ Observation Operators

- Concentration observation operators carried out "online" during simulation
- High resolution aircraft measurements averaged to the simulation time step
- Surface sites compared to temporal model average in nearest ground-level grid cell



[Guerrette and Henze (*GMD*, 2015)]

Obs./Model Error Covariance, $\mathbf{R}$

$$\sigma_{k,k}^2 = \sigma_k^2 = \sigma_{k,\mathrm{obs}}^2 + \sigma_{k,\mathrm{model}}^2$$

$$J(\boldsymbol{x}) = \frac{1}{2}\left(\boldsymbol{x} - \boldsymbol{x}^b\right)^{\mathrm{T}}\mathbf{B}^{-\mathbf{1}}\left(\boldsymbol{x} - \boldsymbol{x}^b\right) + \frac{1}{2}\left[H(\boldsymbol{x}) - \boldsymbol{y}^{\boldsymbol{o}}\right]^{\mathrm{T}}\mathbf{R}^{-\mathbf{1}}\left[H(\boldsymbol{x}) - \boldsymbol{y}^{\boldsymbol{o}}\right]$$

- Observation variance
  - Instrument uncertainty
  - Representativeness (for aircraft grid cell average)

- Model variance from 156 ensemble members
  - 3 LSM options
  - 4 Surface Layer options
  - 7 PBL options
  - 2 LW/SW Radiation options
  - Microphysics on/off
  - Cumulus Convection on/off

[Guerrette and Henze (*GMD*, 2015)]

First Application

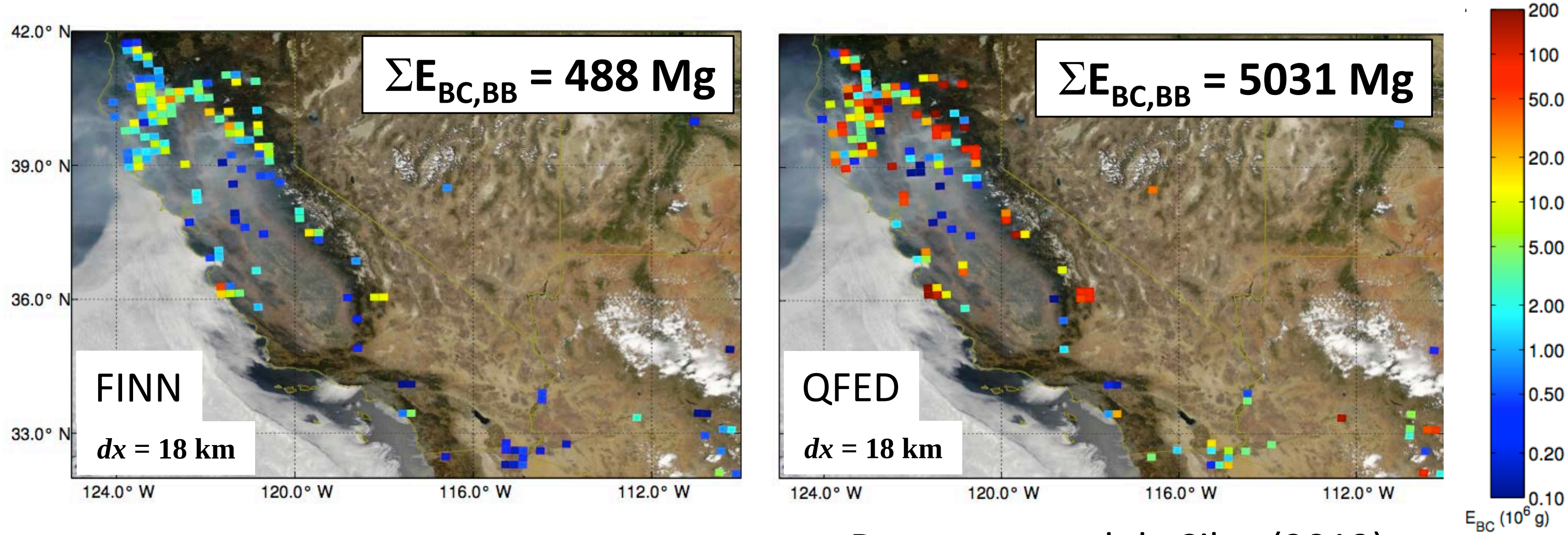
Submitted to ACP:
Guerrette, J.J. and D.K. Henze. Four dimensional variational inversion of black carbon emissions during ARCTAS-CARB with WRFDA-Chem.

2008 ARCTAS-CARB case study

- MODIS True Color is cloud free over California
  26 May – 20 June
- High mountain clouds on 21 June, widespread fire ignition on or before 22 June
- 20 June: First DC8 flight + IMPROVE observe "clean" anthropogenic sources and chemistry
- All measurements thereafter influenced by fire emissions

California BC Emissions

Total Biomass Burning BC Emissions, Jun 20-27, 2008 (Southwest U.S.)



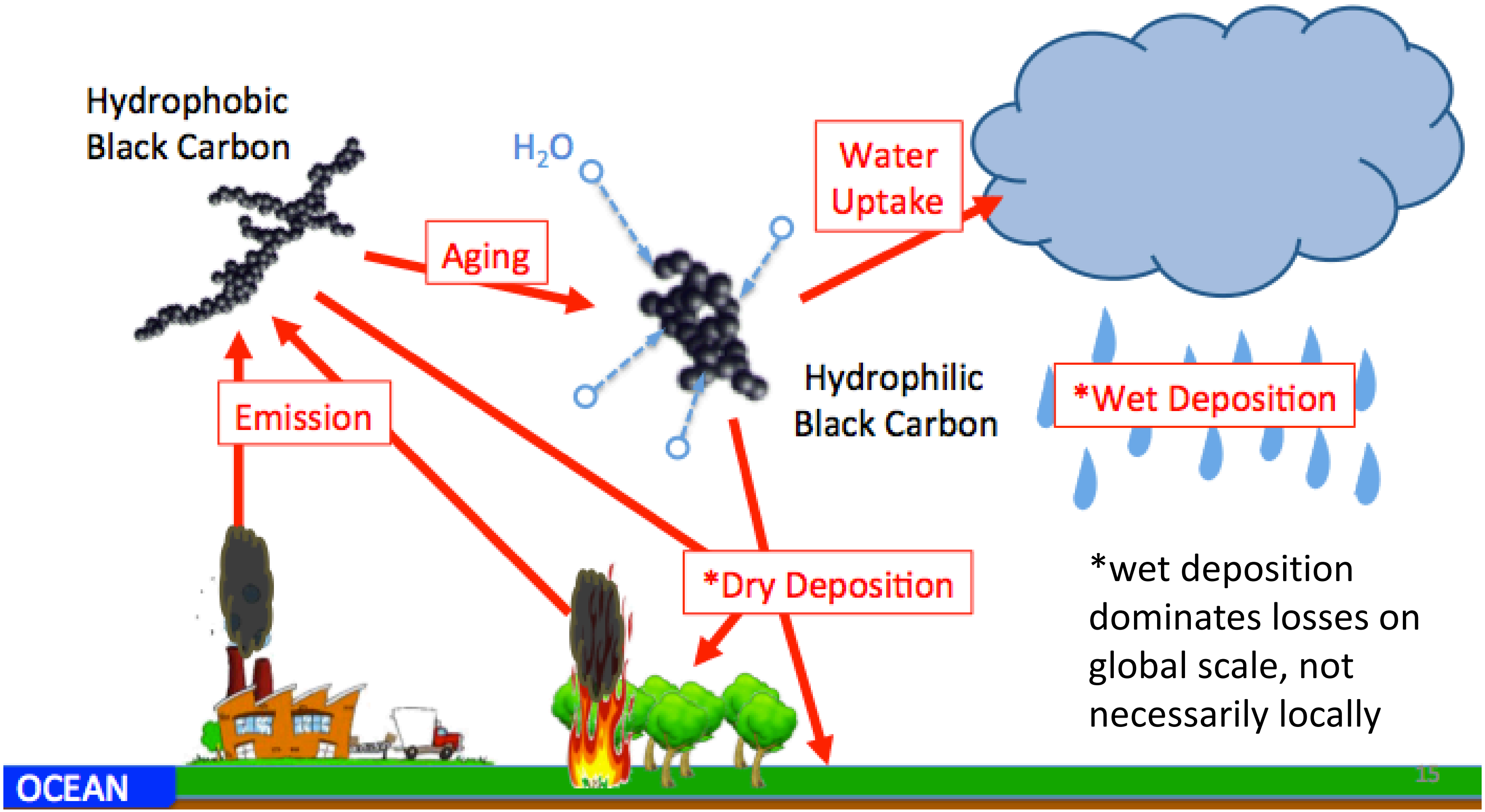
Wiedinmyer et al. (2011)

Darmenov and da Silva (2013)

ANTHROPOGENIC: National Emission Inventory (NEI2005)

$\Sigma E_{BC,ANT}$ = 548 Mg

BC Chemical Processes



*wet deposition dominates losses on global scale, not necessarily locally

Forward Modeling

Time Period

- 7 days, starting 2008, Jun 20 00Z

*Forward model only (Adjoint not developed yet)

Model Setup

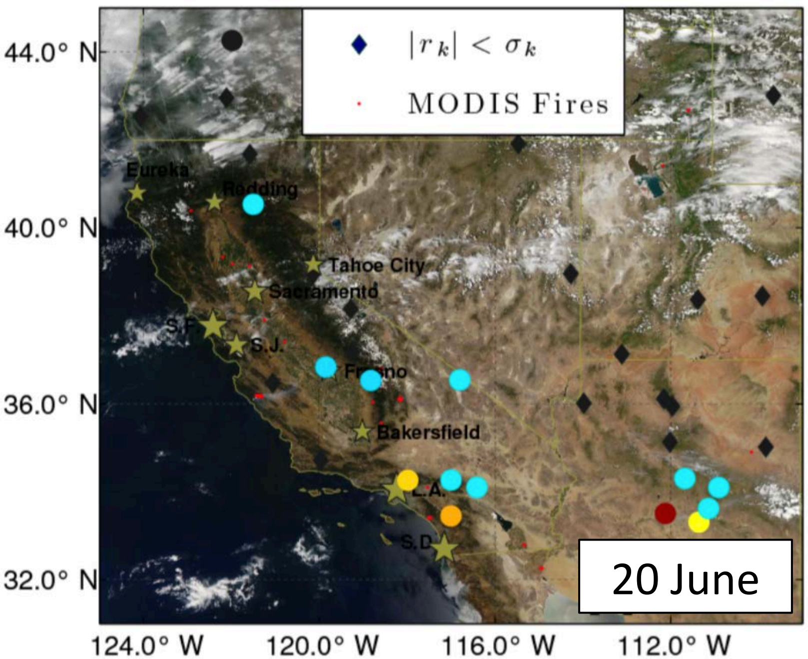
- WRF-Chem V3.6
- 18km – 79 x 79 x 42 levels
- I.C.'s & B.C.'s

  MET: 32km NARR Reanalysis

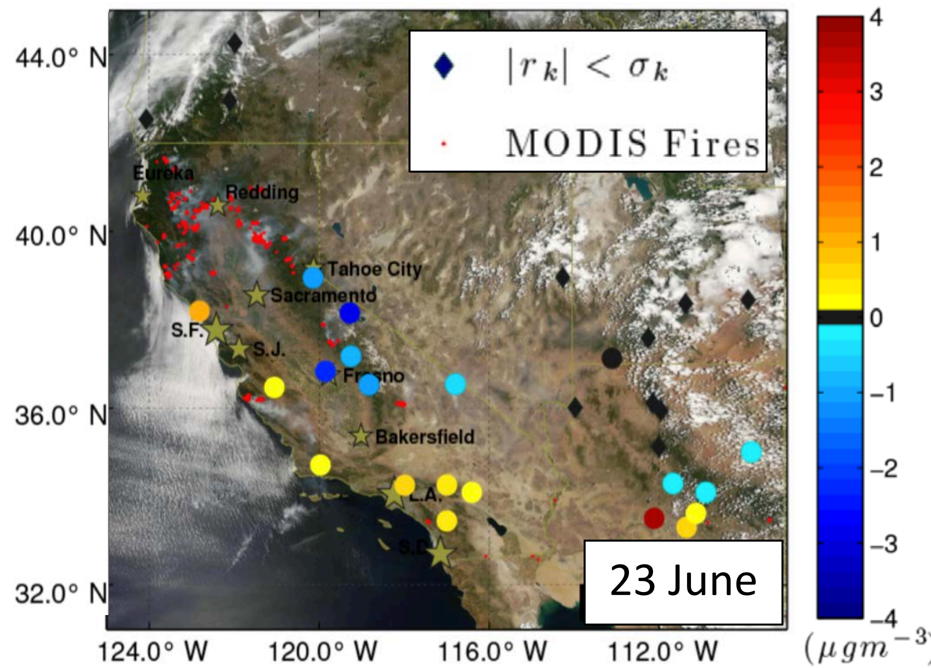
  CHEM: spun up from Jun 15, $[BC]_{bound}$=0.01μg/m^3
- GOCART Aerosols
- NEI2005 Anthro. Emissions
- BB Emissions w/ plumerise: FINN
- PBL: ACM2
- SFCLAY & LSM: Pleim-Xiu
- Radiation*: RRTM-LW and GSFC SW
- No Microphysics
- No Cumulus Convection/Removal

Model - Obs. Mismatch
(IMPROVE surface sites)

Before Fires



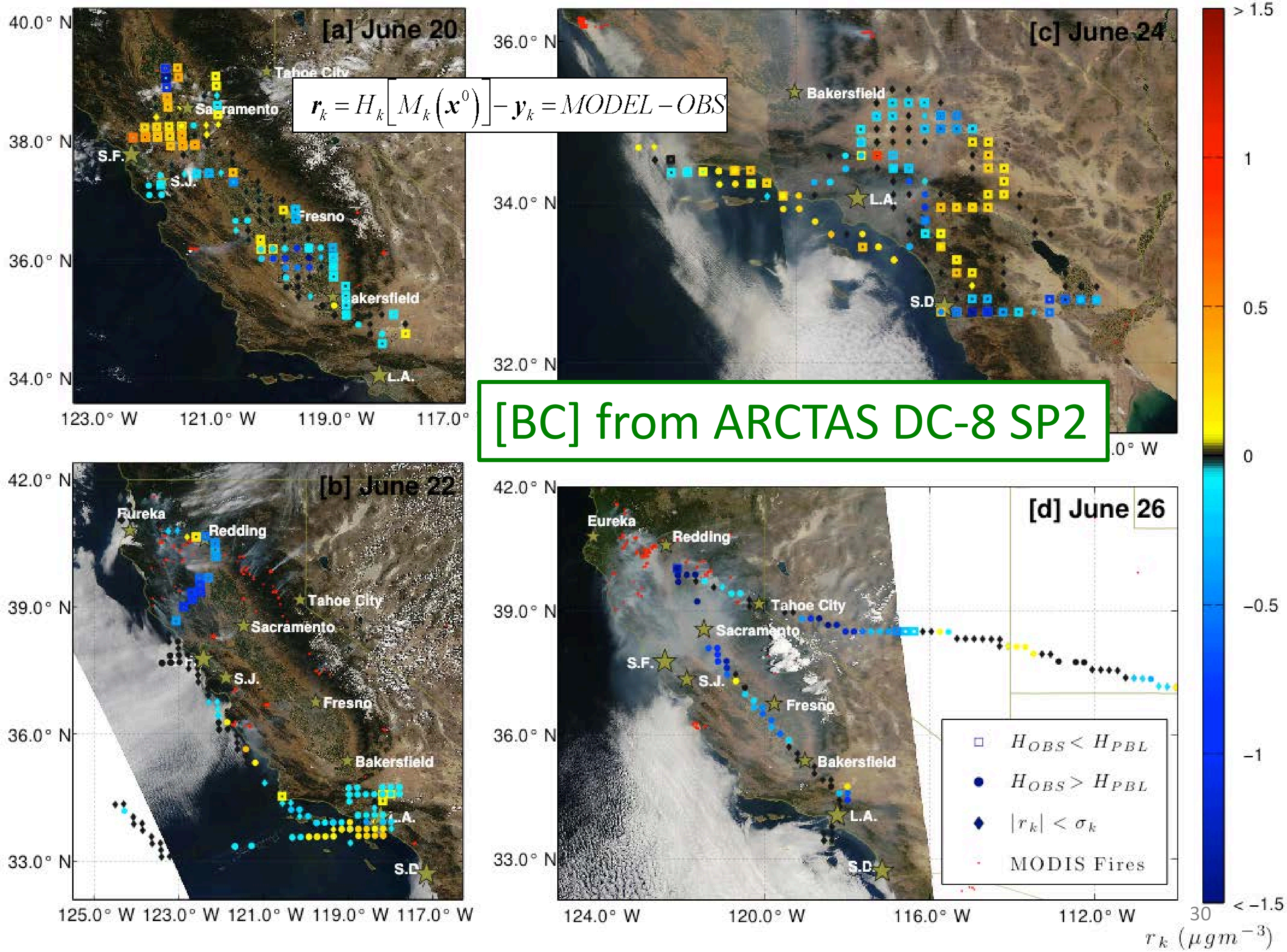
Includes Fires



$$\boldsymbol{r}_k = H_k\left[M_k\left(\boldsymbol{x}^0\right)\right] - \boldsymbol{y}_k = MODEL - OBS$$

[BC] from ARCTAS DC-8 SP2

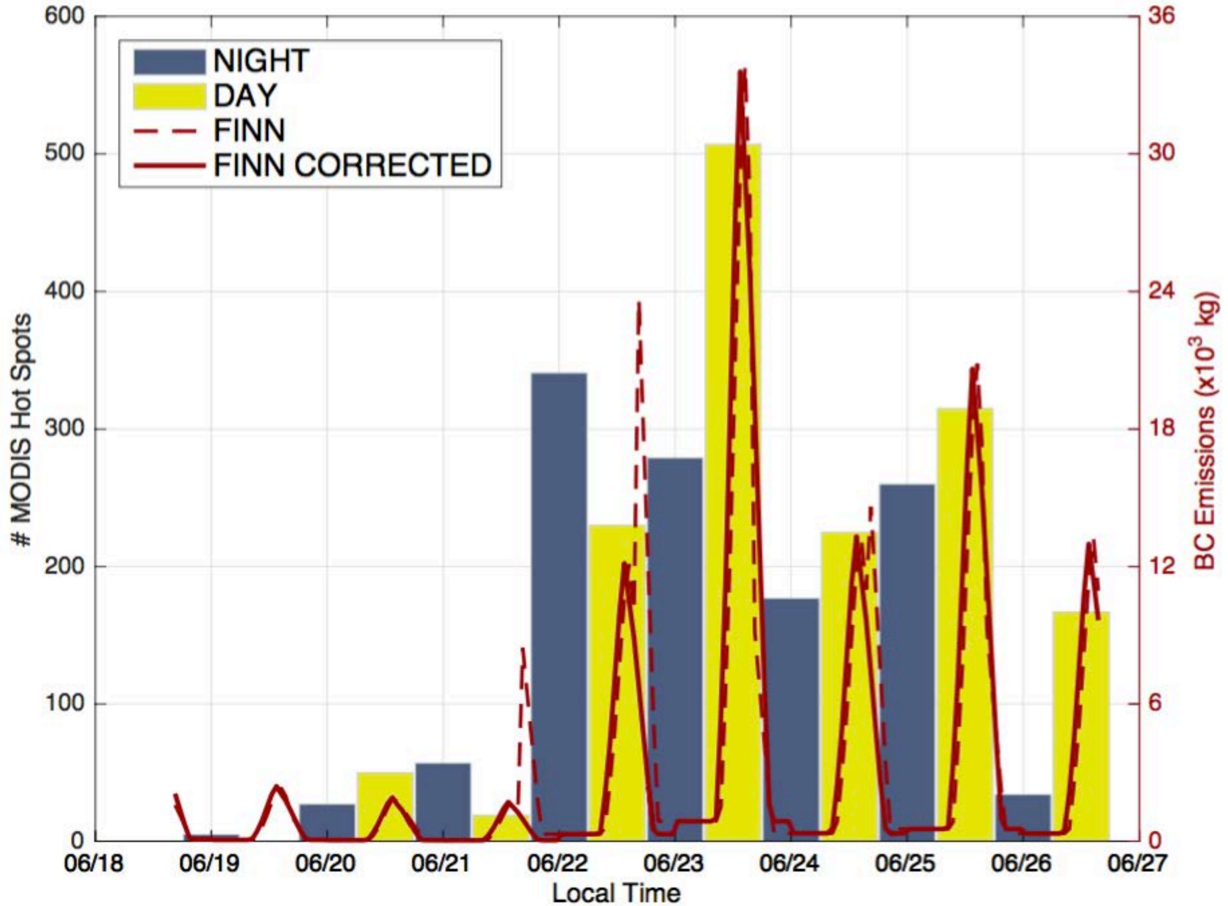
$$r_k = H_k\left[M_k\left(x^0\right)\right] - y_k = MODEL - OBS$$



Prior BB Diurnal Correction

1. Shift late afternoon emissions 24 hours from UTC day to local day

2. Determine Local Time of day from continuous solar schedule instead of discrete 15° longitude zones



WRFDA-Chem Setup

2 Time Periods

- 24 hours, starting 2008, Jun 22 00Z
- 48 hours, starting 2008, Jun 23 00Z

Observations for inversion

- ARCTAS-CARB (DC-8): 22 June & 24 June

  Kondo et al. (2011), Sahu et al. (2012)

- IMPROVE: 23 June - 13 sites in CA

  Malm et al. (2014)

Wall Time for 60 iterations and 24 hour inversion
→ 17 hours on 96 cores
(8 NASA Pleiades Westmere nodes)

Priors

- NEI2005 Anthro. Emissions
- BB Emissions
  - FINN
  - QFED x 1/3

DA Setup (STD)

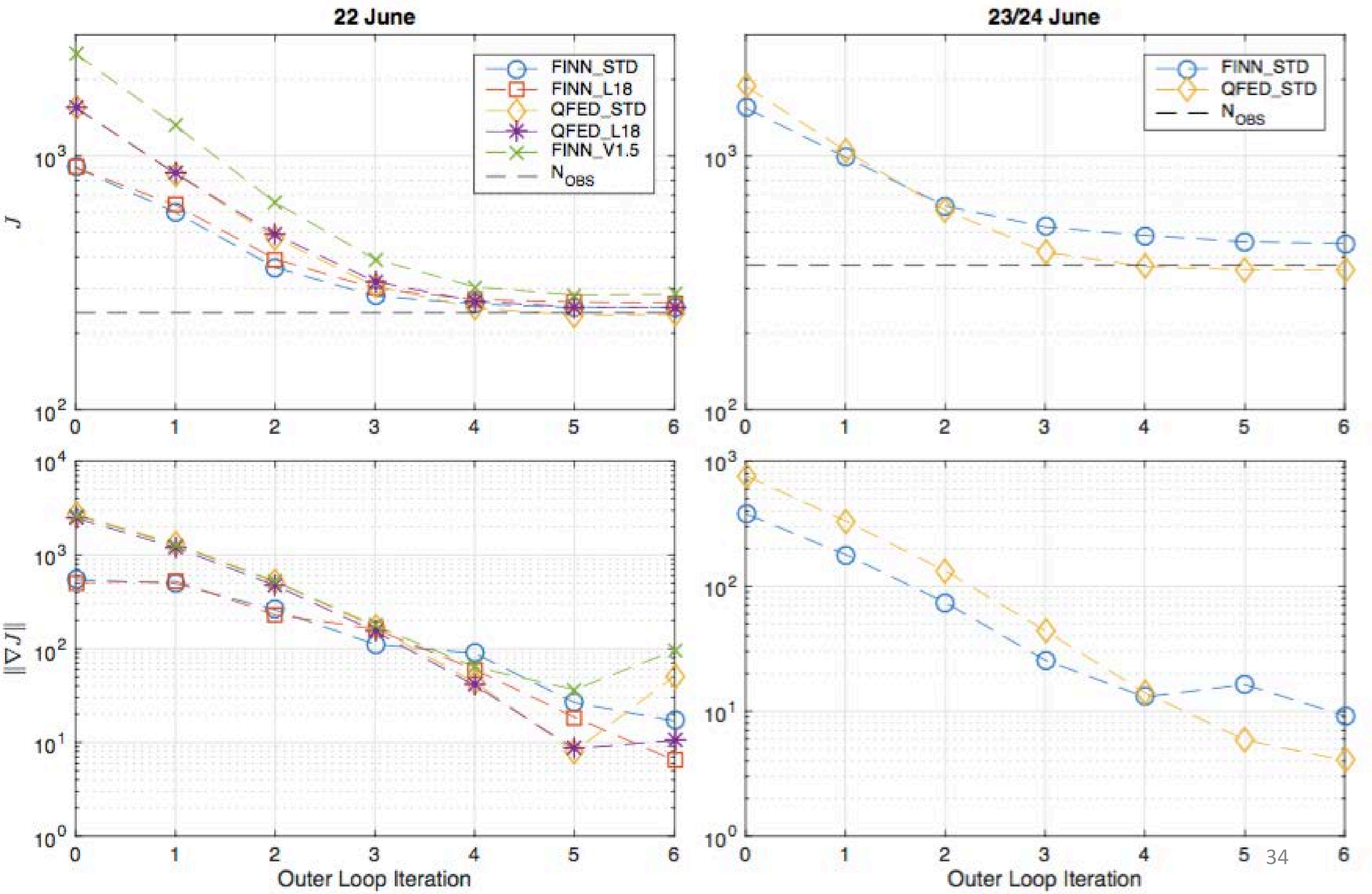
- $dx = 18$ km
- $L_{x,y} = 2*dx = 36$ km
- $L_t = 4$ hours
- Relative emission uncertainty
  - BB → ×3.8
  - ANTHRO → ×2.0

- 6 outer iterations, with 10 inner iterations each (60 total)

Available Posterior Results

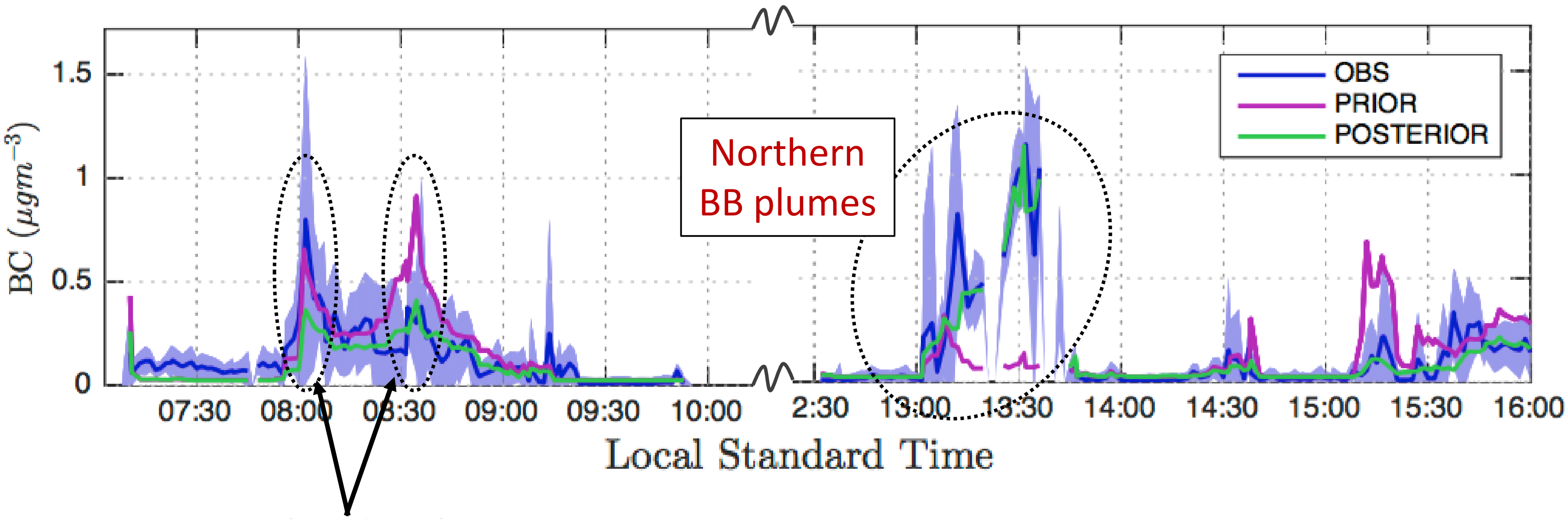
- Cost function and gradient reduction
- Model and observation time series
- Regressions: prior and posterior versus observations
- Spatial Maps: → { Anthropogenic / Biomass Burning / Surface obs. only / Aircraft obs. only / Surface + Aircraft }
  - Posterior emissions
  - Scaling Factors
  - Analysis Increments
- Hourly diurnal posteriors for Emission Areas (EA) of interest

Cost Function Minimization



22 June aircraft time series: FINN_STD

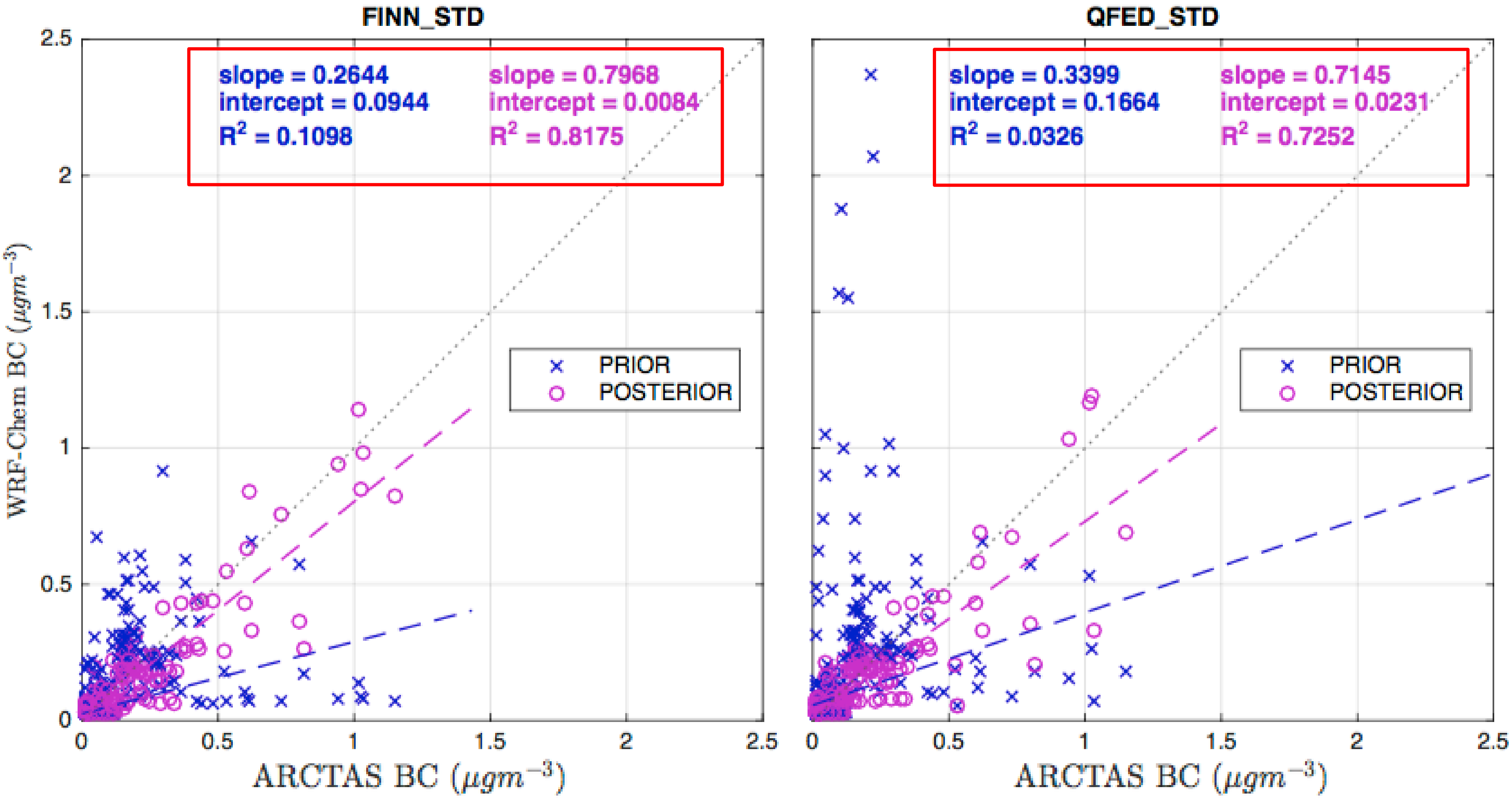
(similar posterior results for other inversion scenarios)



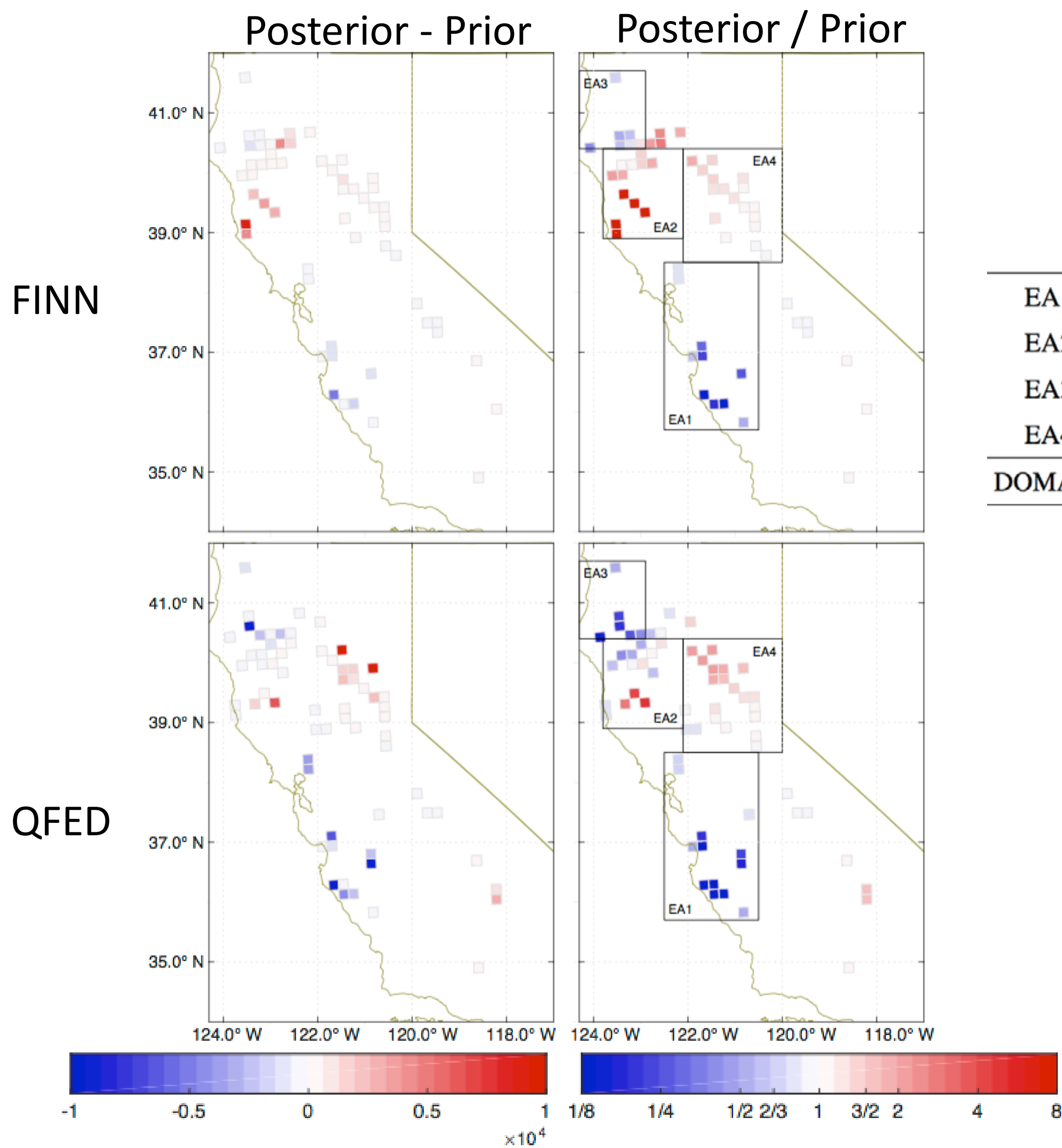
- Correlated anthropogenic emission errors
- Uneven observation uncertainty

22 June Statistics

(data that was used in inversion)



22 June BB Increments

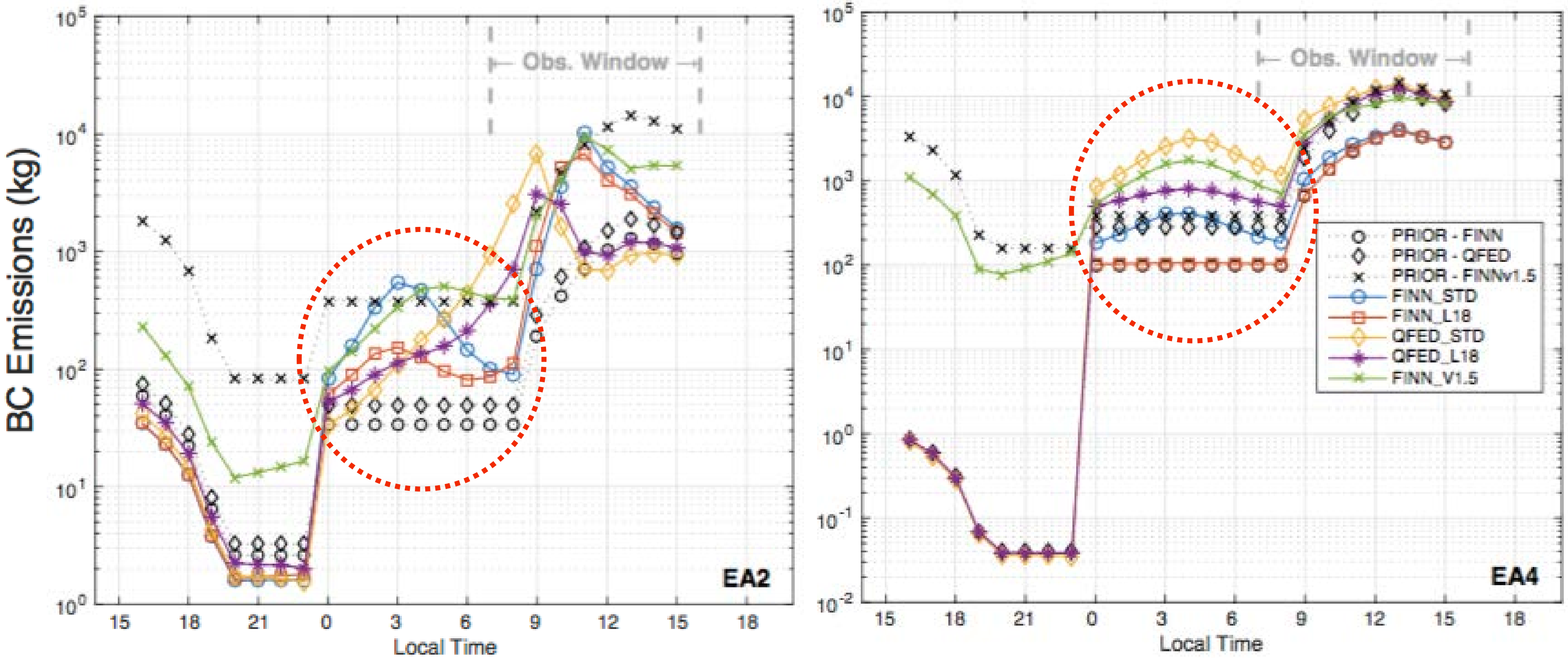


b = background
a = analysis

	FINN_STD			QFED_STD		
	ΣE_b	ΣE_a	Δ	ΣE_b	ΣE_a	Δ
EA1	14	4	-10	82	26	-55
EA2	6	30	+24	9	15	+6
EA3	6	4	-2	29	7	-22
EA4	18	22	+4	52	83	+31
DOMAIN	59	83	+34	209	171	-38

	$\frac{\Sigma E_{\text{QFED}}}{\Sigma E_{\text{FINN}}}$	
	b	a
EA1	$\times 5.8$	$\times 6.4$
EA2	$\times 1.5$	$\times 0.5$
EA3	$\times 4.5$	$\times 1.6$
EA4	$\times 2.8$	$\times 3.8$
DOMAIN	$\times 3.5$	$\times 2.1$

22 June BB Diurnal behavior



Possible early morning emission peak not captured in the prior description

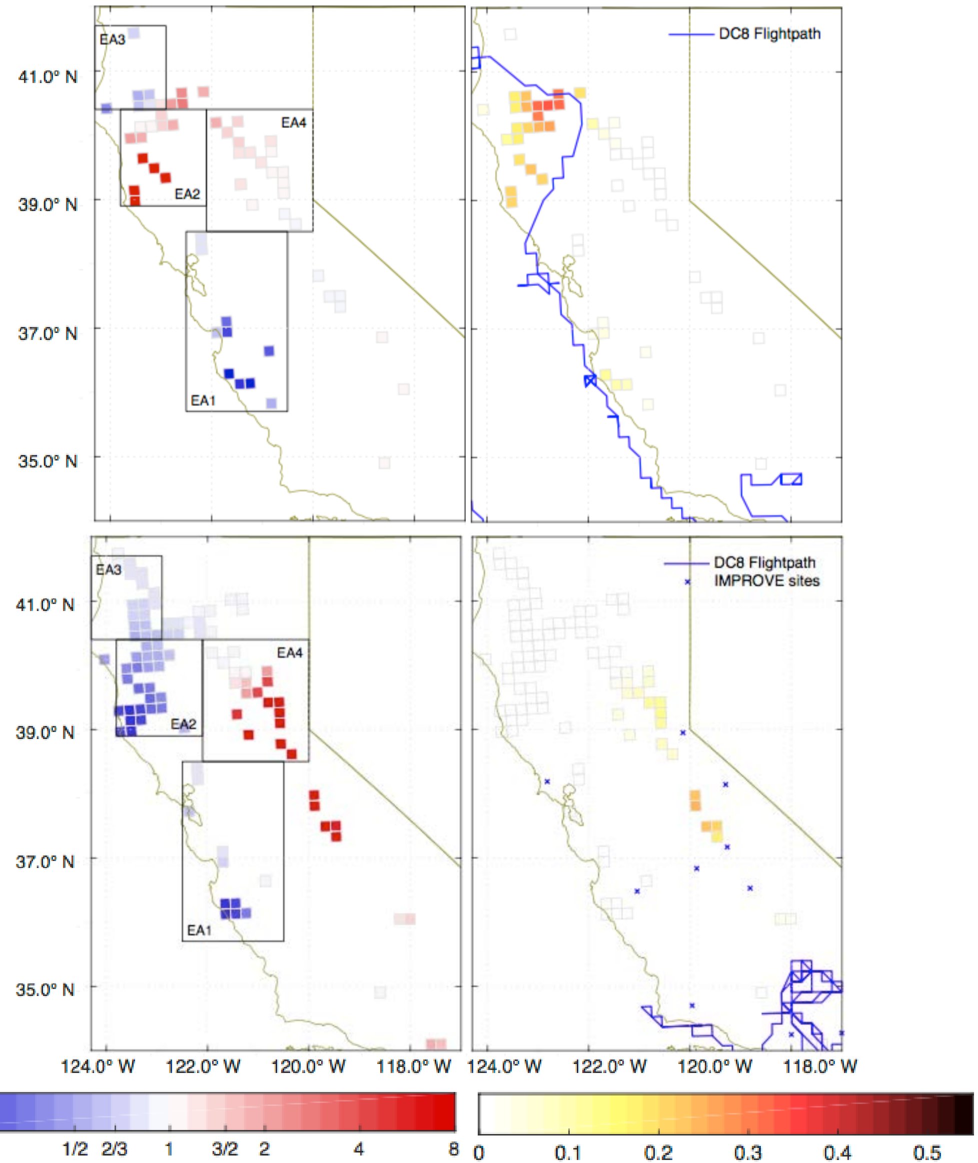
Statistical Significance (BB)

Posterior / Prior

Variance Reduction $= 1 - \frac{\mathbf{A}_{i,i}}{\mathbf{B}_{i,i}}$

22 June

23/24 June



B = Background Covariance

A = Posterior Covariance

Statistical Significance (ANTHRO)

FINN_STD

Posterior / Prior

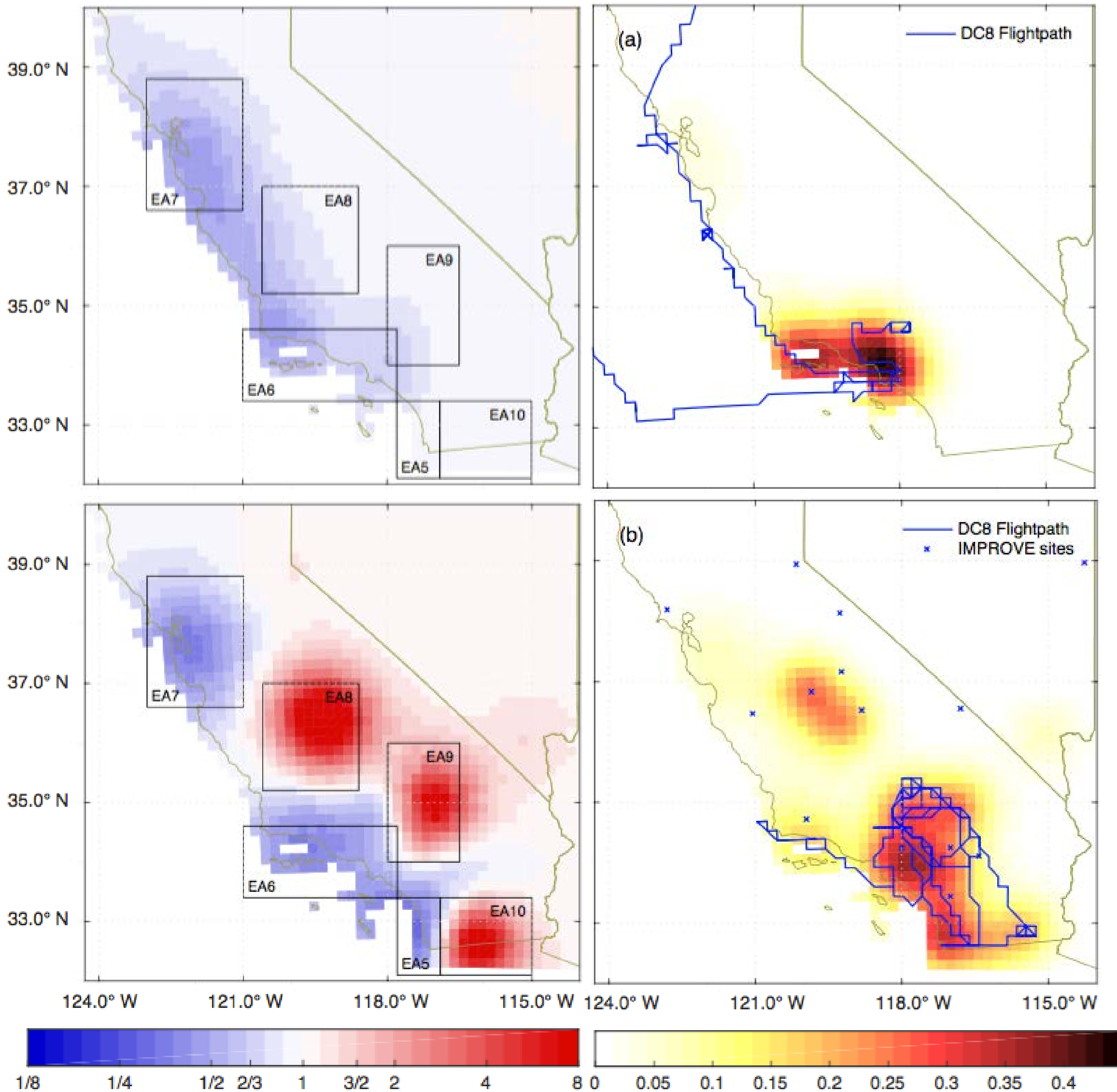
Variance Reduction $= 1 - \frac{\mathbf{A}_{i,i}}{\mathbf{B}_{i,i}}$

$\mathbf{B}$ = Background Covariance

$\mathbf{A}$ = Posterior Covariance

22 June (Sunday)

23/24 June (Mon, Tues)



Additional Diagnostics (submitted manuscript)

- Degrees of freedom of signal (DOF) for observing system assessment and comparison
- Cross validation
- Comparisons to other anthropogenic studies
  - McDonald et al. (2015), BC
  - Kim et al. (2016), CO

Conclusions

- WRFDA-Chem 4D-Var is fully functional for BC and other tracer emission inversions
- Spread in domain-wide fire BC sources is reduced on daily time scale, but grid-scale ratios remain large
- There is a possible early morning peak in fires for some local areas
- Both temporal and spatial BB errors contribute to model concentration errors

Next Steps

- Release WRFDA-Chem to the community
- Find interested users & developers
- Compare to other methods
- Apply the system to a time period with repeated near-source observations
- Add satellite observation operators (e.g., for AOD, NO_2, CO_2)
- Add reactive species to AD and TL
- Simultaneously constrain initial conditions

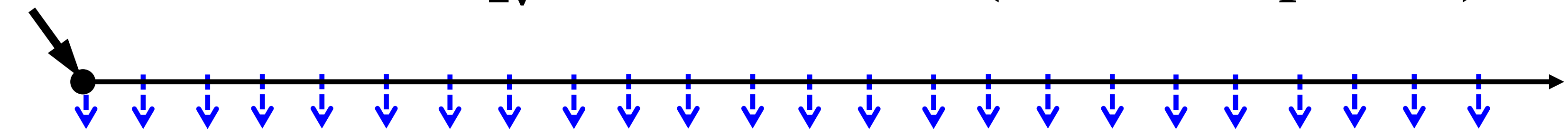
Submitted to ACP:
Guerrette, J.J. and D.K. Henze. Four dimensional variational inversion of black carbon emissions during ARCTAS-CARB with WRFDA-Chem.

Extra Slides

WRFPLUS 1st order checkpointing

① Run forward model; write state variable trajectory @ each time step (**u**, **v**, **θ**, **Φ**, **μ**, **moist**, **chem**)

$\mathbf{x} = \{\mathbf{E}, \mathbf{u}^{0}, \mathbf{T}^{0}, \mathbf{q_v}^{0}, [BC]^{0}, \text{etc.}\}$ (known *a priori*)



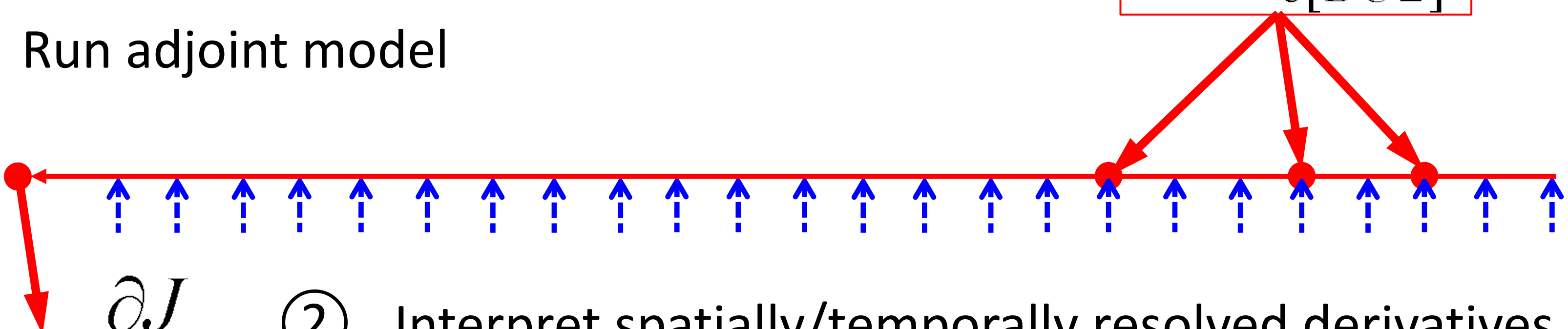
② Devise useful cost function and forcing

$$J = \sum_{m}^{M} \{H_m[M_m(\mathbf{x})] - y_m\}^T \mathbf{R}^{-1} \{H_m[M_m(\mathbf{x})] - y_m\}$$

$$\lambda_{BC1}^{n} = \frac{\partial J}{\partial [BC1]^{n}}$$

$$\lambda_{BC2}^{n} = \frac{\partial J}{\partial [BC2]^{n}}$$

① Run adjoint model



$$\underline{\lambda}_{\chi} = \frac{\partial J}{\partial \mathbf{x}_{\chi}}$$

② Interpret spatially/temporally resolved derivatives

Nonlinear Cost Function

Non-Gaussian J, due to nonlinear model, M

$$J(\mathbf{x}) = \frac{1}{2}\left(x - x^b\right)^{\mathbf{T}} \mathbf{B}^{-1}\left(x - x^b\right) + \frac{1}{2}\left(y - y^0\right)^{\mathbf{T}} \mathbf{R}^{-1}\left(y - y^0\right)$$

$$\boldsymbol{y} = H\left[M(\mathbf{x})\right]$$

$\mathbf{M}$ – TL model (M Jacobian)
$\mathbf{H}$ – TL obs. operator
k – obs. time index
n – minimization iteration

$\boldsymbol{x}$ – control variable
$\boldsymbol{y}^{\mathbf{0}}$ – observations
$\boldsymbol{y}$ – modeled observations

Courtier et al., 1994

*

Incremental 4D-Var Cost Function

Non-Gaussian J, due to nonlinear model, M

$$J(\mathbf{x}) = \frac{1}{2}\left(x - x^b\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(x - x^b\right) + \frac{1}{2}\left(y - y^0\right)^{\mathrm{T}} \mathbf{R}^{-1}\left(y - y^0\right)$$

Tangent Linear (TL) Approximation

$$y(x + \delta x) \approx H\left[M(x)\right] + \mathbf{HM}\delta x$$

max log-likelihood of approximate pdf

$$J\left(\boldsymbol{\delta x}^n\right) = \frac{1}{2}\sum_k \left[\mathbf{H}_k\mathbf{M}_k\boldsymbol{\delta x}^n + \boldsymbol{r}_k\right]^{\mathrm{T}} \mathbf{R}_k^{-1}\left[\mathbf{H}_k\mathbf{M}_k\boldsymbol{\delta x}^n + \boldsymbol{r}_k\right]$$

$$+ \frac{1}{2}\left[\boldsymbol{\delta x}^n + \boldsymbol{x}^{n-1} - \boldsymbol{x}^b\right]^{\mathrm{T}} \mathbf{B}^{-1}\left[\boldsymbol{\delta x}^n + \boldsymbol{x}^{n-1} - \boldsymbol{x}^b\right]$$

$$\boldsymbol{r}_k = H_k\left[M_k\left(\boldsymbol{x}^{n-1}\right)\right] - \boldsymbol{y}_k^0 = MODEL - OBS$$

$\mathbf{M}$ – TL model (M Jacobian)
$\mathbf{H}$ – TL obs. operator
k – obs. time index
n – minimization iteration

$\boldsymbol{x}$ – control variable
$\boldsymbol{y}^{\mathbf{0}}$ – observations
$\boldsymbol{y}$ – modeled observations

Courtier et al., 1994

*

Increment by Damped Gauss Newton

$$\delta \boldsymbol{x}^n = \eta^n \left. \mathcal{H}^{-1} \right|_{\boldsymbol{x}^{n-1}} \left. \nabla_{\boldsymbol{x}} J \right|_{\boldsymbol{x}^{n-1}}$$

The gradient is evaluated through the adjoint model at the previous guess, x^{n-1}

The inverse Hessian ($\mathcal{H}^{-1}$) is approximated by sequential application of the adjoint and tangent linear models in a linear optimization (e.g., Lanczos recurrence, conjugate gradient)

Damping based on Armijo Rule enables nonlinear optimization

$$J_{nonlinear} \,|_{\eta \delta \boldsymbol{x}} \leq J_{nonlinear} \,|_{\delta \boldsymbol{x} = \boldsymbol{0}} \quad \text{when} \quad 0 < \eta \leq 1$$

Control Variables (preconditioned exponential scaling factors)

NL: $E_i^n = E_i^0 e^{x_i^n}$

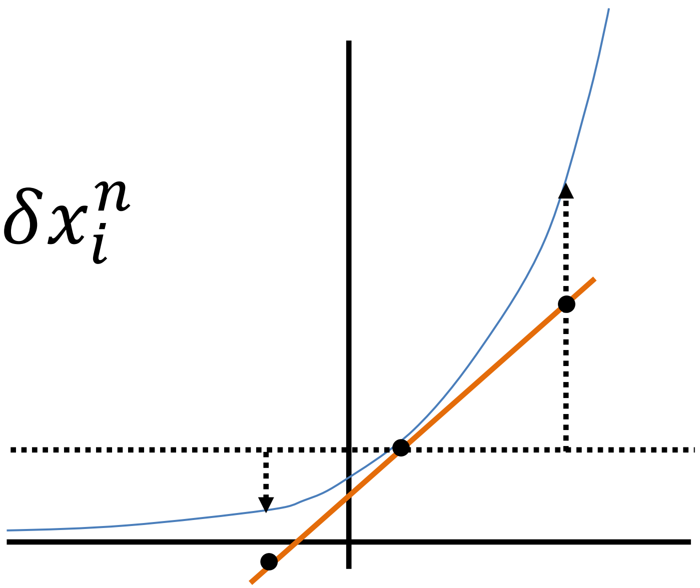
TL: $\delta E_i^n = E_i^0 e^{x_i^{n-1}} \delta x_i^n$

AD: $\delta x_i^* = E_i^0 e^{x_i^{n-1}} \delta E_i^{n*}$

Incremental 4D−Var → δx_i^n

$x_i^n = x_i^{n-1} + \delta x_i^n$

Grid-scale E_i = Emission Strength



All BC Observations during ARCTAS-CARB