Developing adjoint and tangent linear subgrid parameterizations of source, loss, and vertical transport mechanisms for chem. tracers in WRFPLUS

WRF USER WORKSHOP

June 25, 2013

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Image: MODIS true color image on June 24, 2008 (http://cimss.ssec.wisc.edu/)

This research is funded by
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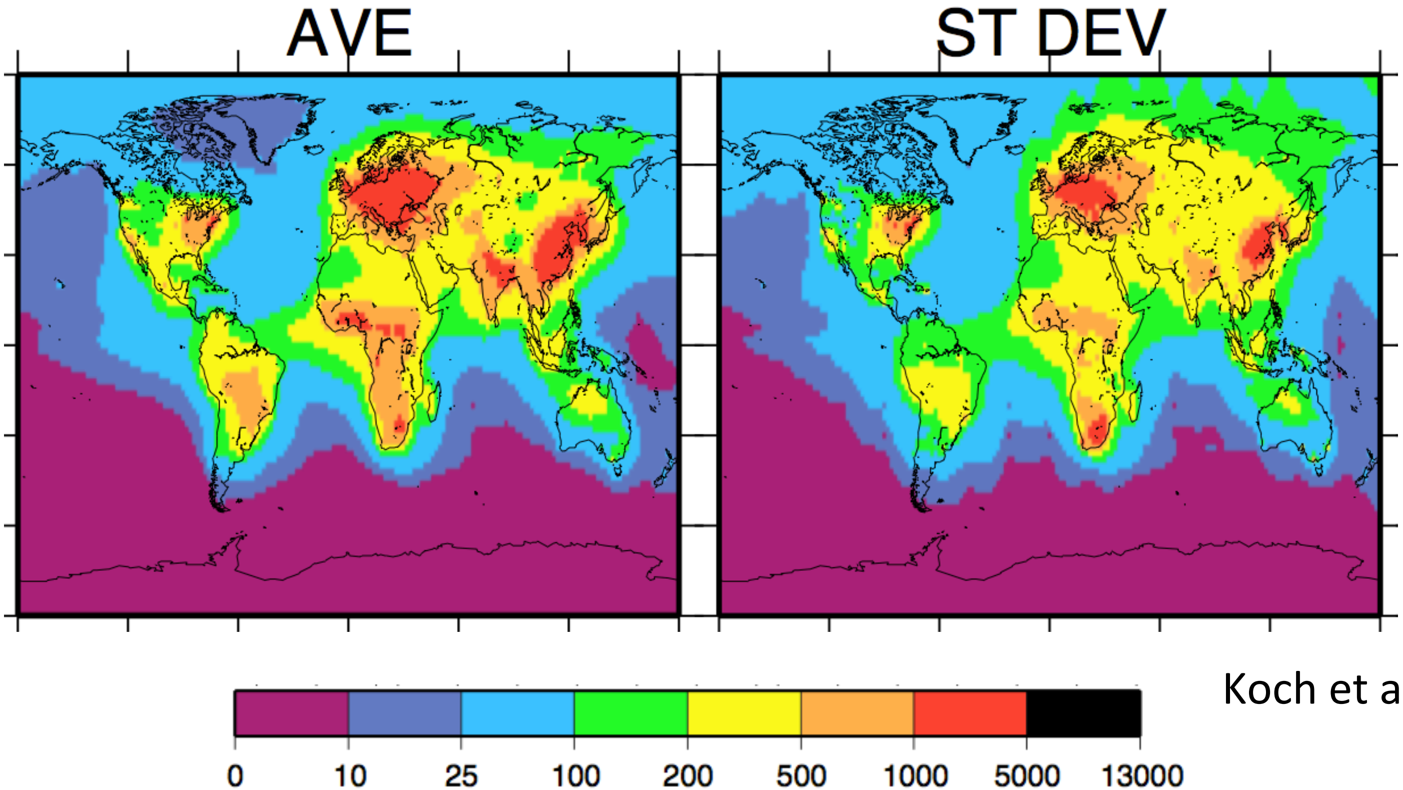
AeroCom Intercomparison (y. 2000)

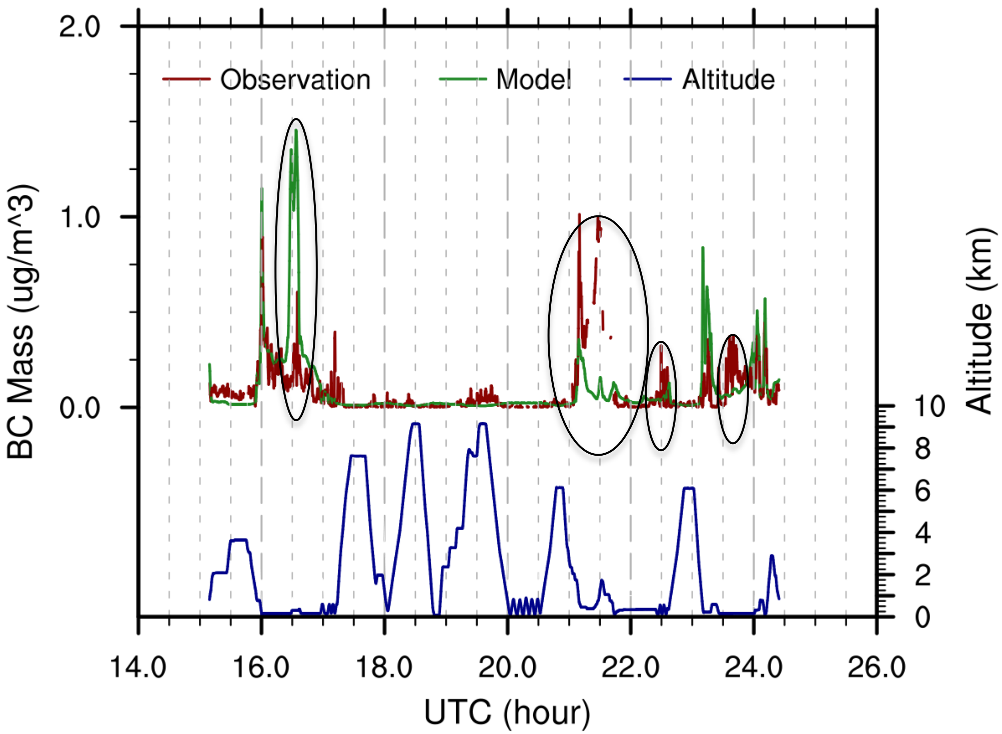


Koch et al. (2009)

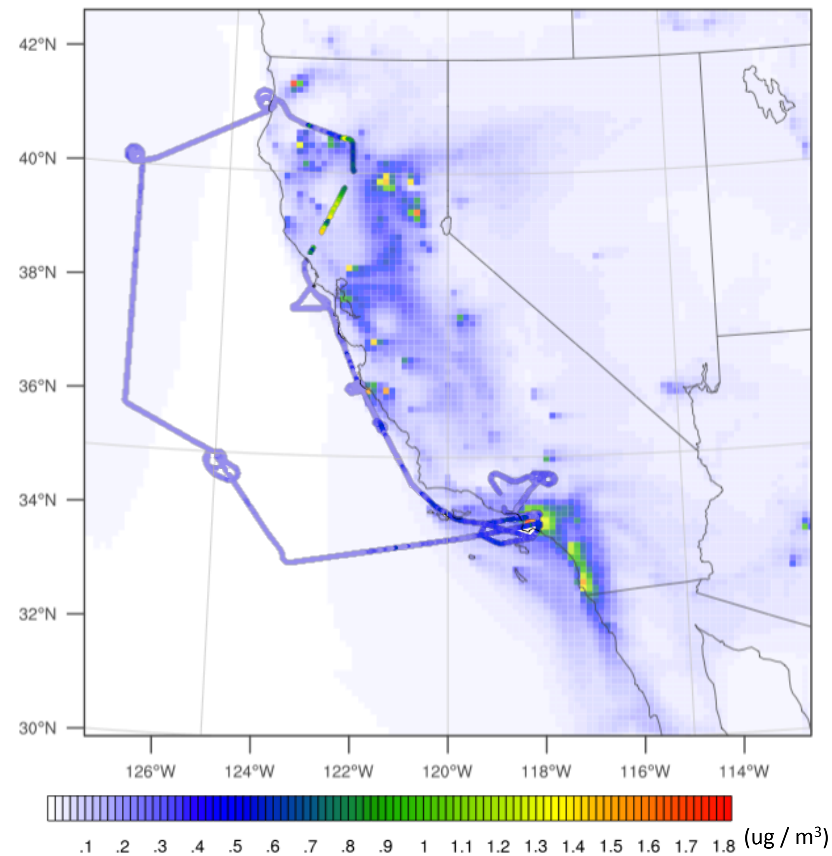
Fig. 2. AeroCom models annual mean BC surface concentrations (ngm^{-3}).

[BC] uncertainty is similar order as [BC] magnitude!!
->Worse above surface and at smaller scales

Jun 22 ARCTAS-CARB Campaign



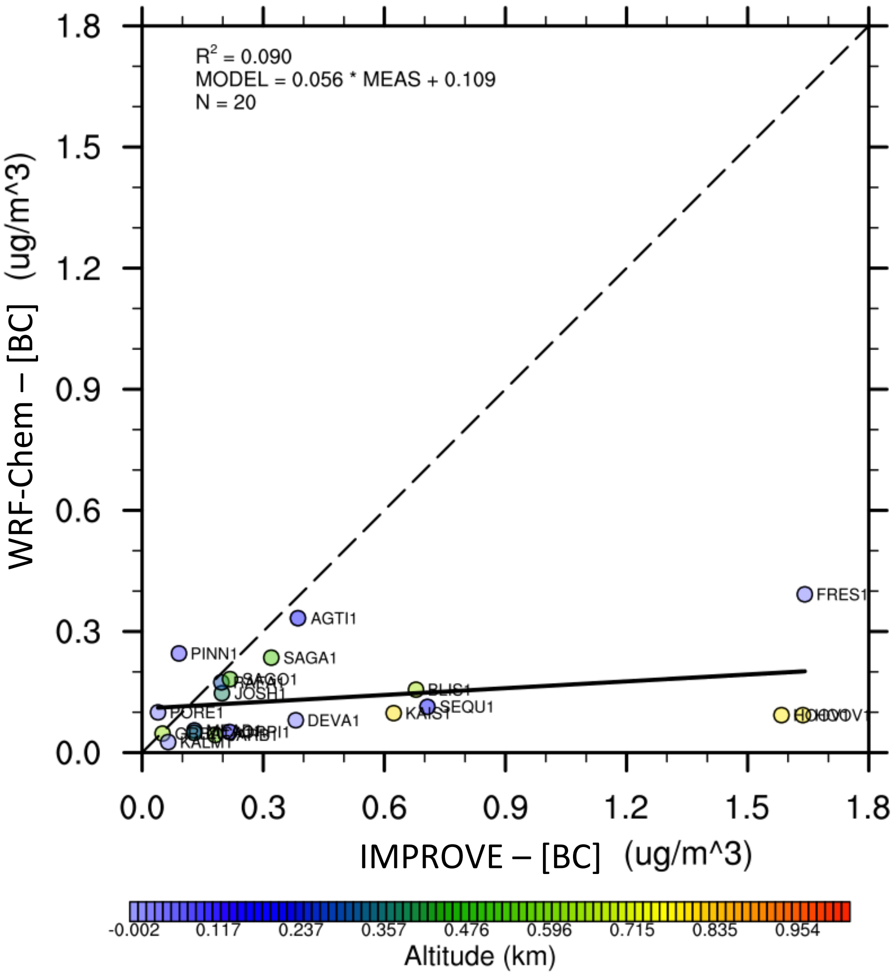
Average Daily Surface BC

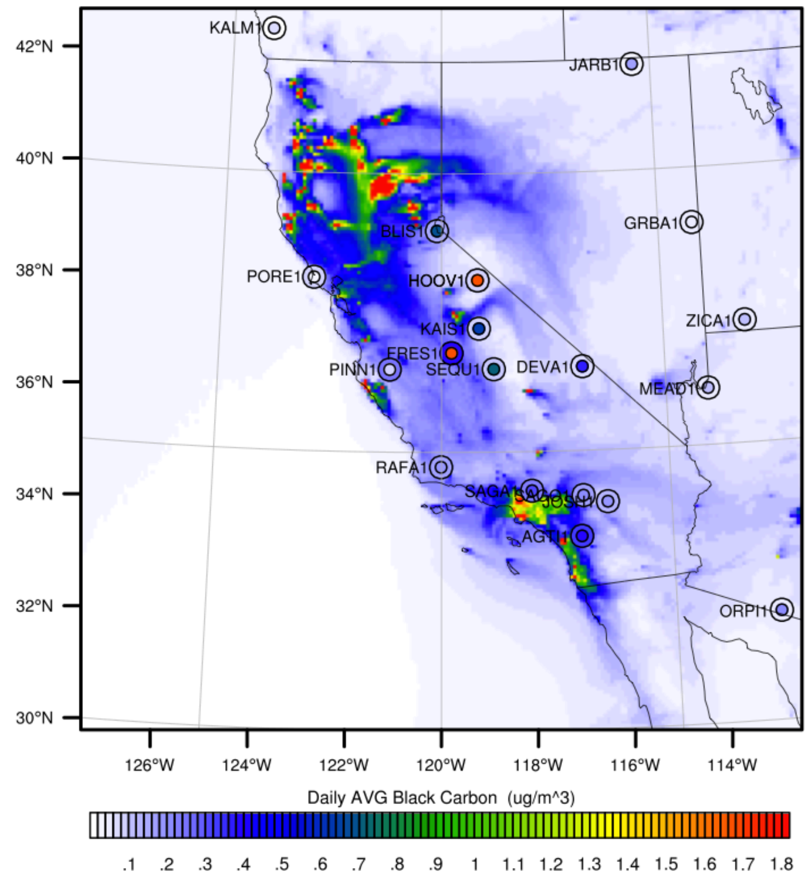


- 10 minute model output interpolated to 10 sec measurement locations, then 30 sec average
- 30 sec average observation (10 sec from instrument)

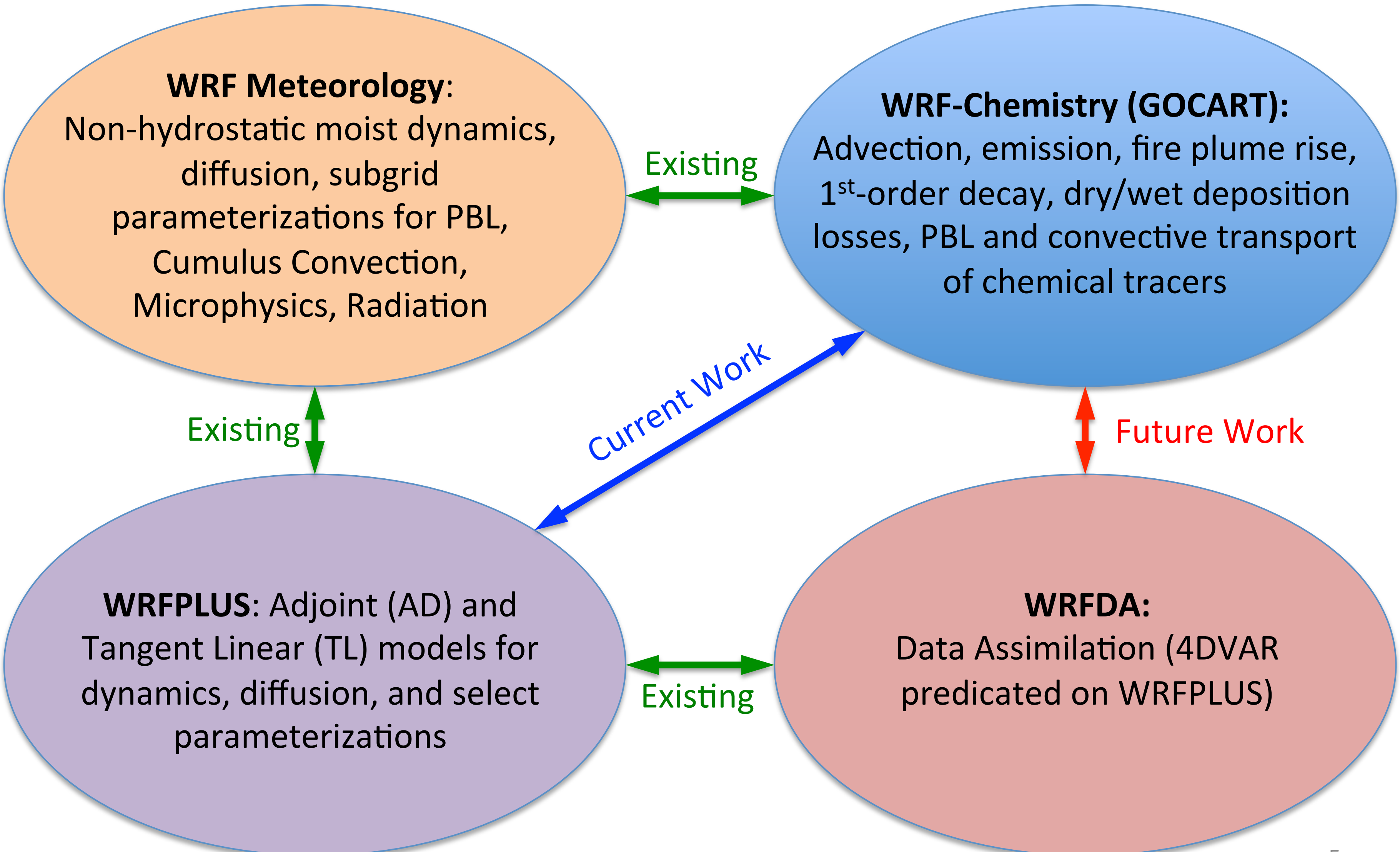
LOW bias near BB, HIGH bias near ANTHRO

June 23, 2008 IMPROVE Results





WRF Models


WRF Meteorology:
Non-hydrostatic moist dynamics, diffusion, subgrid parameterizations for PBL, Cumulus Convection, Microphysics, Radiation
Existing
WRF-Chemistry (GOCART):
Advection, emission, fire plume rise, 1st-order decay, dry/wet deposition losses, PBL and convective transport of chemical tracers
Existing
Current Work
Future Work
WRFPLUS: Adjoint (AD) and Tangent Linear (TL) models for dynamics, diffusion, and select parameterizations
Existing
WRFDA:
Data Assimilation (4DVAR predicated on WRFPLUS)

WRFPLUS Capabilities

- AD and TL developed for:
  - Emissions (Anthropogenic and Biomass Burning for GOCART)
  - ACM2 PBL (Pleim et al. 2007) w/ integrated tracer transport (2013) (7)
  - Pleim-Xiu and SFCLAY surface layer schemes (7,1)
  - Pleim-Xiu and SLAB LSMs (7,1)
  - Wesely Dry Deposition
  - chem advection (similar to tracer advection by Xin Zhang in 2012)
  - GOCART Aerosols
    - BC aging
    - PM summation
    - Sulfate chemistry (pending testing)

- New forcing scheme for in-situ chemical observations

- 2nd-order checkpointing for long duration (> 6 hr) sensitivity studies

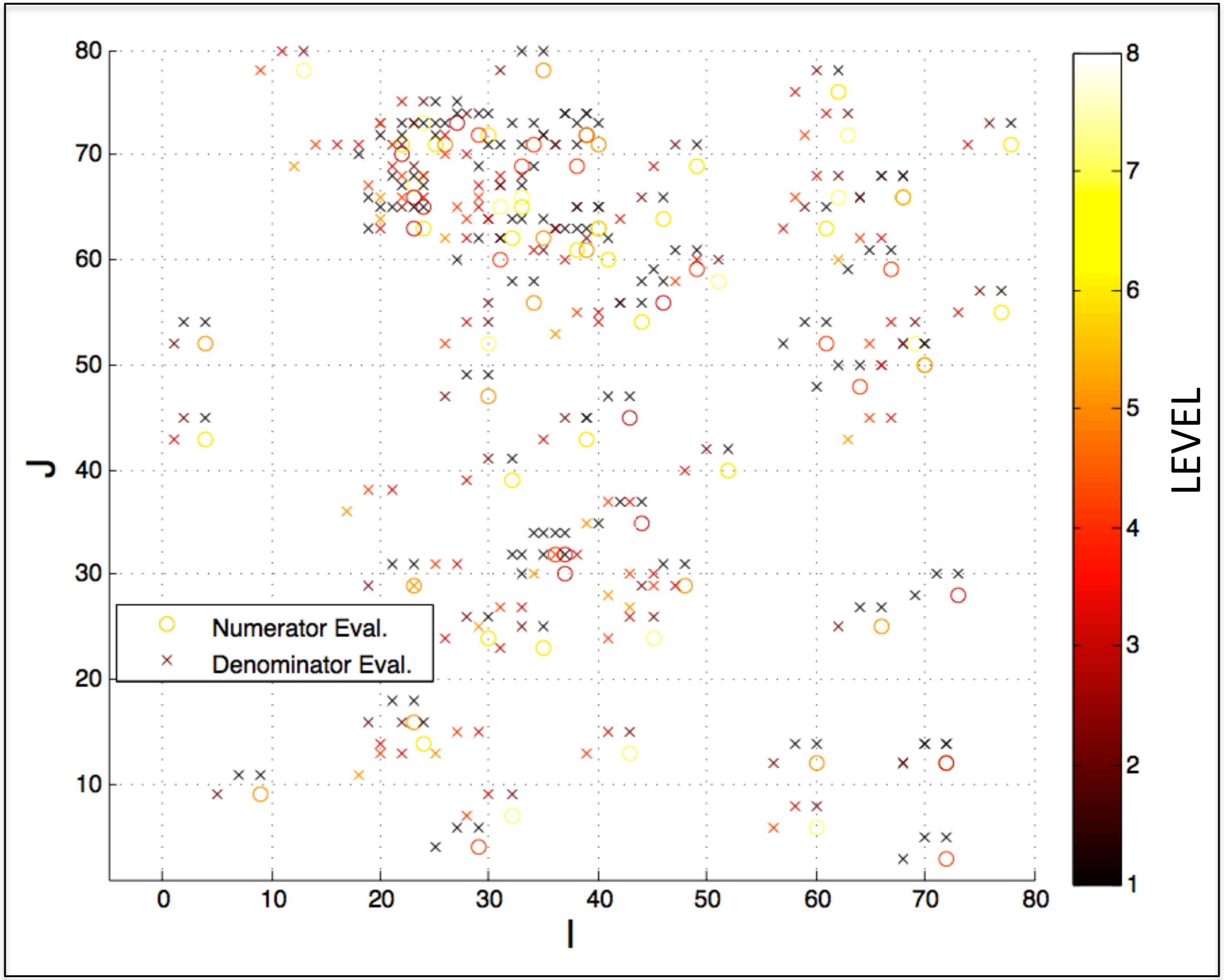
- Standalone AD and TL:
  - Grell-Freitas Convection (2013) [chemical tracers in development]

3 hour Derivative Tests

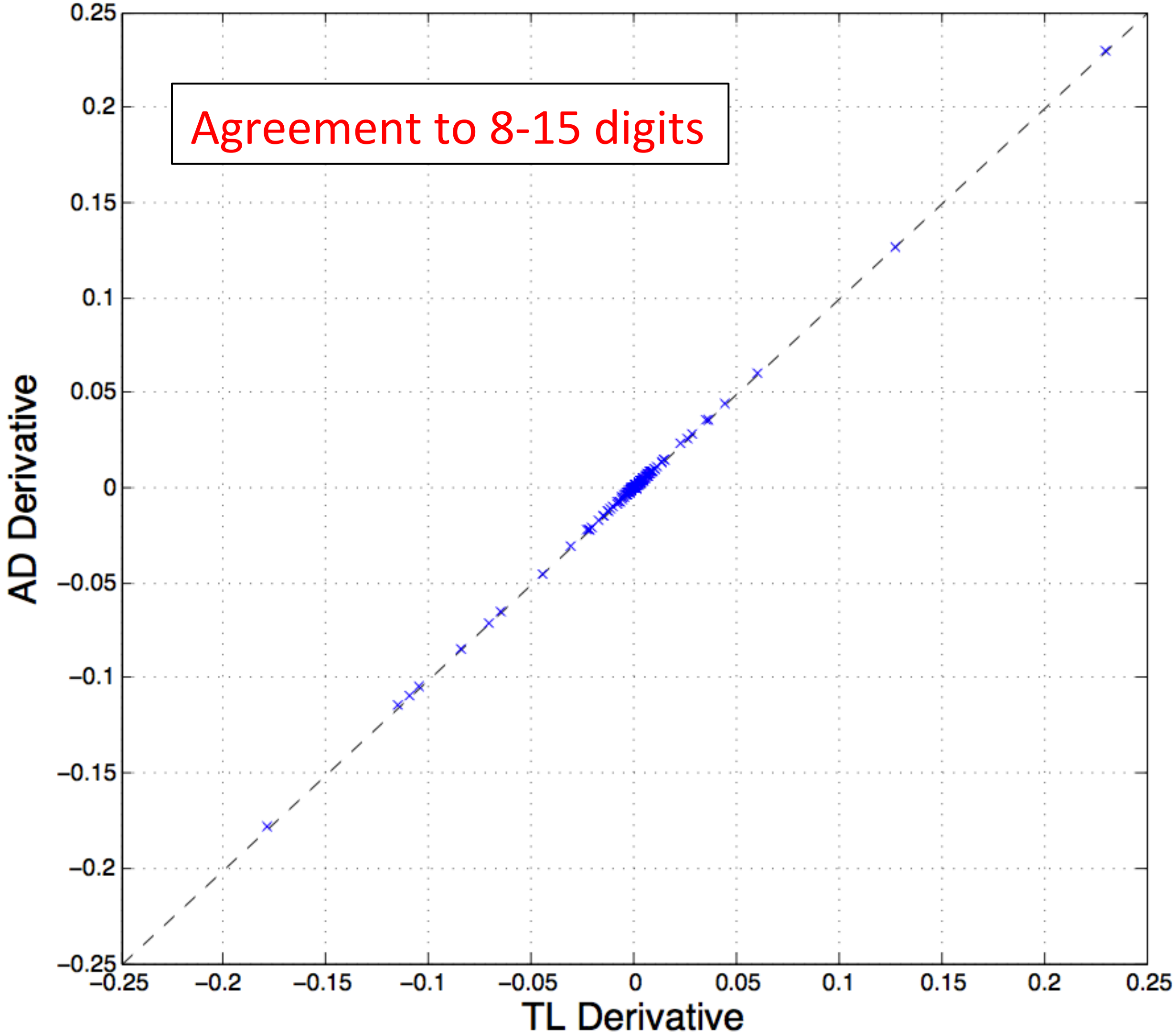
- Tangent Linear test
- Finite Difference linearity test
- 300 grid pairings per sensitivity type

- Sensitivities tested:

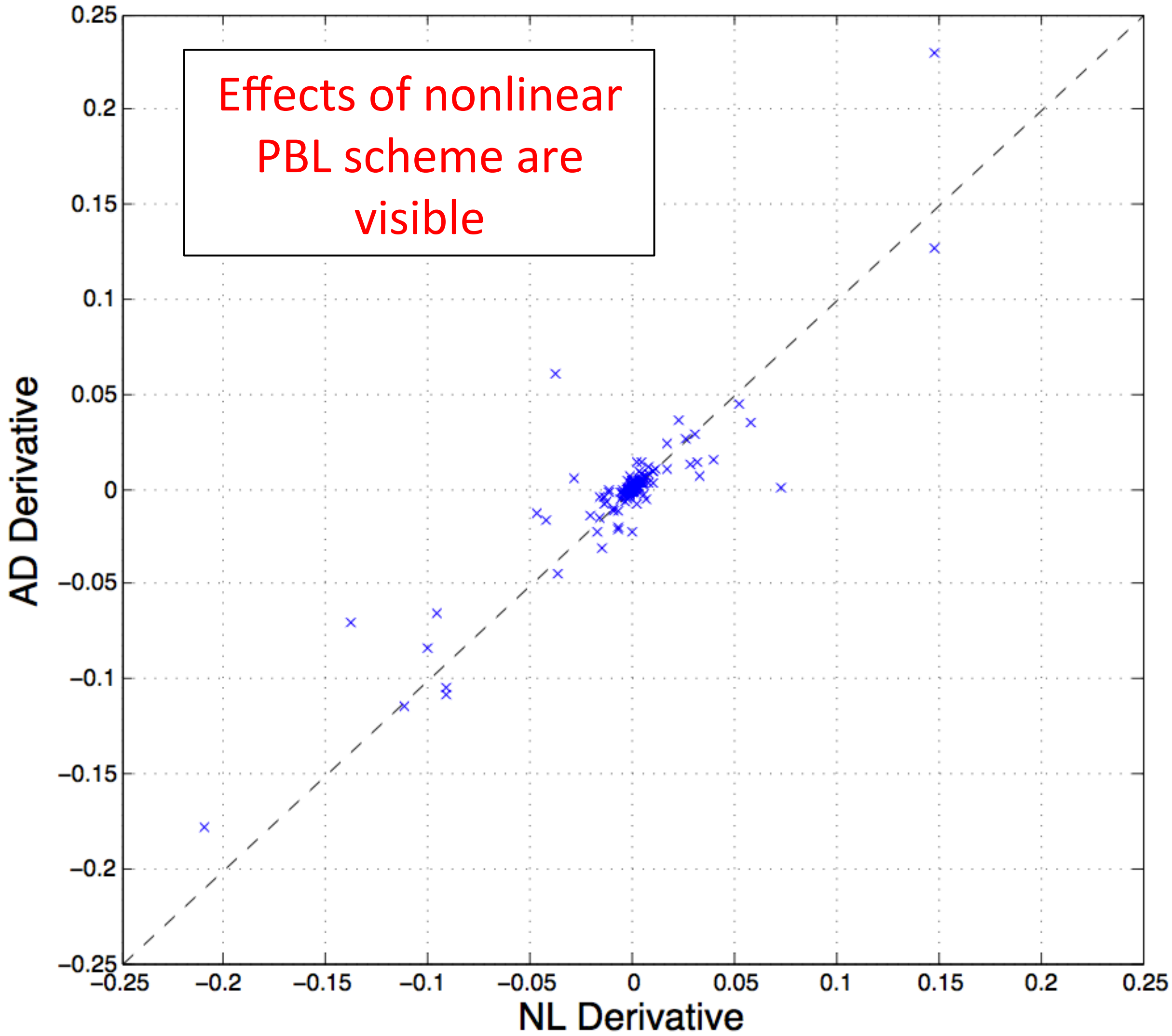
$$\frac{\partial[BC1]}{\partial u}, \frac{\partial[BC1]}{\partial T}, \frac{\partial[BC1]}{\partial q_v}, \frac{\partial[BC1]}{\partial[BC1]}, \frac{\partial[BC1]}{\partial E_{BC1}}$$



Tangent Linear Validation



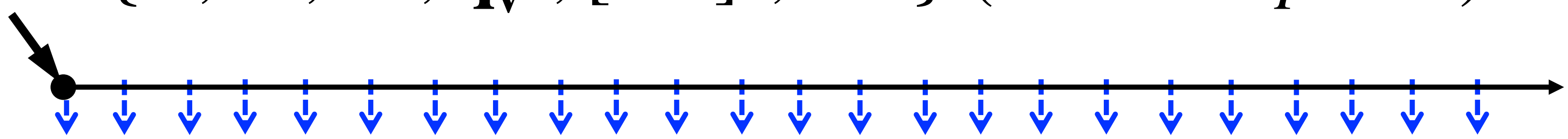
Centered Difference Nonlinearity



WRFPLUS w/ 1st order checkpointing

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

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



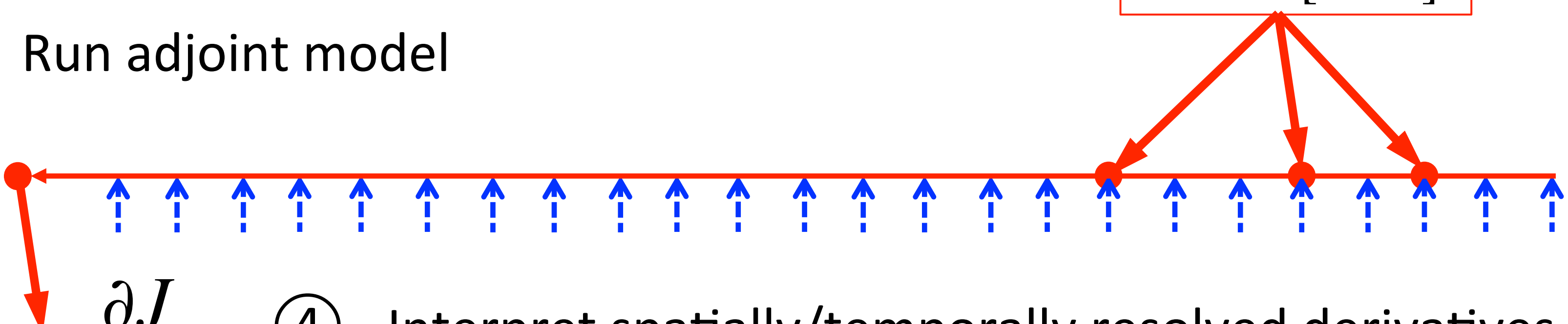
② Devise useful cost function and forcing

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

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

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

③ Run adjoint model



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

④ Interpret spatially/temporally resolved derivatives

New 2nd-Order Checkpointing in WRFDA

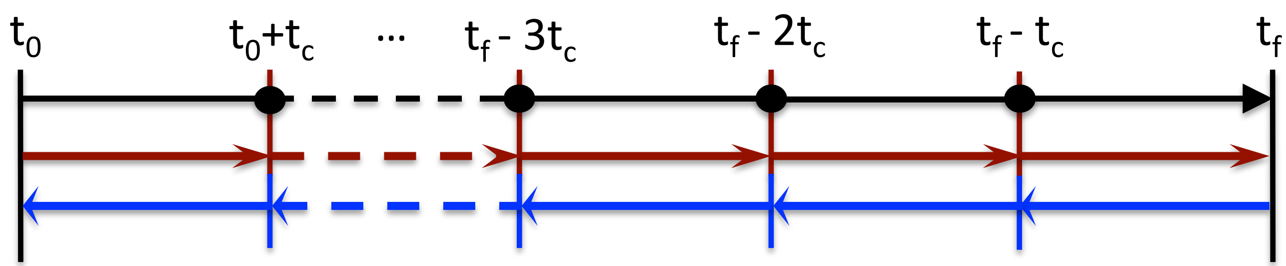
Trajectory – All model state variables stored at every grid cell and every time step (u, v, w, t, ph, mu, moist x1-3, chem x19)

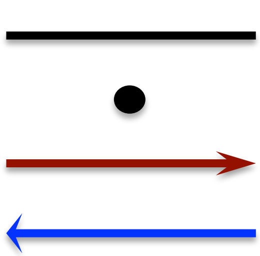
coarse 18km grid (10 boundary cells)

3 hr for dt=90s

1 CORE: RAM_1 ~ 89 x 89 x 31 x 26 variables x 8 bytes x 120 time steps = 5.8GB (single core)

64 CORES: **RAM_{64}** ~ 5.8GB * 1.5^6 = 66GB -> **1GB per core** + normal memory requirements





Initial full forward model run without trajectory IO

Initial run generates RESTART files

Checkpoint forward model run with trajectory output

Checkpoint adjoint model run with trajectory input

Cost Function & Chem Obs.

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

Assumed only for this demonstration

$$\overline{M}_{m,SURF} = \frac{1}{P_m} \sum_{p=p_{0,m}}^{P_m} M_m^p \left(\mathbf{x} \right) \qquad \overline{y}_{m,AIR} = \frac{1}{Q_m} \sum_{q=q_{0,m}}^{Q_m} y_m^q$$

Two Preprocessed Observation Sets:

	m	n_i	n_f	i	j	k	[BC] …
IMPROVE	36	281.000	1240.000	17.746353149414	76.181304931641	1.000000000000	1.149e-01
	37	281.000	1240.000	70.141807556152	11.226648330688	1.000000000000	1.857e-01
	38	241.000	1200.000	58.793373107910	32.409439086914	1.000000000000	3.750e-02
	39	3161.000	4120.000	40.150882720947	9.093823432922	1.000000000000	3.861e-01
	40	3161.000	4120.000	25.215013504028	43.165985107422	1.000000000000	6.785e-01
	41	3121.000	4080.000	63.426769256592	35.204486846924	1.000000000000	9.070e-02
ARCTS-CARB	2641	1008.000	1008.111	35.719543457031	17.366888046265	4.452124834061	1.202e-01
	2642	1008.111	1008.222	35.693733215332	17.304485321045	4.621666073799	7.801e-02
	2643	1008.222	1008.333	35.672988891602	17.241428375244	4.776512444019	8.249e-02
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Model Demonstration

Time Period

- Jun 20 00Z to Jun 27 09Z, 2008

Observations

- Jun 20, 23, 26 (IMPROVE)
  – Daily avg. @ ~40 sites
- Jun 20, 22, 24, 26 (DC-8)
  – Single Particle Soot Photometer (SP2)
  – 10 sec sample rate
  – $0.01 \mu g/m^3$ measurement limit
  – 10% accuracy

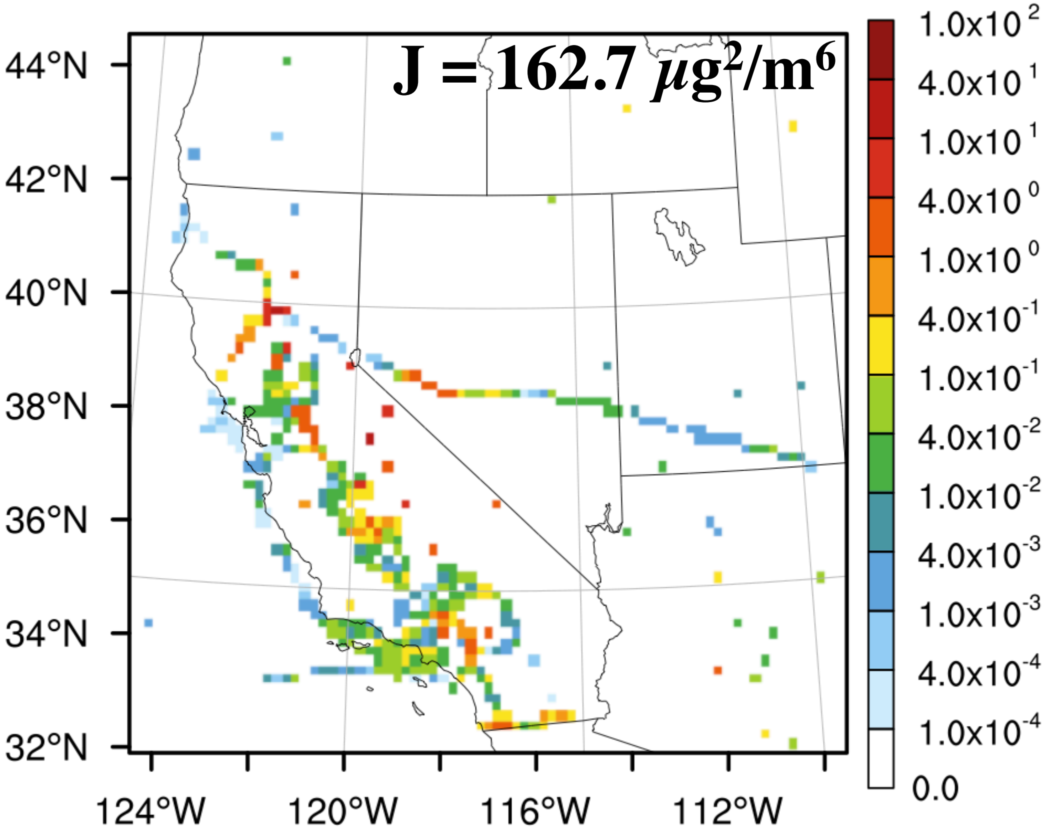
Adjoint Model Setup

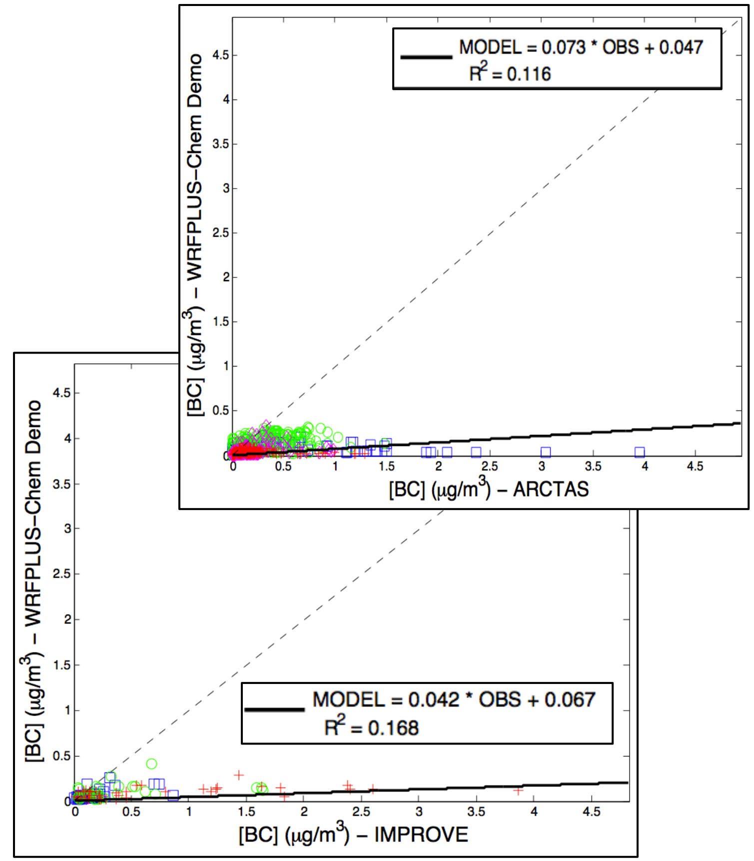
- WRF V3.5
- 18km – 79 x 79 x 31 levels
- I.C.'s & B.C.'s
  MET: 32km NARR Reanalysis
  CHEM: spun up from Jun 15, $[BC]_{bound} = 0.01 \mu g/m^3$
- GOCART Aerosols
- NEI2005 Anthro. Emissions (4km)
- FINN BB Emissions (1km) w/ plumerise
- ACM2 PBL Mixing (7)
- Pleim-Xiu SFCLAY (7)
- No LSM → No dry deposition
- No Microphysics
- No Cumulus scheme
- No LW or SW Radiation

*Forward model only (Adjoint not developed yet)

Cost Function Evaluation

Column Summed Cost Function ($\mu g^2/m^6$)





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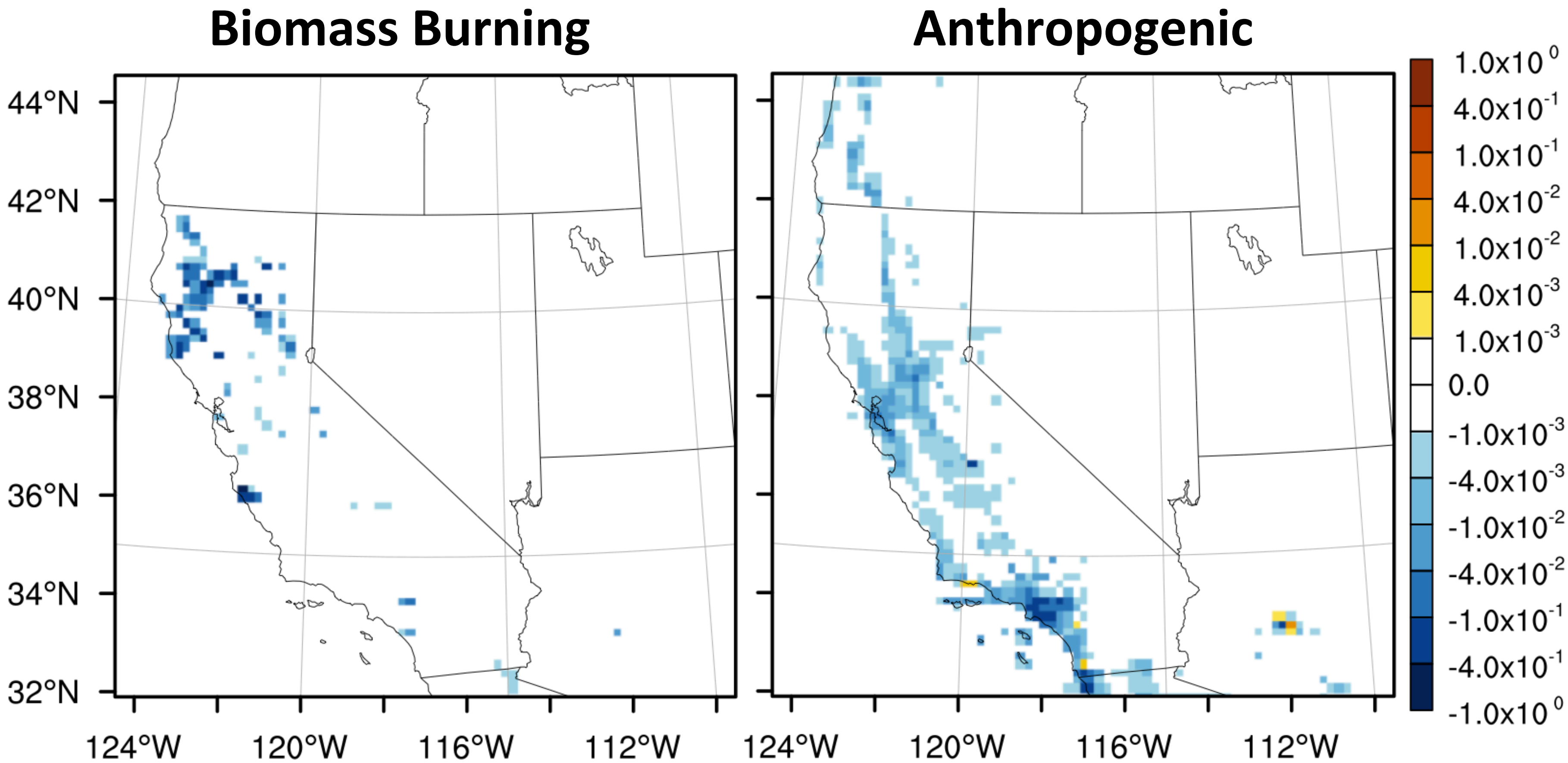
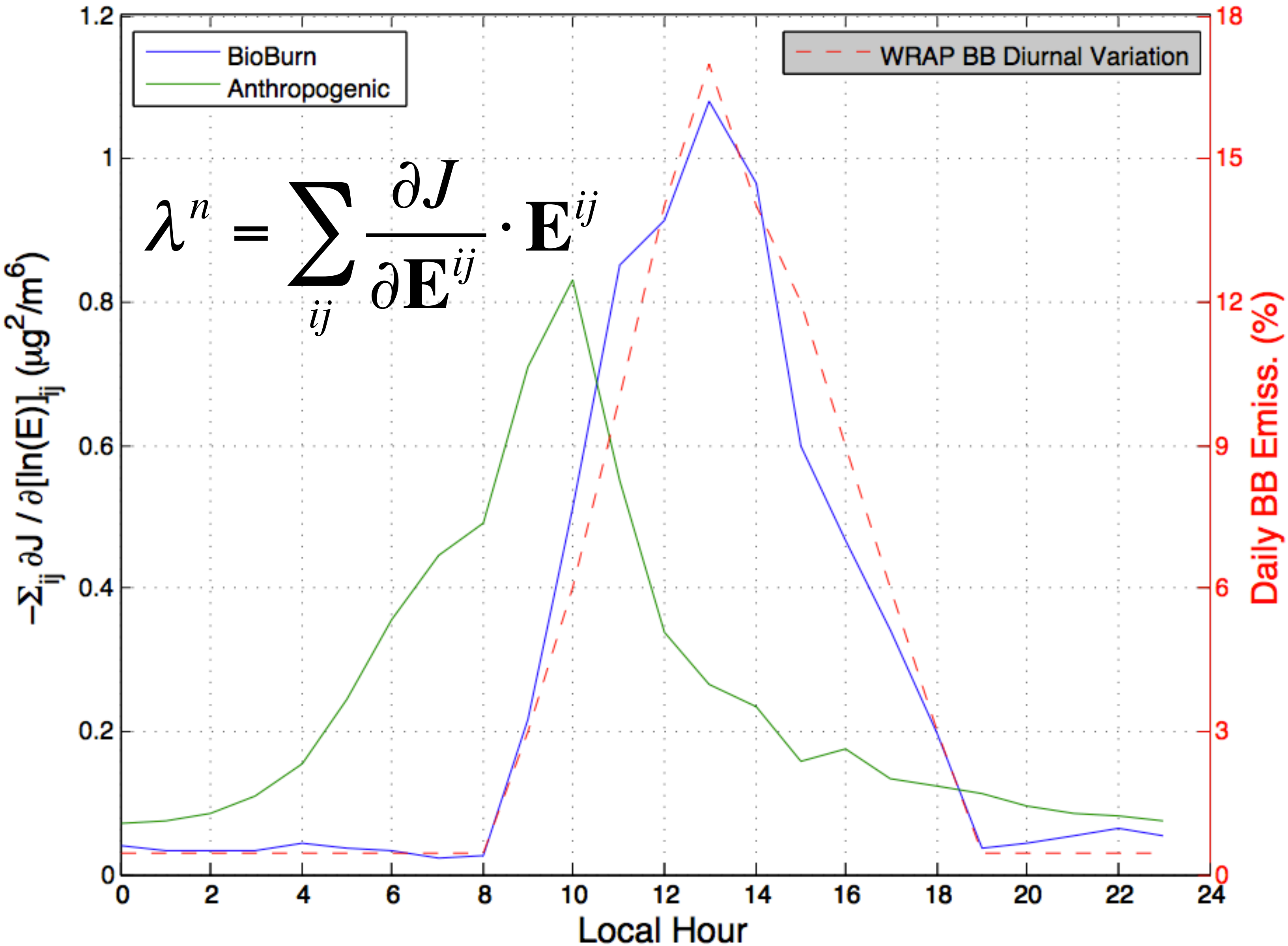
Spatially Aggregated Sensitivities



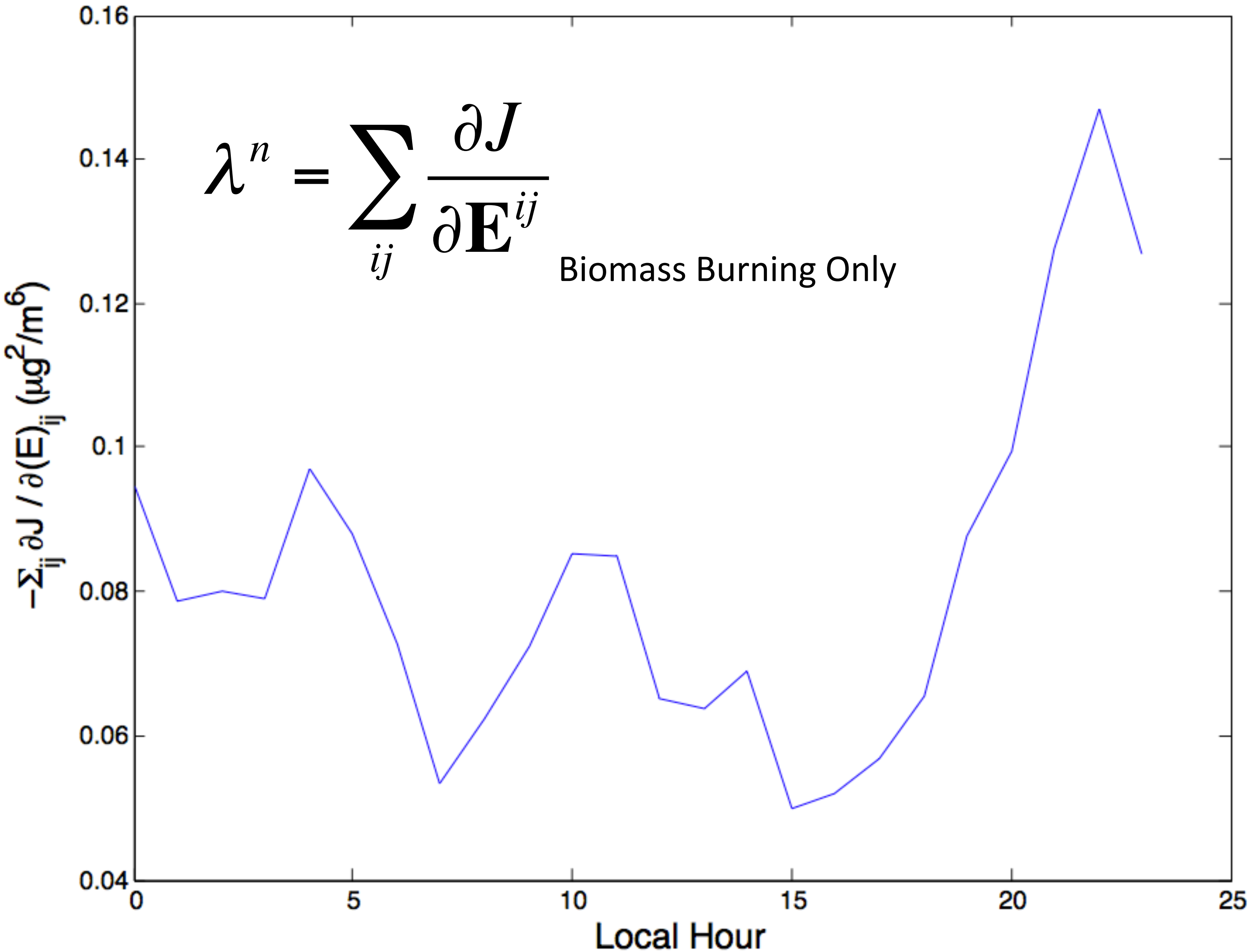
$$\sum_{n}^{N_e} \frac{\partial J}{\partial \mathbf{E}^n} \cdot \mathbf{E}^n$$

N_e = # of emission intervals

Temporally Aggregated Sensitivities



Temporally Aggregated Sensitivities



Next Steps

- Incorporate more AD and TL pieces into WRFPLUS
  - Cumulus Convection (shallow possible too?)
  - Radiative feedbacks
  - Mix-activate for aerosol-cloud interactions
  - Dust
  - Observation Operators
    - AOD & AAOD diagnostic
    - 3D spatial interpolation for in-situ observations

- Tune the PBL, including adding more grid levels
- Investigate which SFCLAY and LSM schemes work best in forward model

- 4DVar Data Assimilation

References

Koch, D. and Schulz, M. and Kinne, S. and McNaughton, C. and Spackman, J. R. and Balkanski, Y. and Bauer, S. and Berntsen, T. and Bond, T. C. and Boucher, O. and Chin, M. and Clarke, A. and De Luca, N. and Dentener, F. and Diehl, T. and Dubovik, O. and Easter, R. and Fahey, D. W. and Feichter, J. and Fillmore, D. and Freitag, S. and Ghan, S. and Ginoux, P. and Gong, S. and Horowitz, L. and Iversen, T. and Kirkevåg, A. and Klimont, Z. and Kondo, Y. and Krol, M. and Liu, X. and Miller, R. and Montanaro, V. and Moteki, N. and Myhre, G. and Penner, J. E. and Perlwitz, J. and Pitari, G. and Reddy, S. and Sahu, L. and Sakamoto, H. and Schuster, G. and Schwarz, J. P. and Seland, Ø. and Stier, P. and Takegawa, N. and Takemura, T. and Textor, C. and van Aardenne, J. A. and Zhao, Y. Evaluation of black carbon estimations in global aerosol models, Atmos. Chem. Phys., 9, 9001-9026, 2009.

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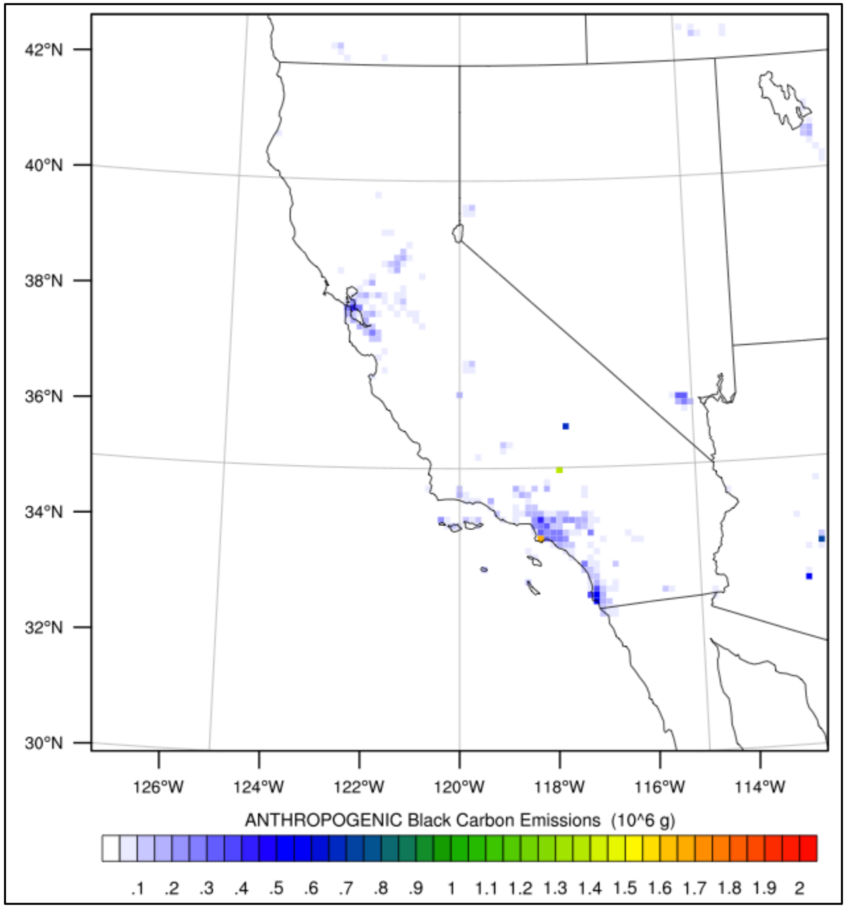
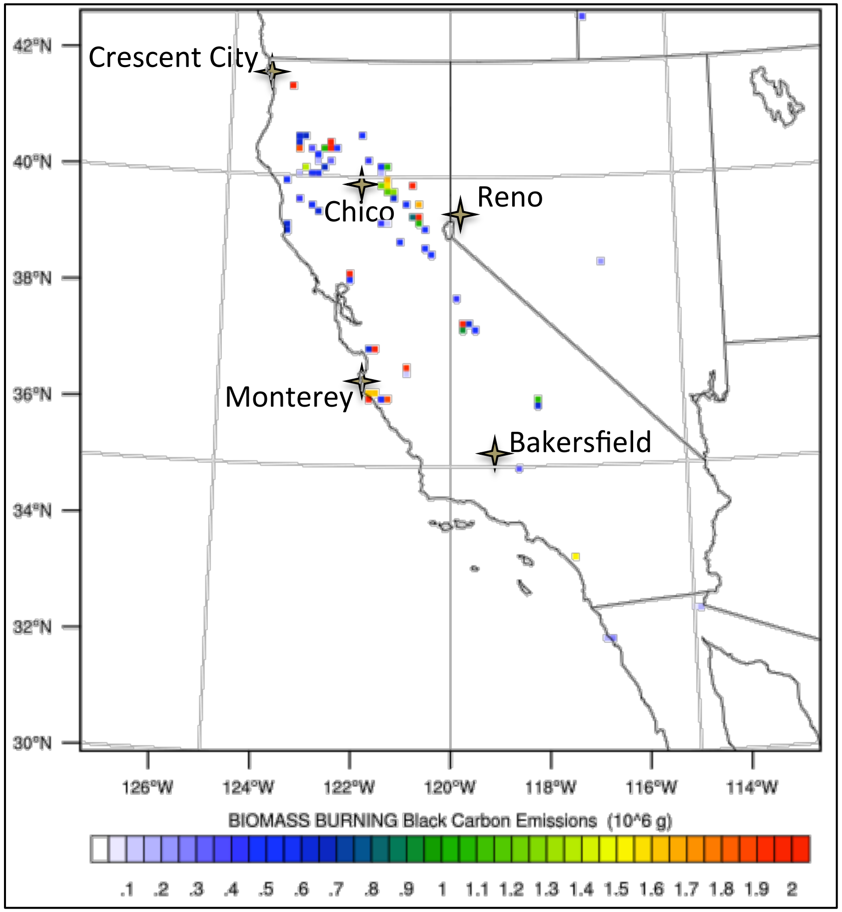
Jun 22, 2008 Emissions

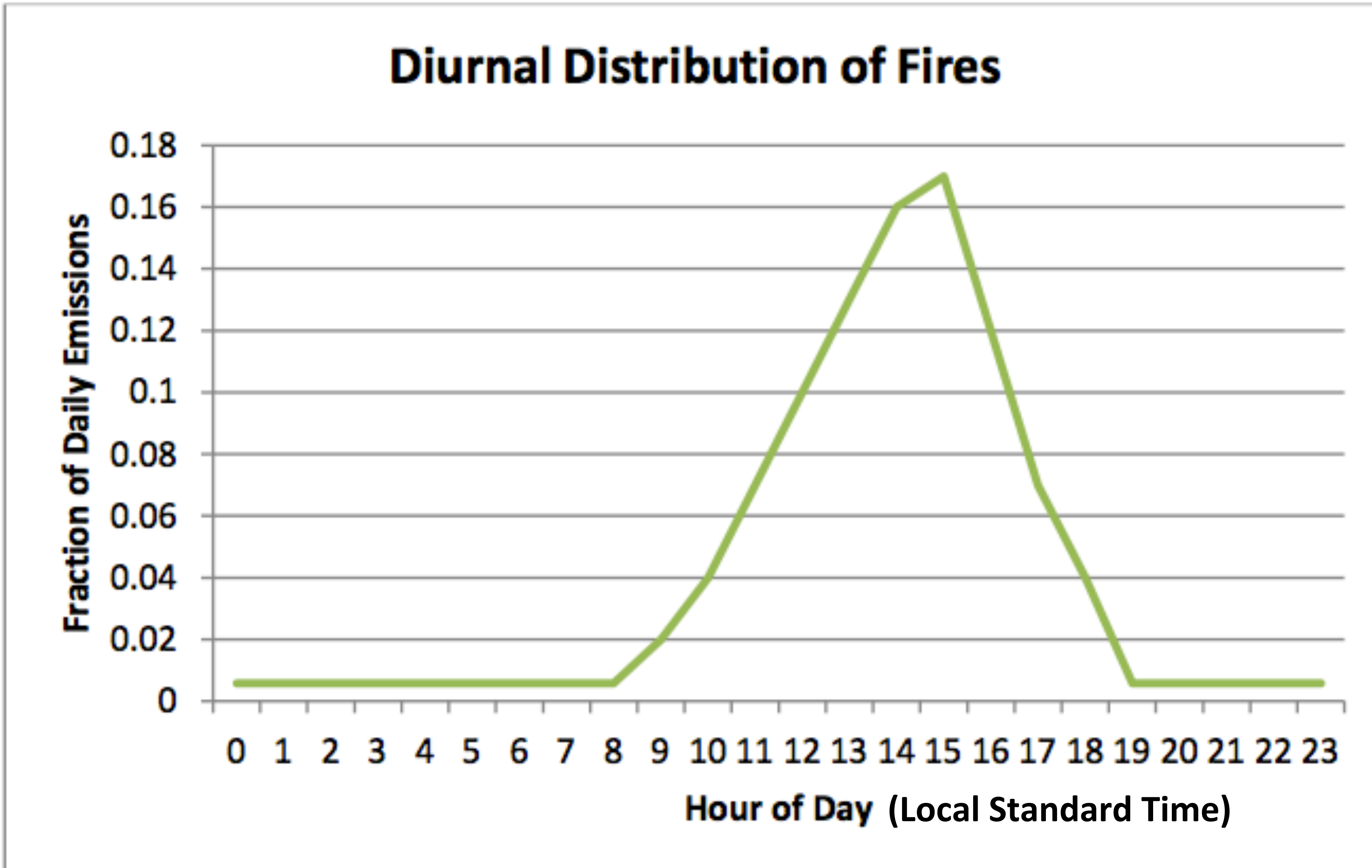
NEI2005 Anthropogenic Emissions



FINN Biomass Burning Emissions

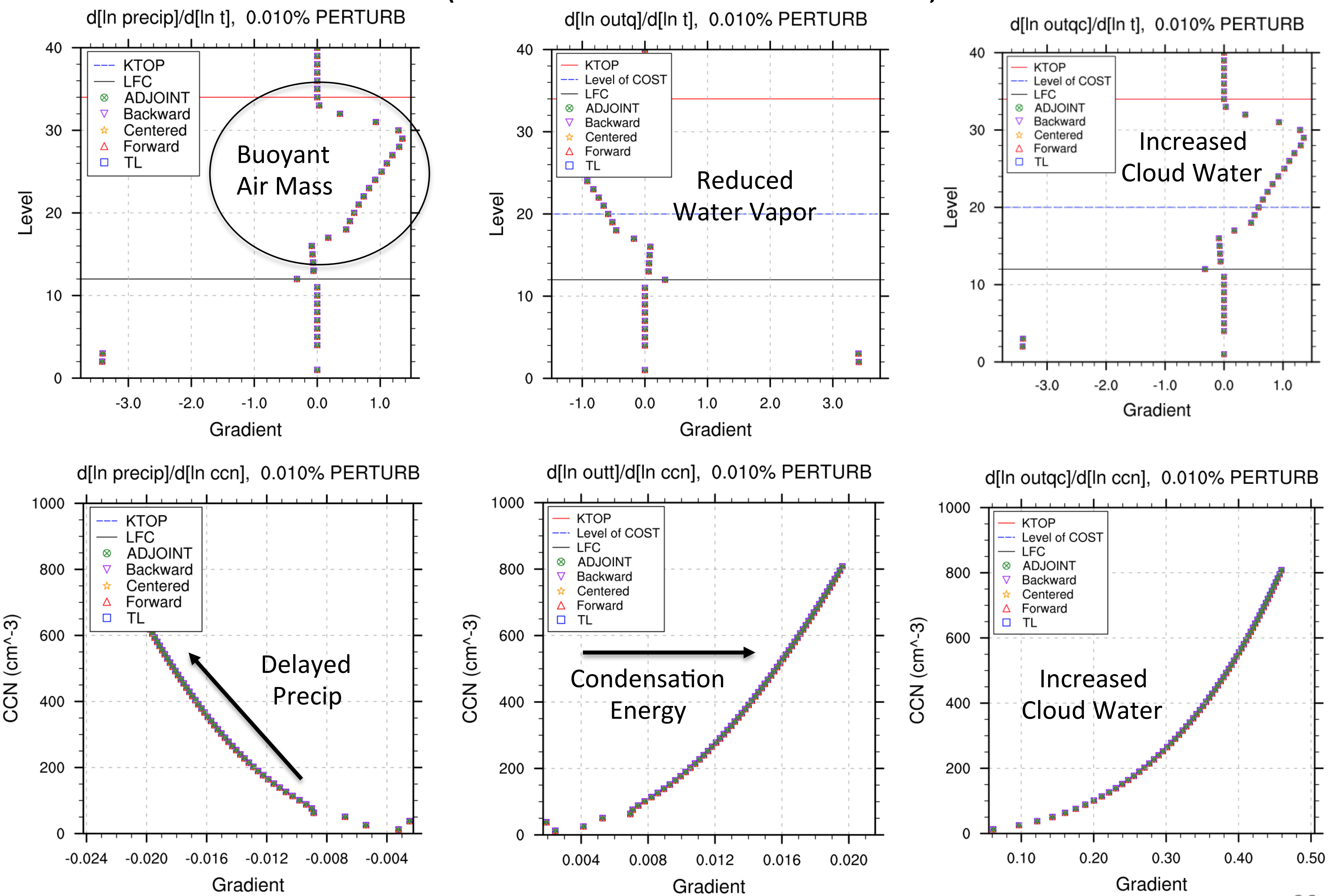


BC Biomass Emissions Diurnal Cycle



Standalone G-F Convection Verification

(lowest 40 of 64 vertical levels)



Code Modifications (not up to date)

NEW TL FILES

chem/chem_driver_tl.F
chem/mechanism_driver_tl.F
chem/aerosol_driver_tl.F
chem/emissions_driver_tl.F
chem/module_emissions_anthropogenics_tl.F
chem/module_gocart_aerosols_tl.F
chem/module_gocart_chem_tl.F

NEW AD FILES

chem/chem_driver_ad.F
chem/mechanism_driver_ad.F
chem/aerosol_driver_ad.F
chem/emissions_driver_ad.F
chem/module_emissions_anthropogenics_ad.F
chem/module_gocart_aerosols_ad.F
chem/module_gocart_chem_ad.F

MODIFIED FILES

chem/chem_driver.F
chem/mechanism_driver.F
chem/aerosol_driver.F
chem/emissions_driver.F
chem/module_emissions_anthropogenics.F
chem/module_add_emiss_burn.F
chem/module_plumerise1.F
chem/chemics_init.F
chem/module_input_chem_data_tl.F
chem/module_input_chem_data_ad.F

chem/depend.chem
chem/Makefile

share/solve_interface.F
share/mediation_pertmod_io.F
share/mediation_integrate.F
share/module_adtl_grid_utilities.F

main/real_em.F
main/module_wrf_top.F
main/depend.common

Registry/Registry.EM_CHEM
Registry/registry.chemplus
Registry/registry.wrfplus
Registry/Registry.EM_COMMON

frame/module_integrate.F

dyn_em/start_em.F
dyn_em/depend.dyn_em
dyn_em/module_first_rk_step_part1_tl.F
dyn_em/module_em_tl.F
dyn_em/solve_em_tl.F
dyn_em/start_em_tl.F

dyn_em/module_first_rk_step_part1_ad.F
dyn_em/module_em_ad.F
dyn_em/solve_em_ad.F
dyn_em/start_em_ad.F