Enabling sensitivity analysis in CMAQ with the complex-step approach

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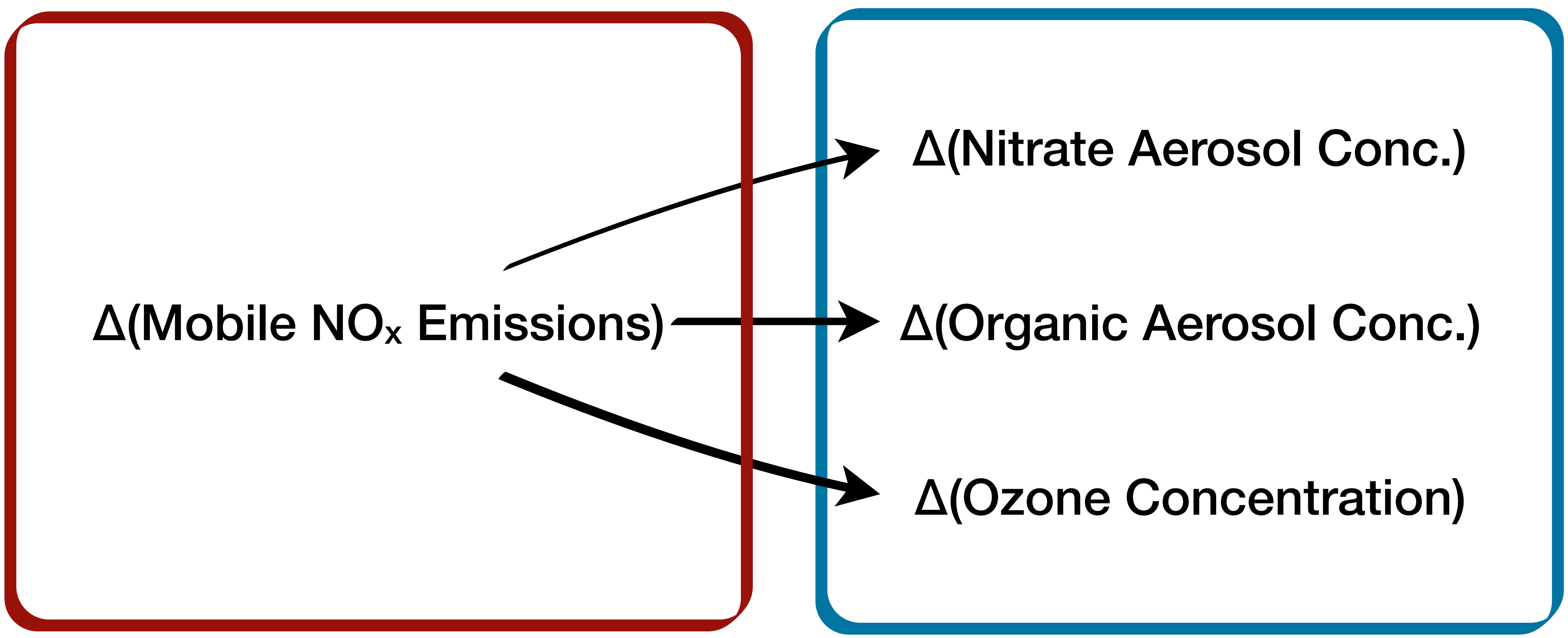
Sensitivity Analysis with Finite Differences

$$\Delta \mathbf{y} = \frac{F(x_0+\Delta x)-F(x_0)}{\Delta x}$$



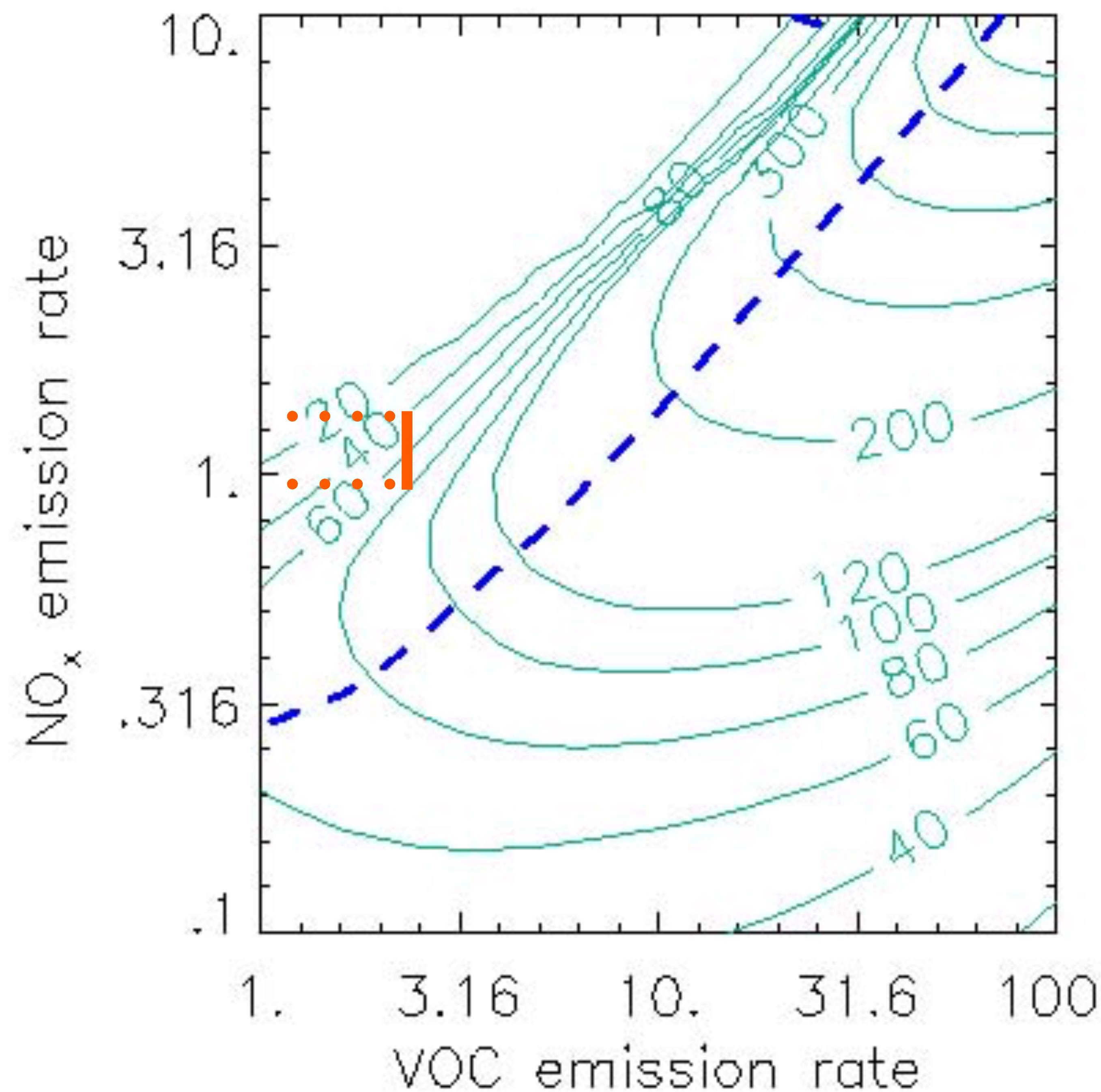
$$\frac{\Delta \textbf{Model Output Fields}_{i,j}}{\Delta \text{Mobile Emissions}}$$

Sensitivity Analysis with Finite Differences

$$\Delta O_3 = \frac{F(\mathbf{x_0}+\Delta NO_x)-F(\mathbf{x_0})}{\Delta NO_x}$$

Accuracy of the difference is limited by the numerical noise of the model.

ozone (ppb)



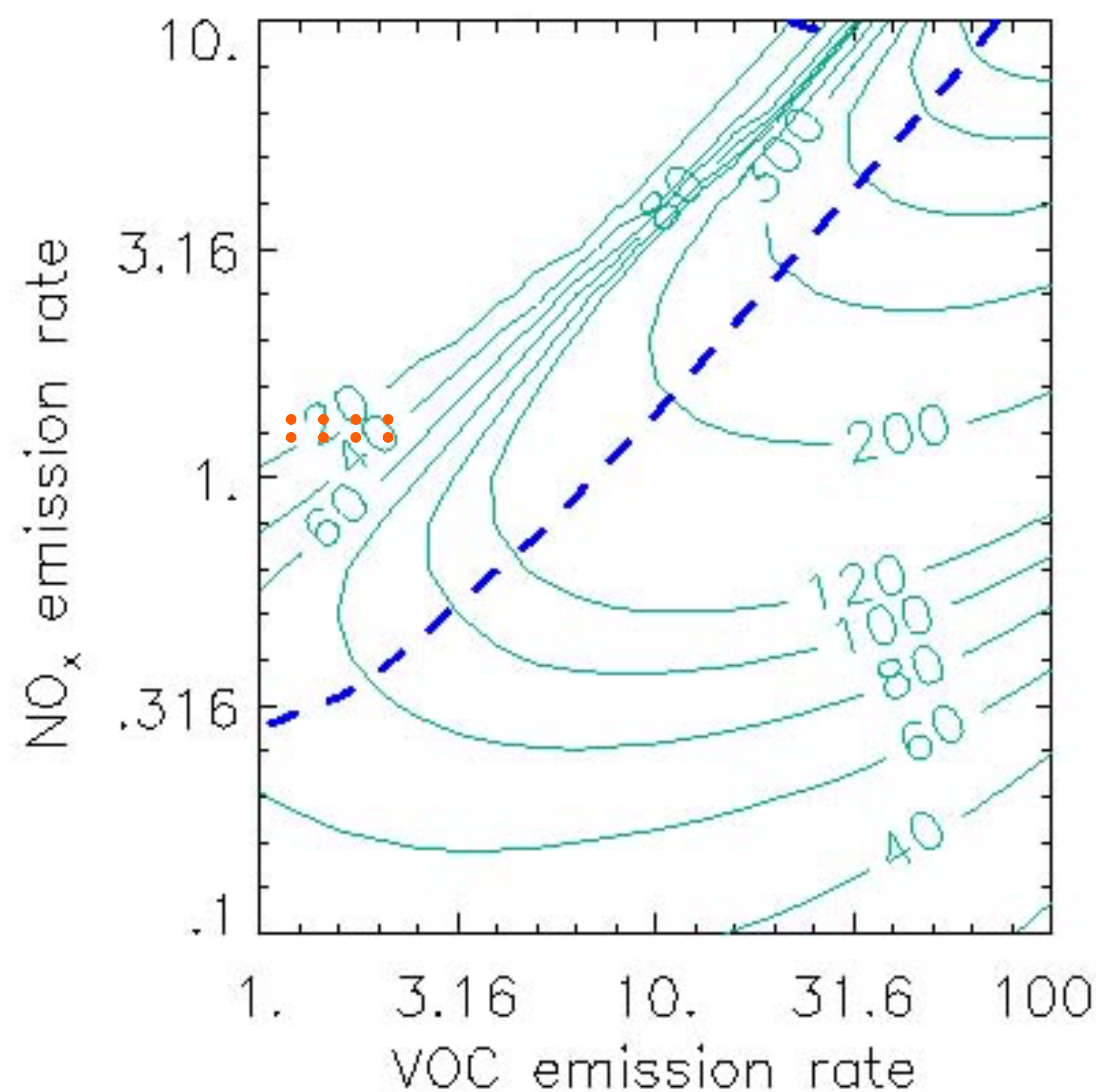
Sillman and He (2002)

Sensitivity Analysis with Finite Differences

$$\Delta O_3 = \frac{F(\mathbf{x_0}+\Delta NO_x)-F(\mathbf{x_0})}{\Delta NO_x}$$

With a small enough perturbation, the modeled results may cancel out providing a sensitivity of zero.

ozone (ppb)



Sillman and He (2002)

Decoupled Direct Method in CMAQ

- CMAQ-DDM-3D enables efficient sensitivity analysis without subtractive cancellation errors and minimal model noise influences.

- Sensitivities with respect to emission rates, boundary conditions, initial conditions, reaction rates, potential vorticity, and any combination of these parameters can be calculated.

- Second-order sensitivities can also be calculated.

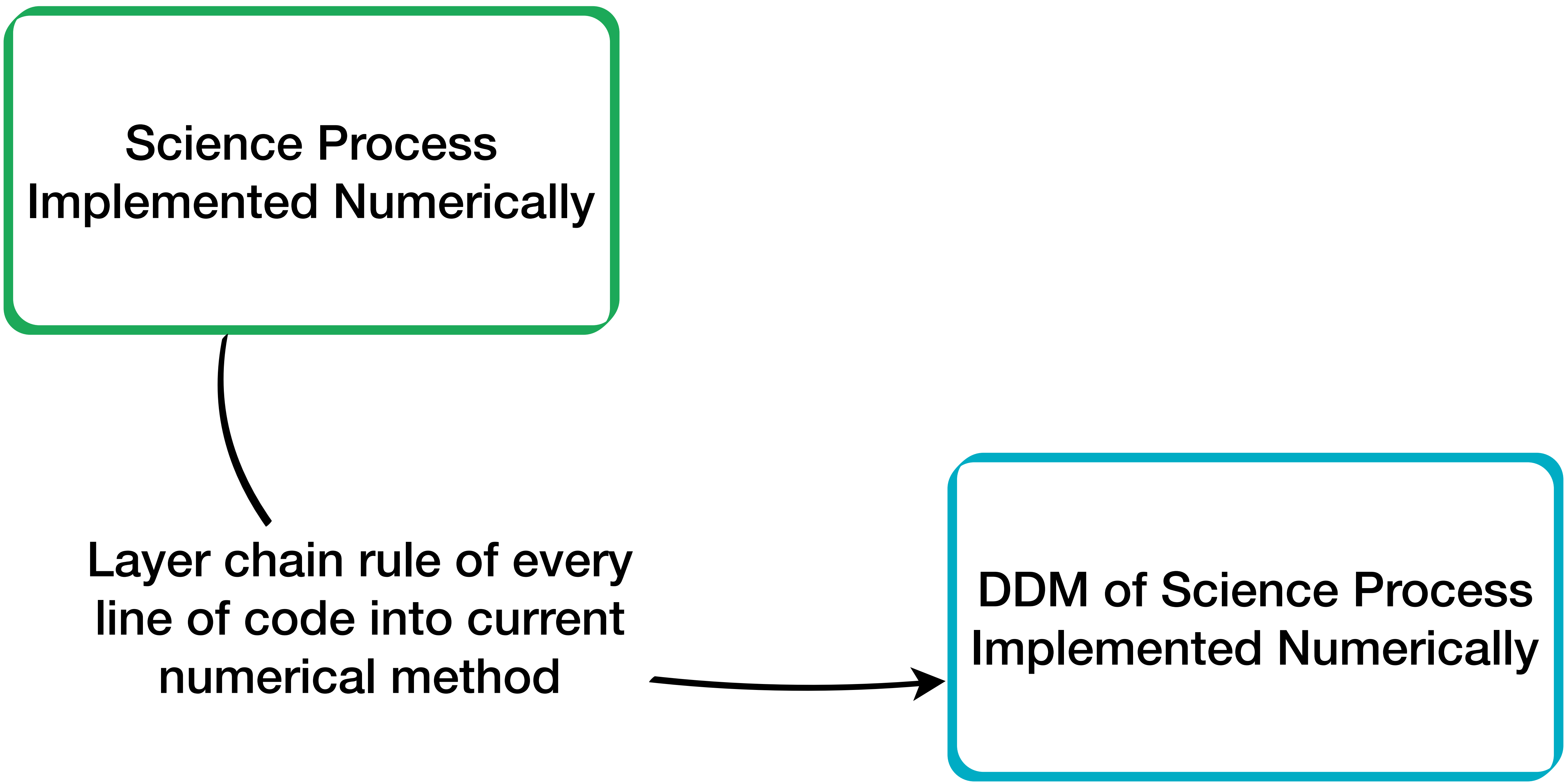
- The computational cost is reasonable because extensive development has layered the derivative of every science process into the model.

Applying the Chain Rule

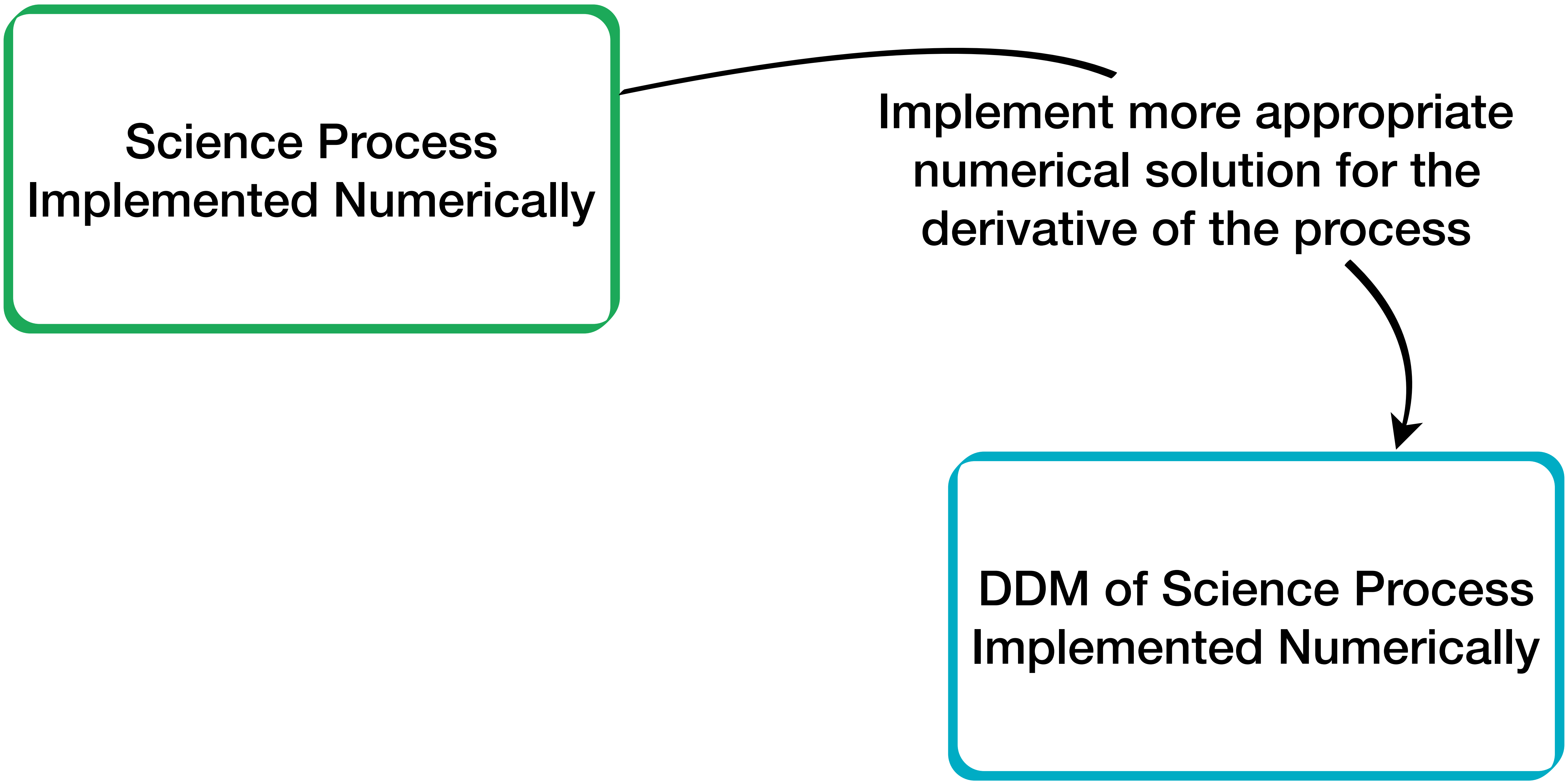
Science Process
Implemented Numerically

DDM of Science Process
Implemented Numerically

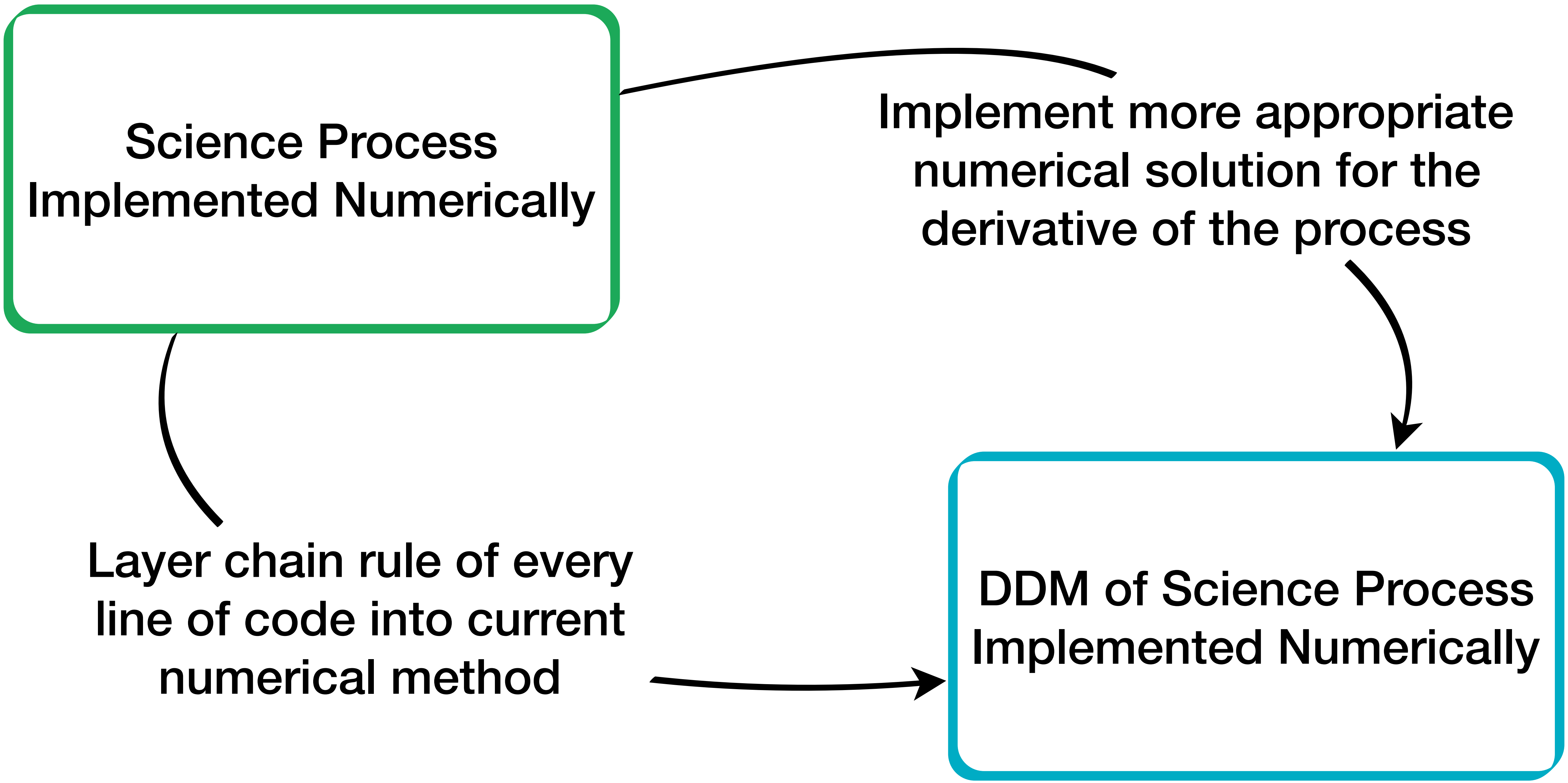
Applying the Chain Rule: *Discrete Method*



Applying the Chain Rule: *Continuous Method*



Applying the Chain Rule: *Continuous Method*



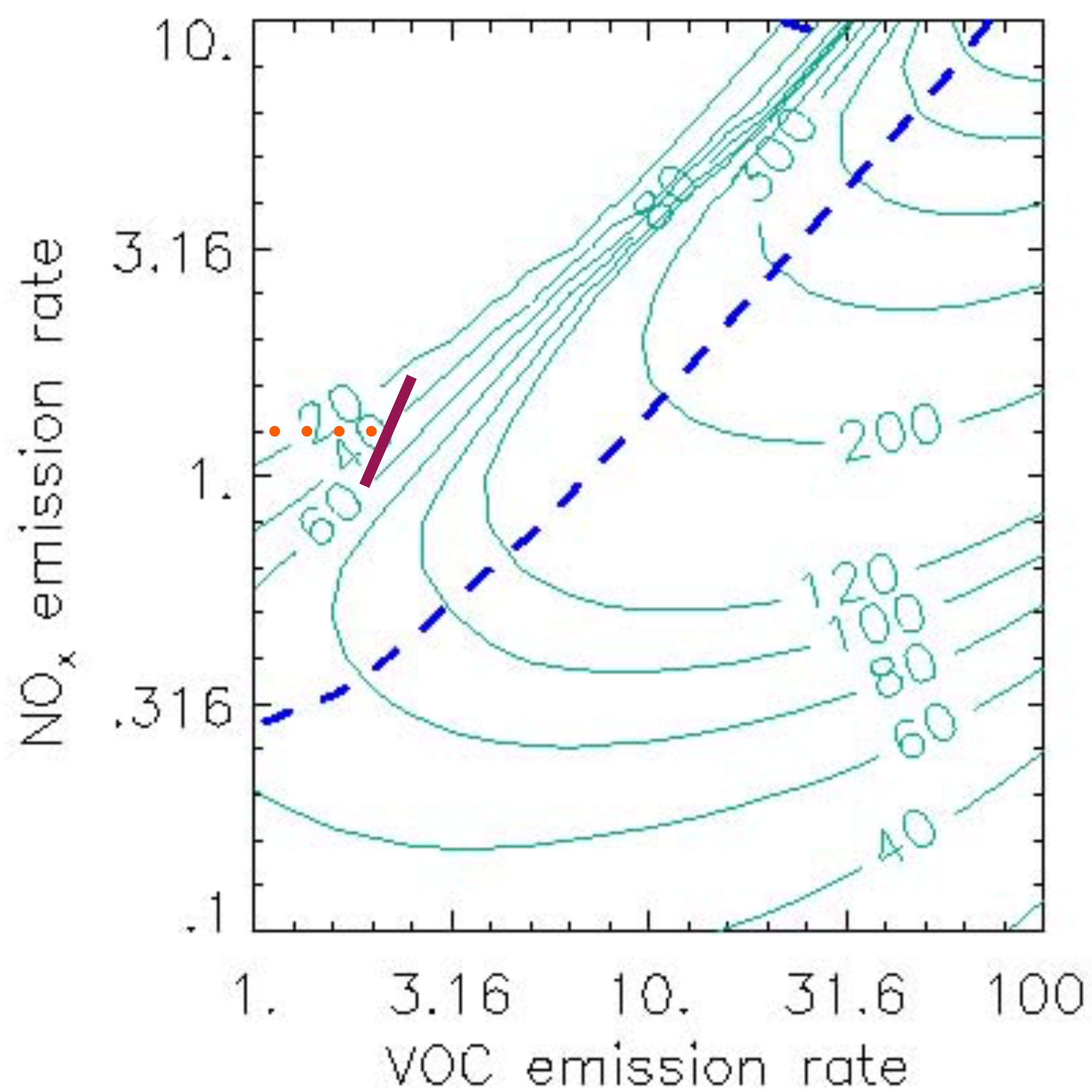
Sensitivity Analysis with Complex Step Method

$$\Delta O_3 = \frac{F(\mathbf{x_0} + i\Delta NO_x)}{\Delta NO_x}$$

Apply the perturbation in imaginary space instead of real space.

Perturbation can now be on the order of 1e-20.

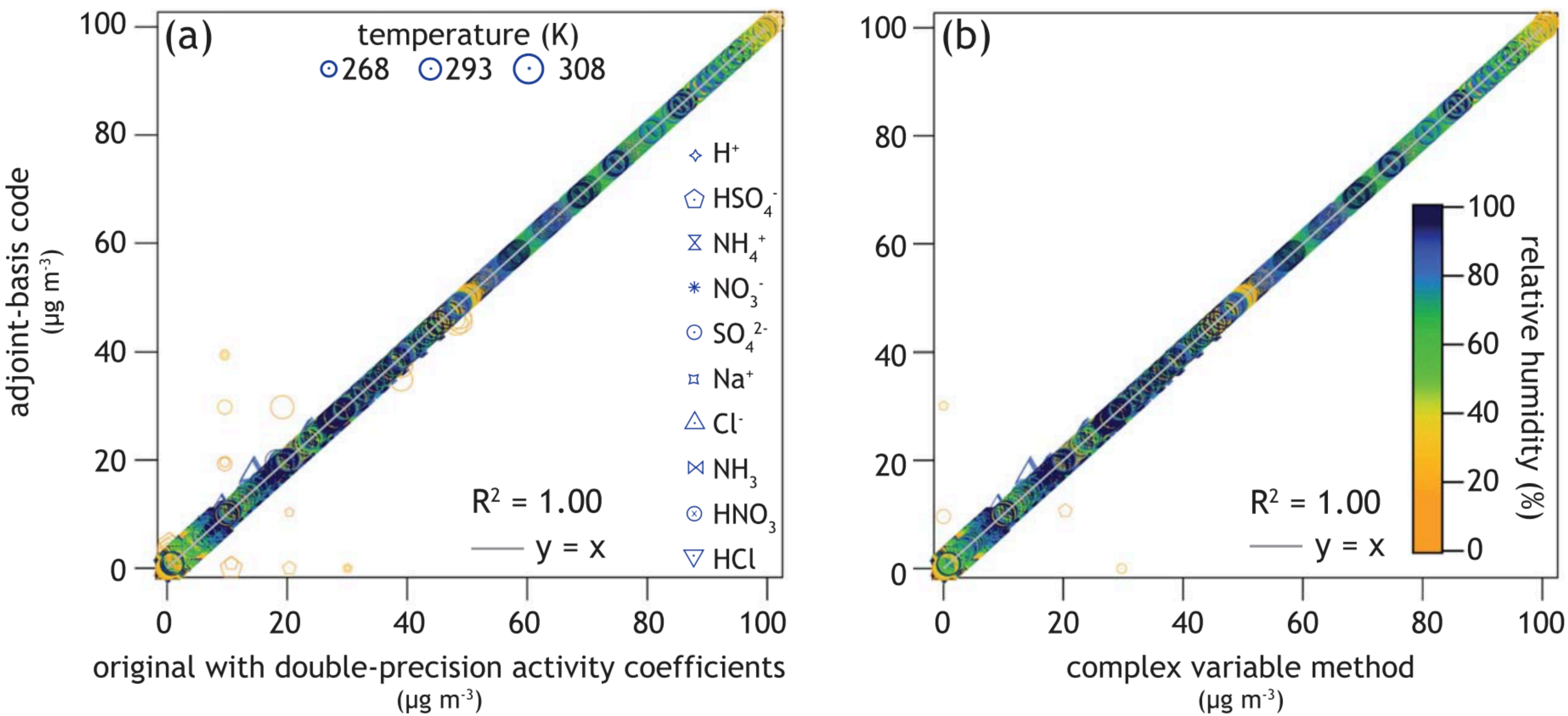
ozone (ppb)



Sillman and He (2002)

Sensitivity Analysis with Complex Variables

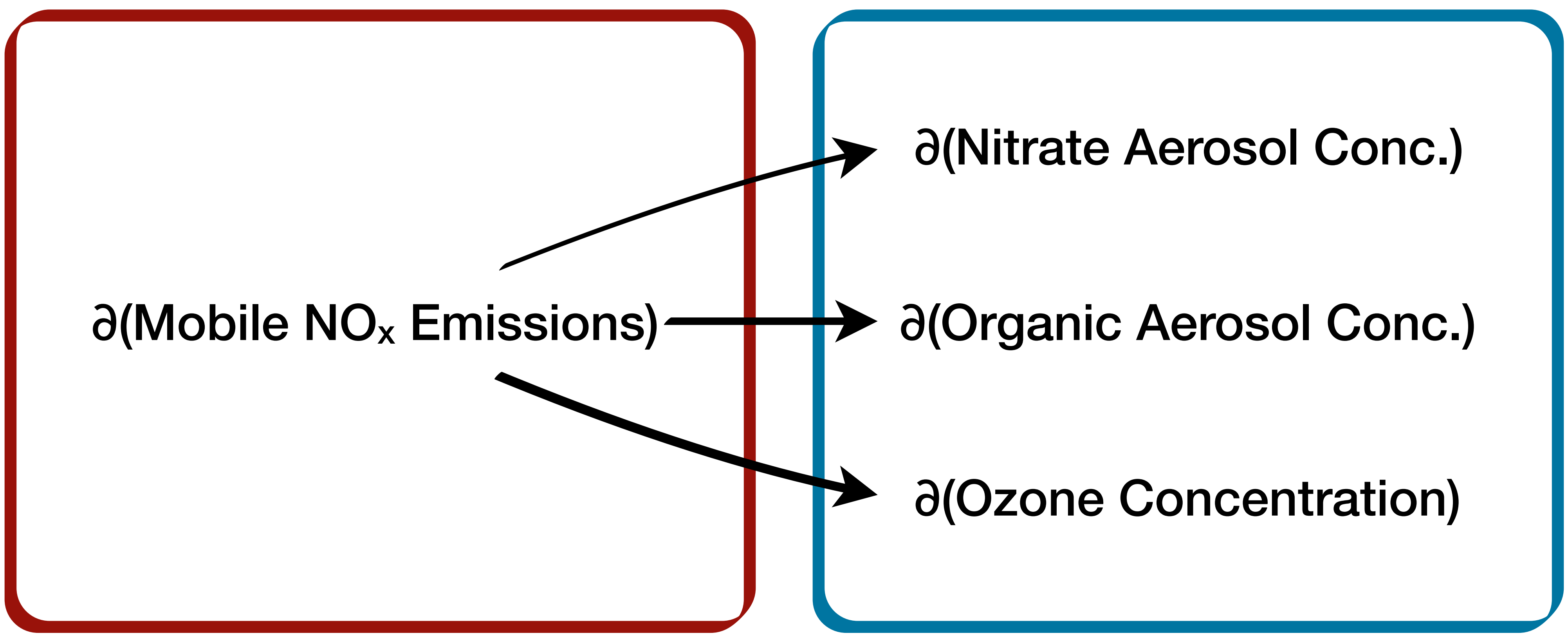
$$\partial \mathbf{y} = \frac{\mathrm{Imag}[F(x_0 + i\Delta x)]}{\Delta x}$$



Capps et al., ACP, 2012

Sensitivity Analysis with Complex Variables

$$\partial \mathbf{y} = \frac{\mathrm{Imag}[F(x_0 + i\Delta x)]}{\Delta x}$$



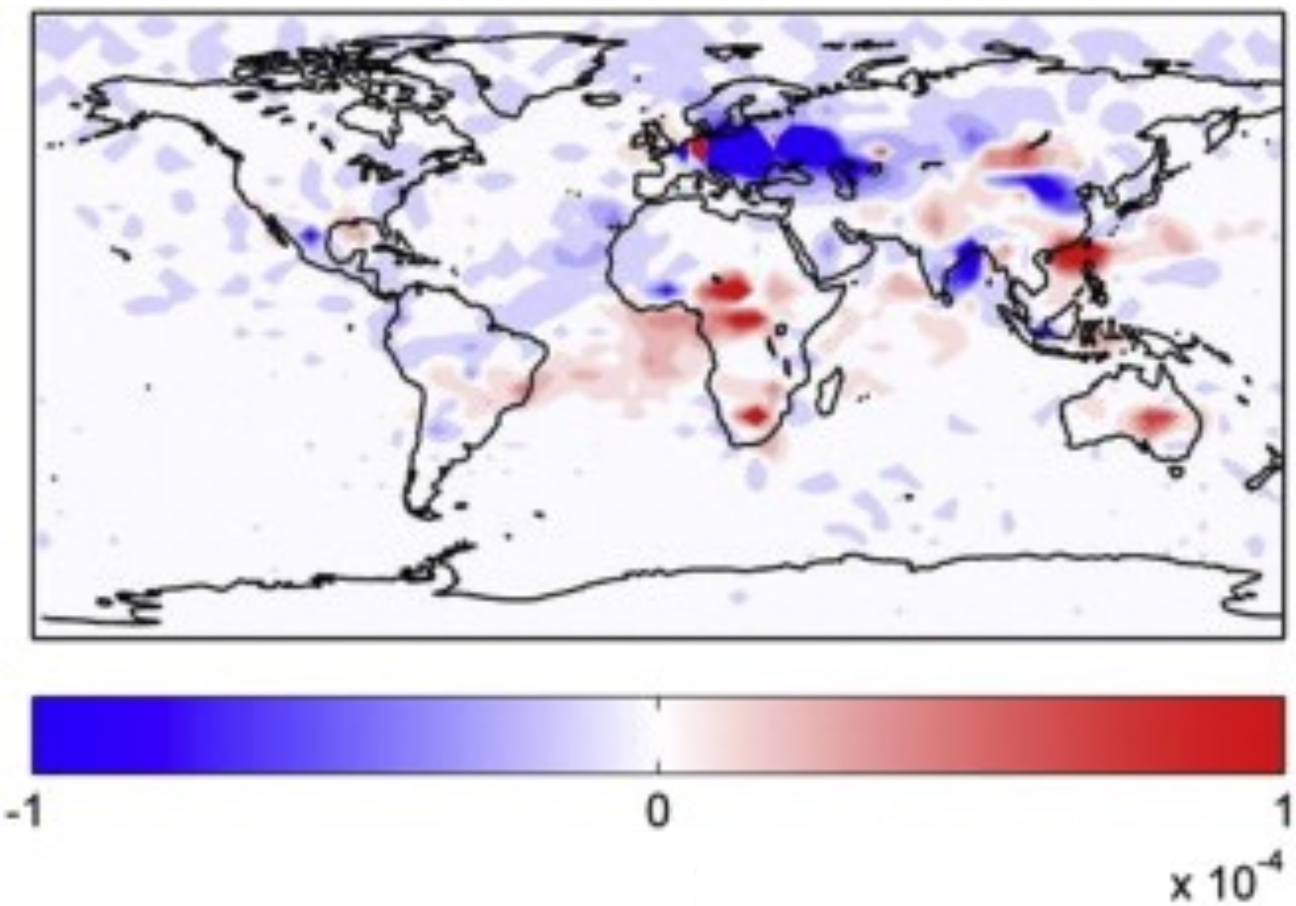
$$\frac{\partial \textbf{Model Output Fields}_{i,j}}{\partial \mathrm{Mobile\ Emissions}}$$

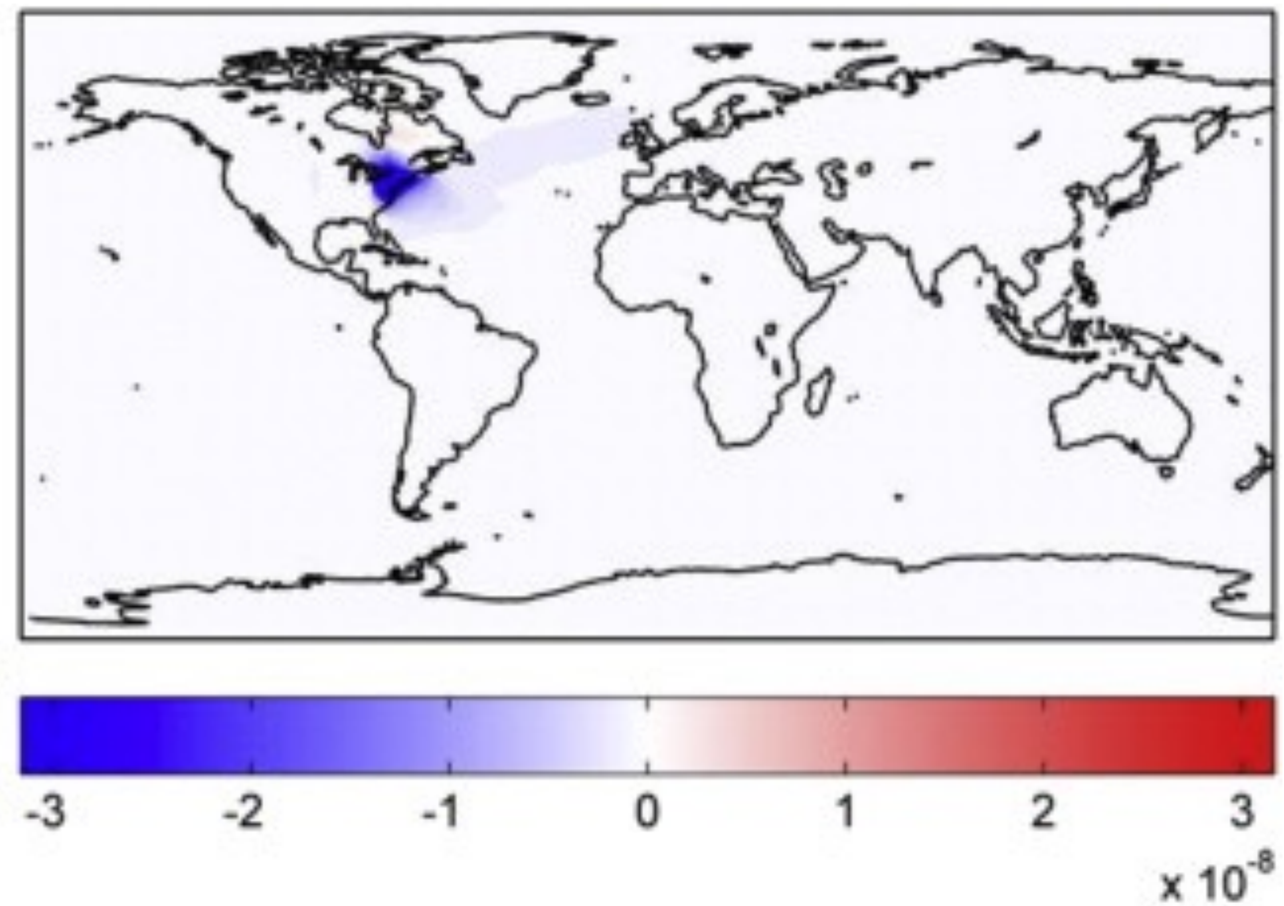
Squire and Trapp, SIAM Rev, 1998; Giles and Pierce, Flow, Turbulence & Combustion, 2001

Advantage of Complex Method

$$\Delta O_{3,surf} = \frac{F(\mathbf{x_0}+\Delta NO_x)-F(\mathbf{x_0})}{\Delta NO_x}$$

$$\partial O_{3,surf} = \frac{F(\mathbf{x_0}+i\Delta NO_x)}{\Delta NO_x}$$



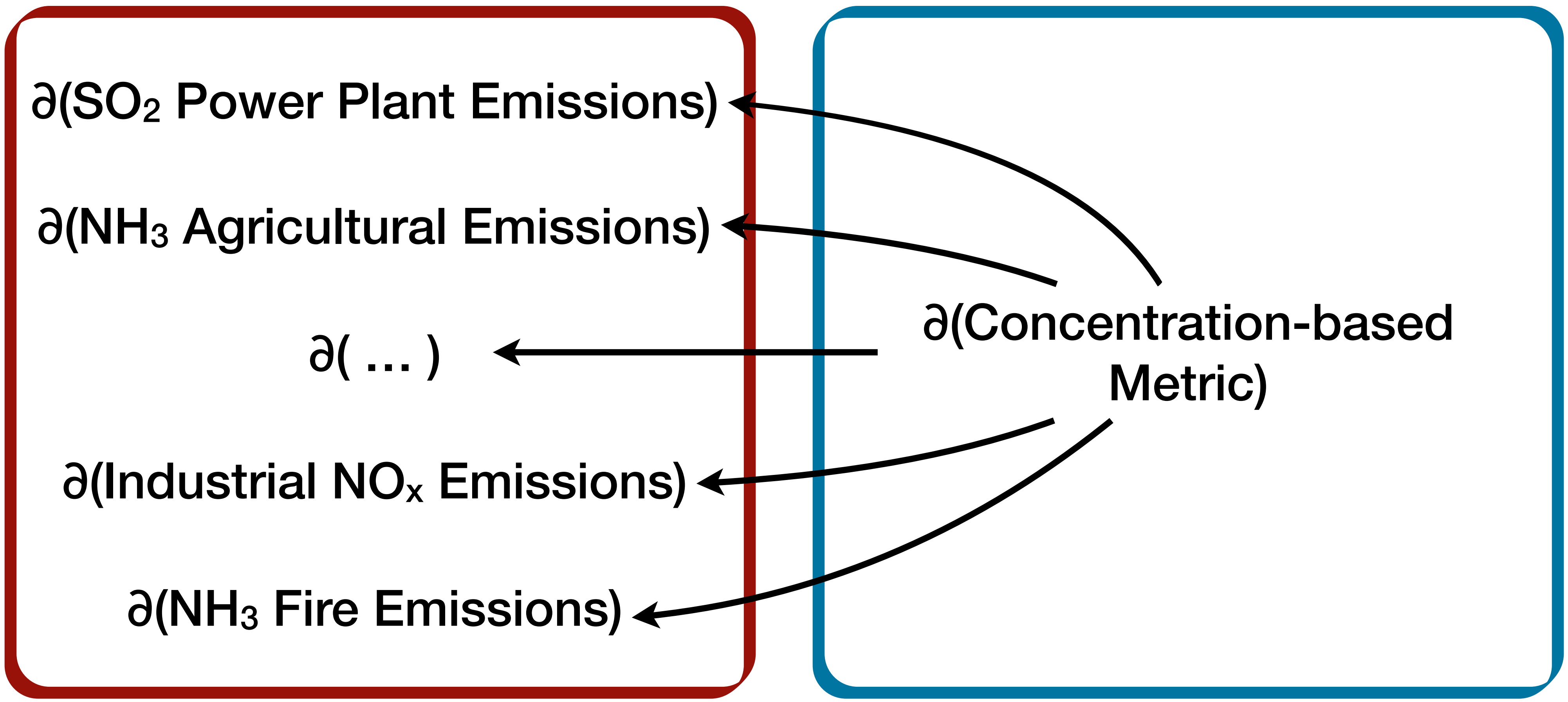


Values shown are ***average monthly sensitivities of ground level O_3 to 1 kg of NO_x*** (ppb kg^{-1}).

Constantin and Barrett, Atmos. Environ., 2014

Efficiency of Adjoint-based Approach

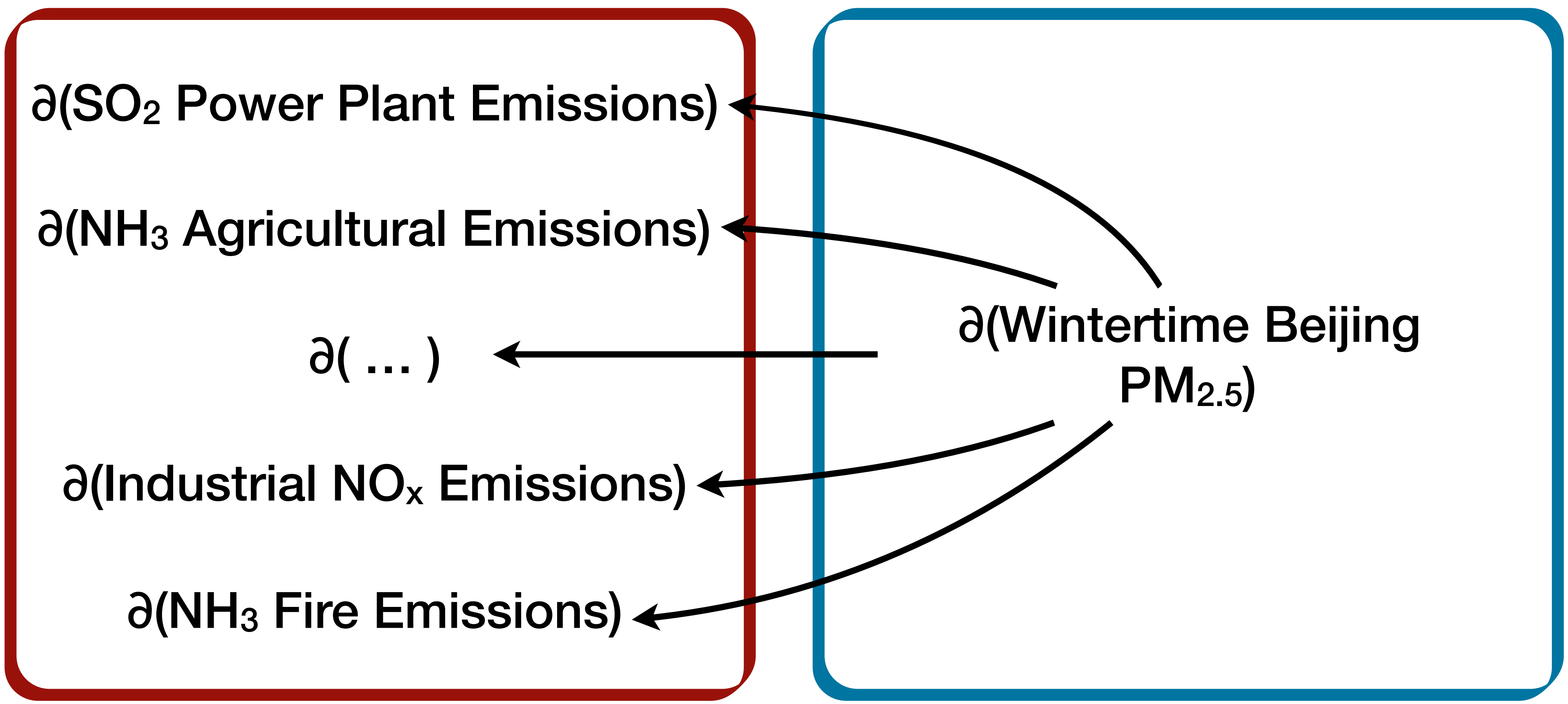
$$\partial \mathbf{x} = F'^{T}(\mathbf{x_0}, \partial y)$$



$$\frac{\partial \text{Concentration-based Metric}}{\partial \mathbf{Emissions}_{i,j,k}}$$

Attributing Beijing $PM_{2.5}$ to Emissions

$$\partial \textbf{Emissions}_{i,j,k} = F'^{T}(\mathbf{x_0}, \partial[\text{Beijing } PM_{2.5}])$$

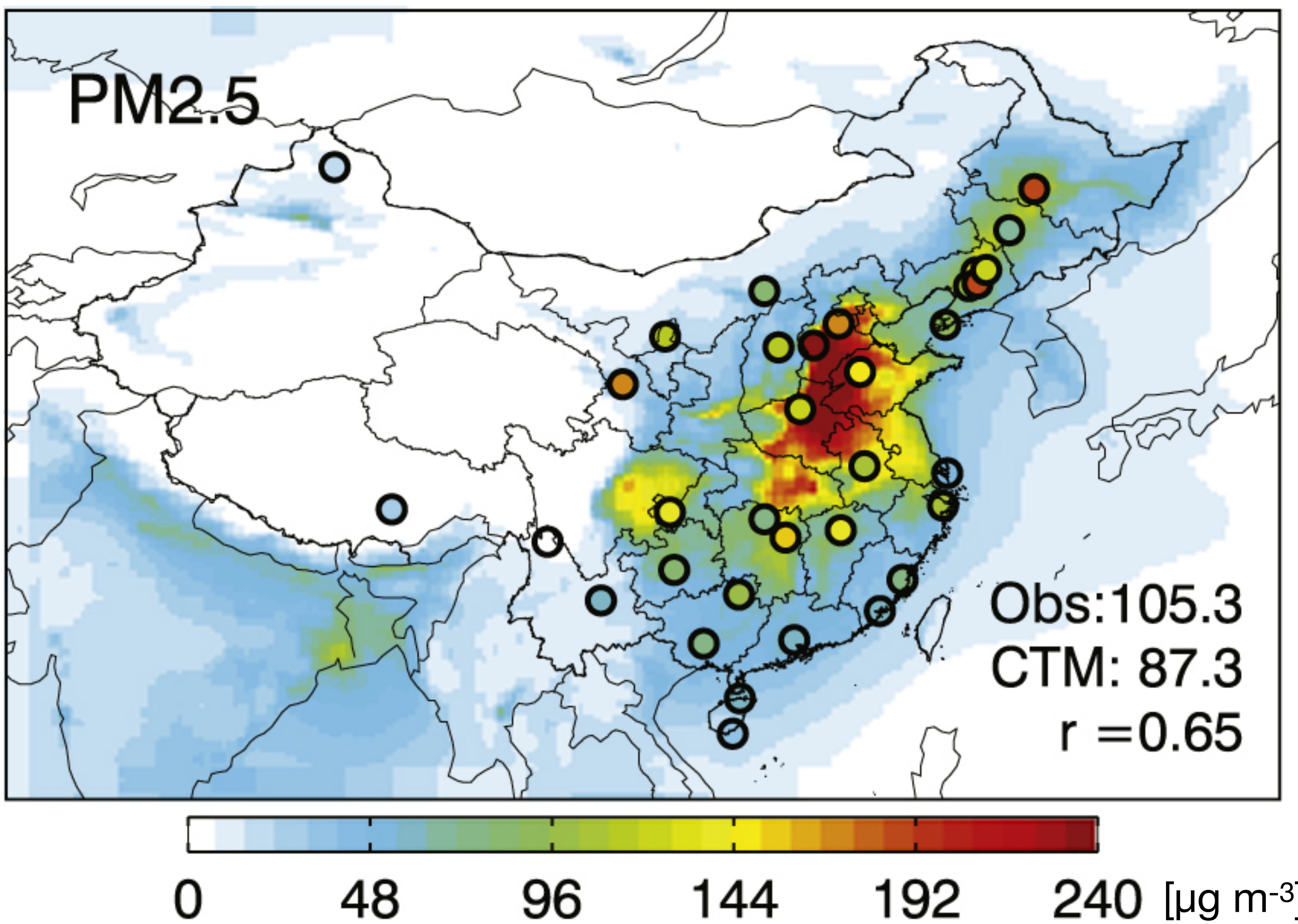


$$\frac{\partial \text{Wintertime } PM_{2.5} \text{ in Beijing}}{\partial \textbf{Emissions}_{i,j,k}}$$

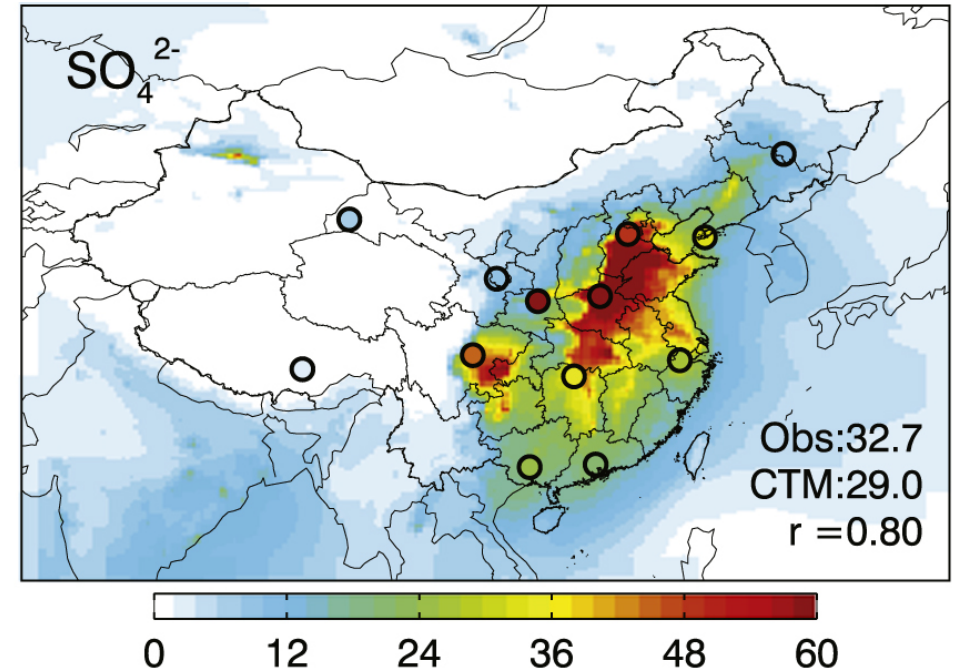
Zhang et al., Environ. Res. Lett., 2015

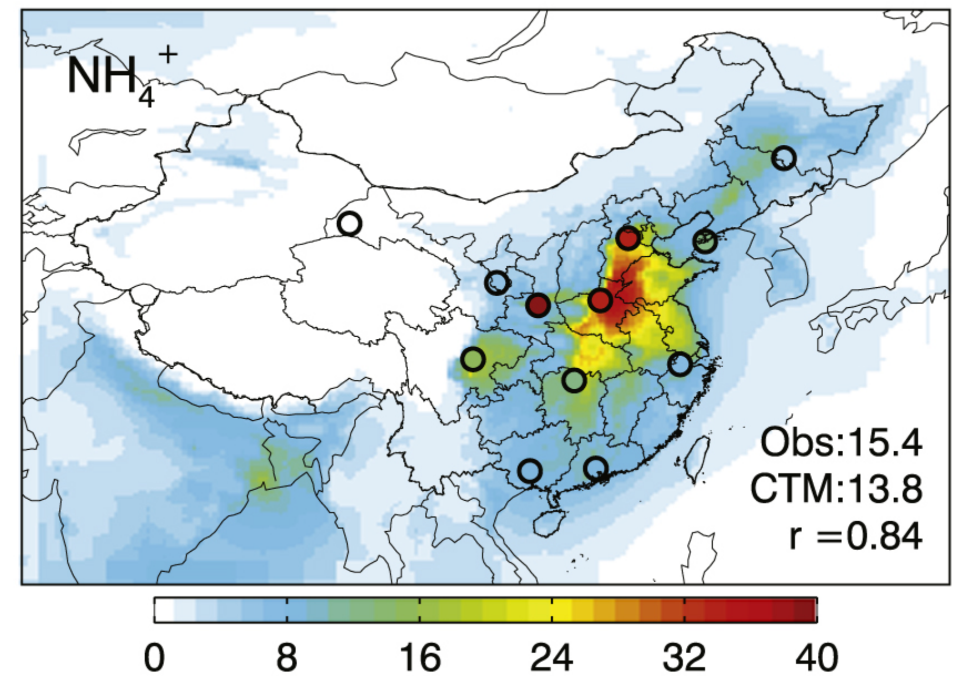
Modeling $PM_{2.5}$ Concentrations

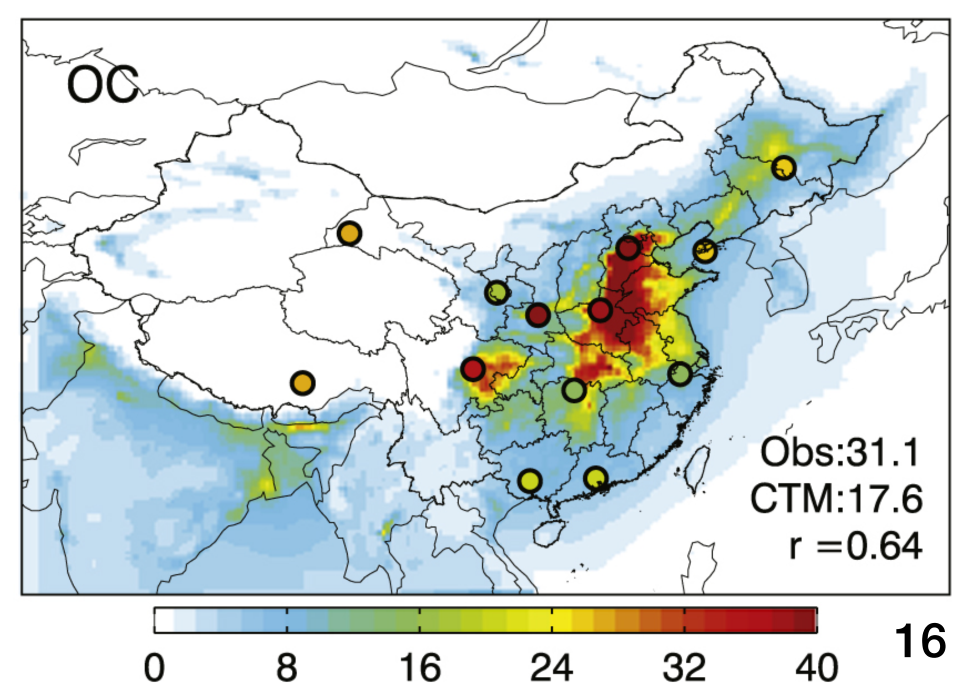
$$PM_{2.5} = F(\mathbf{Emissions}_{i,j,k})$$



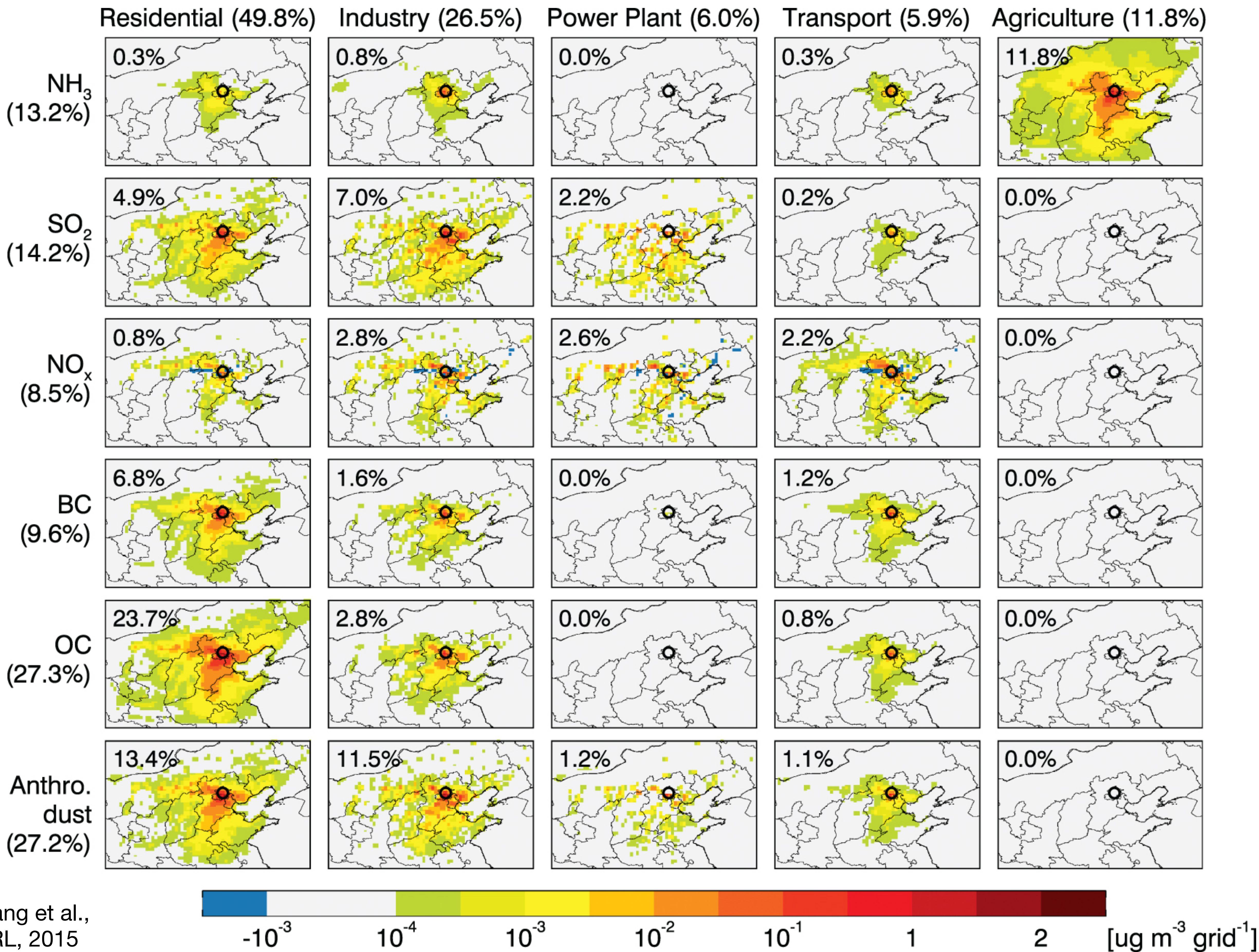
Zhang et al., Environ. Res. Lett., 2015







Attributing Beijing $PM_{2.5}$ to Sources



Zhang et al., ERL, 2015

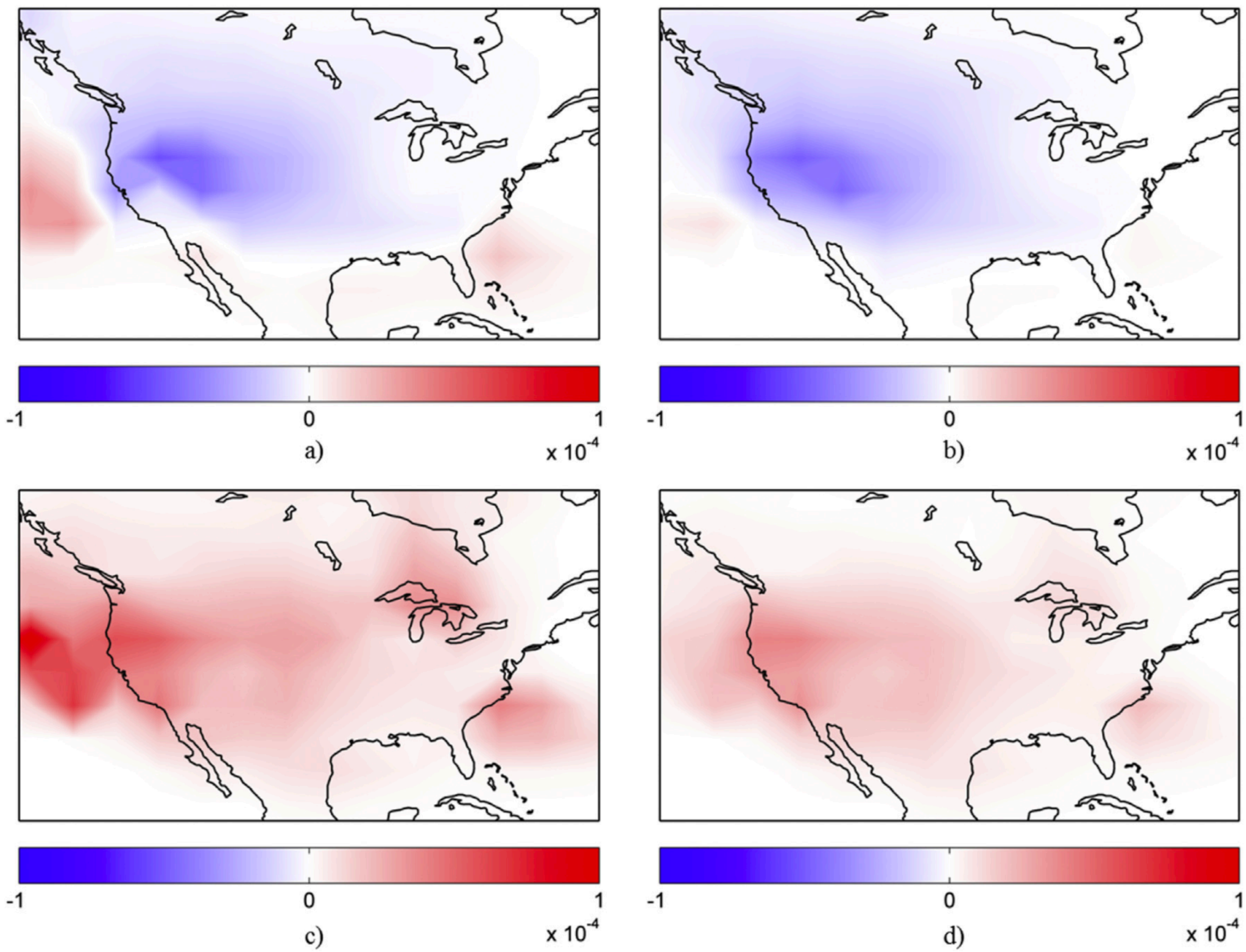
Second-order Combined Sensitivities

$$\frac{\partial^2 PM_{2.5}}{\partial \mathbf{Emis}_{SO_2}\ \partial \mathbf{Emis}_{NO_x}}$$

CS-adjoint | FD-adjoint

January

June



Values shown are ***time-averaged second-order sensitivities of ground level*** $\boldsymbol{PM_{2.5}}$ ***to*** $\boldsymbol{NO_x}$ ***and*** $\boldsymbol{SO_2}$ ***emissions*** ($\mu g\ m^{-3}\ (kg\ h^{-1})^{-2}$).

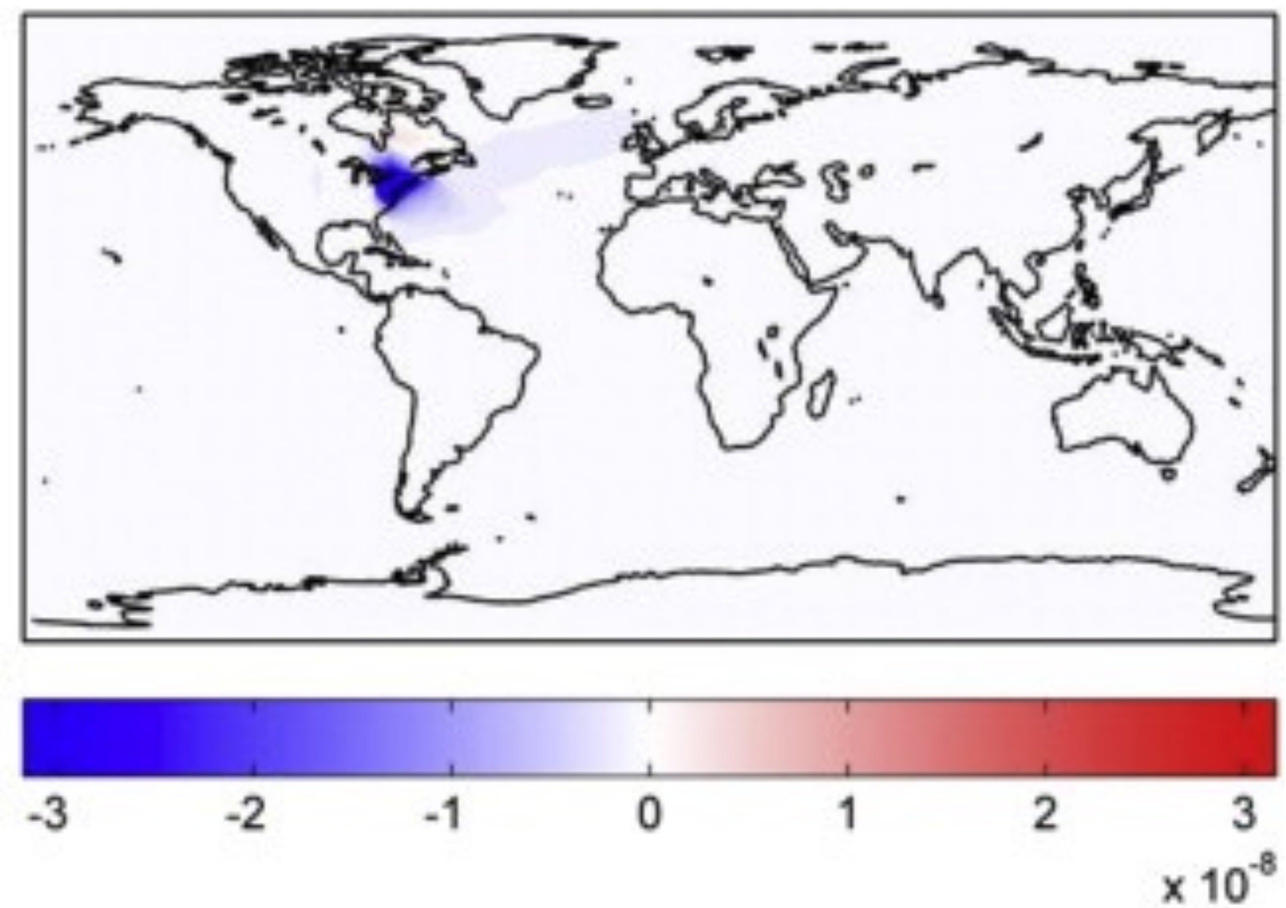
Constantin and Barrett, Atmos. Environ., 2014

Ongoing Work in CMAQ

Implementing the complex step method in CMAQ v.5.2.

Evaluation will be against DDM-3D.

Limitation is that it will only treat one variable at a tir



Constantin and Barrett, Atmos. Environ., 2014