Spatial Reduction Algorithm for Global Atmospheric Chemical Transport Simulation: Algorithm Integration into the GEOS-Chem Solver

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Motivation

- Very Large and Complex: Chemical mechanisms for Global Atmospheric modeling include hundreds of coupled species and thousand of reactions
- Extremely Stiff: Multiscale nature of the chemical system dynamics: Time scales range from milliseconds to many years $\tau_s/\tau_f \sim 10^{10}$

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severe limitations in the spatial resolution

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Inability to resolve or adequately simulate:

- Vertical stratification of the troposphere
- Dynamics of the planetary boundary layer
- Sharp horizontal gradients across fronts and coastlines
- Trans-pacific plume dynamics

Example of code failure due to inadequate spatial resolution

pollution plumes in the remote troposphere can preserve their identity as well-defined layers for two weeks or more as they circle the globe

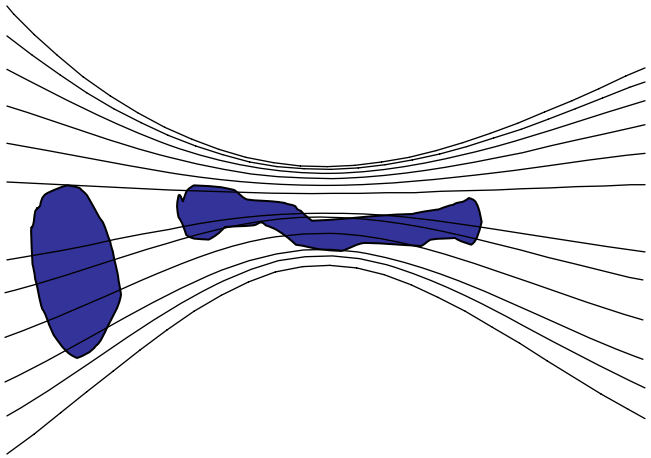
Global 3-D CTMs are completely incapable of reproducing the global-scale plume dynamics

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = 0$$

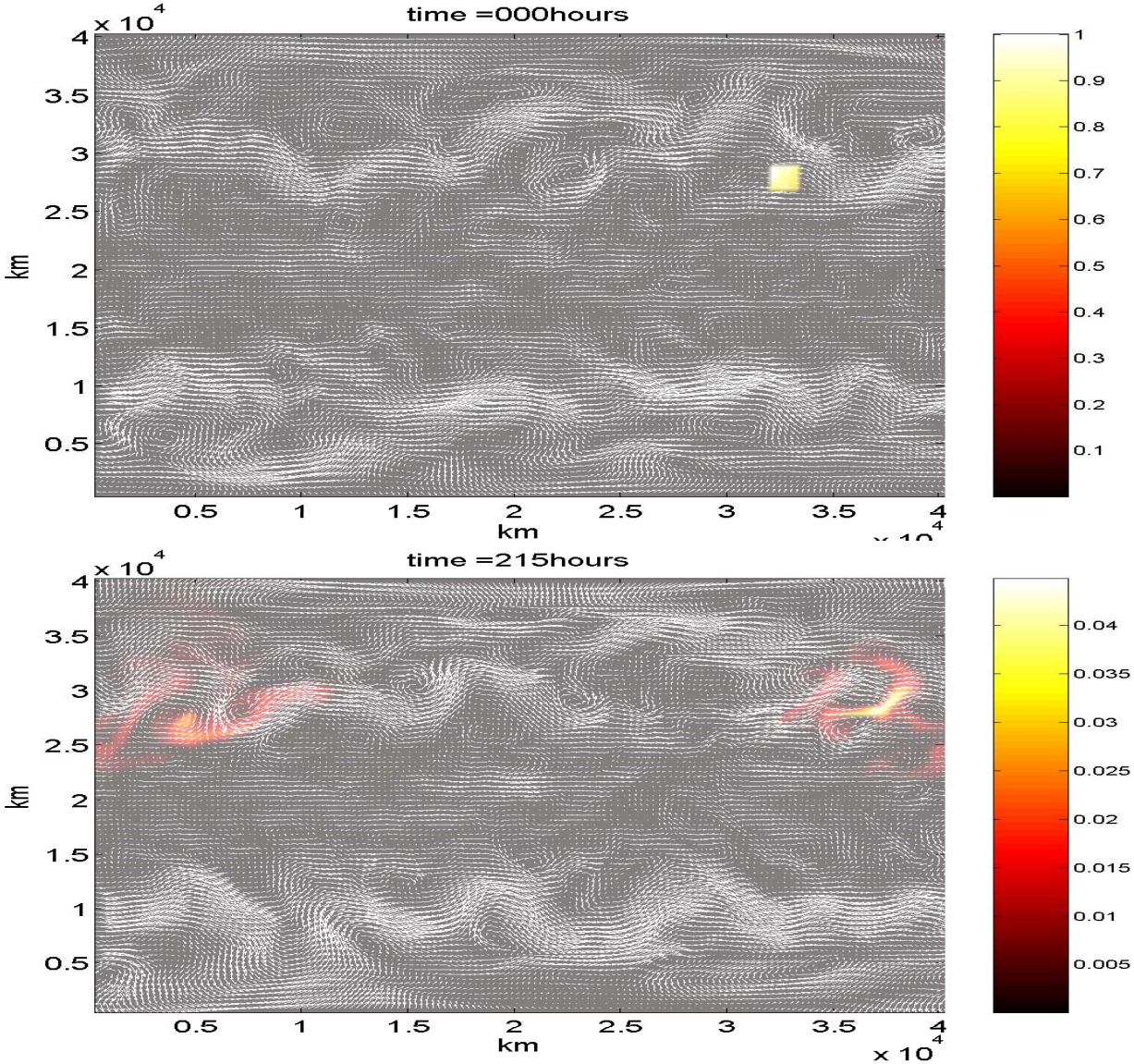
$$\Downarrow$$

$$c = const$$

Along streamlines



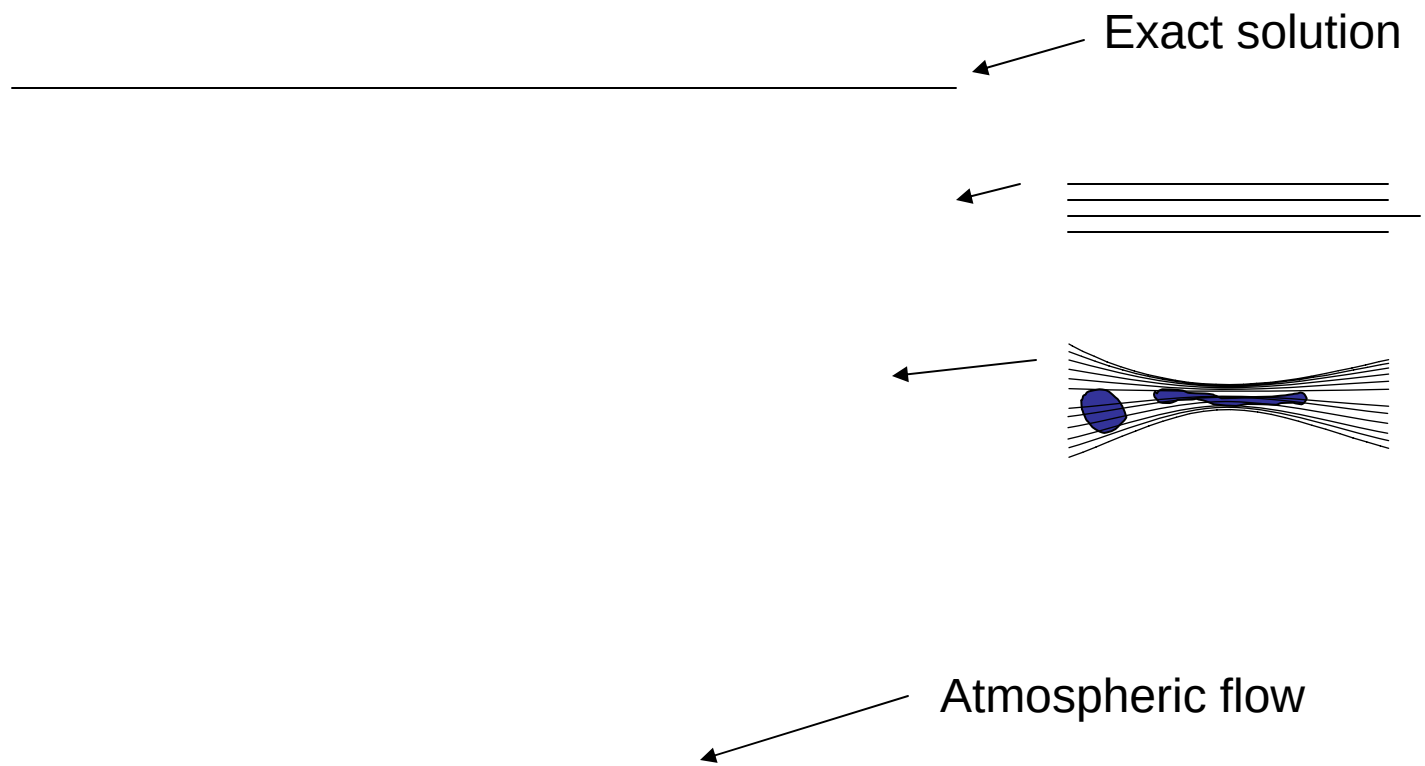
Results of numerical simulation



Why the code failed?

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D_{numer} \Delta c + h.o.t.$$

Numerical diffusion + flow stretching → Strong numerical mixing



Main objective

To create a multi-scale numerical algorithm (Spatial Reduction Method) which provides a significant (at least order of magnitude) reduction in computational cost

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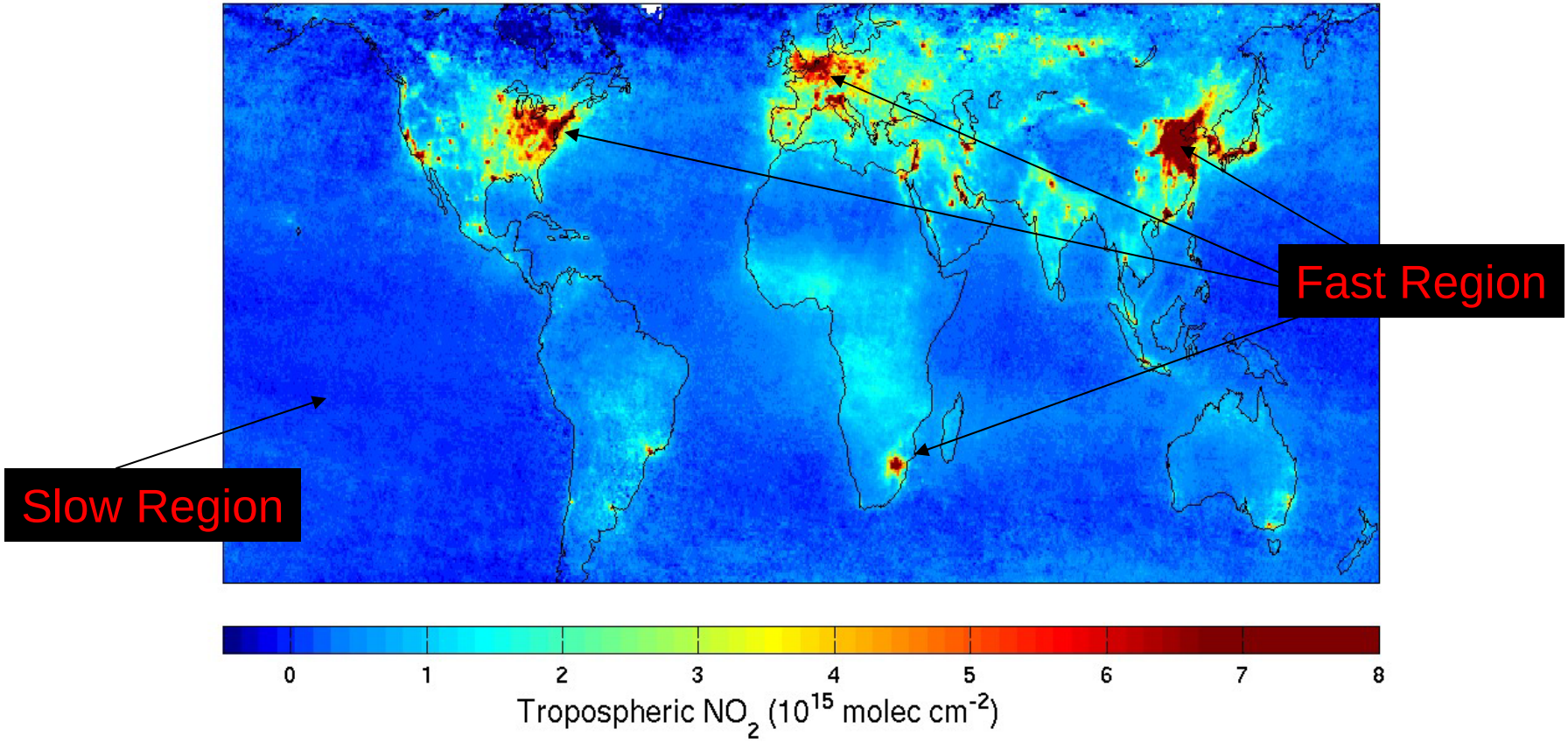
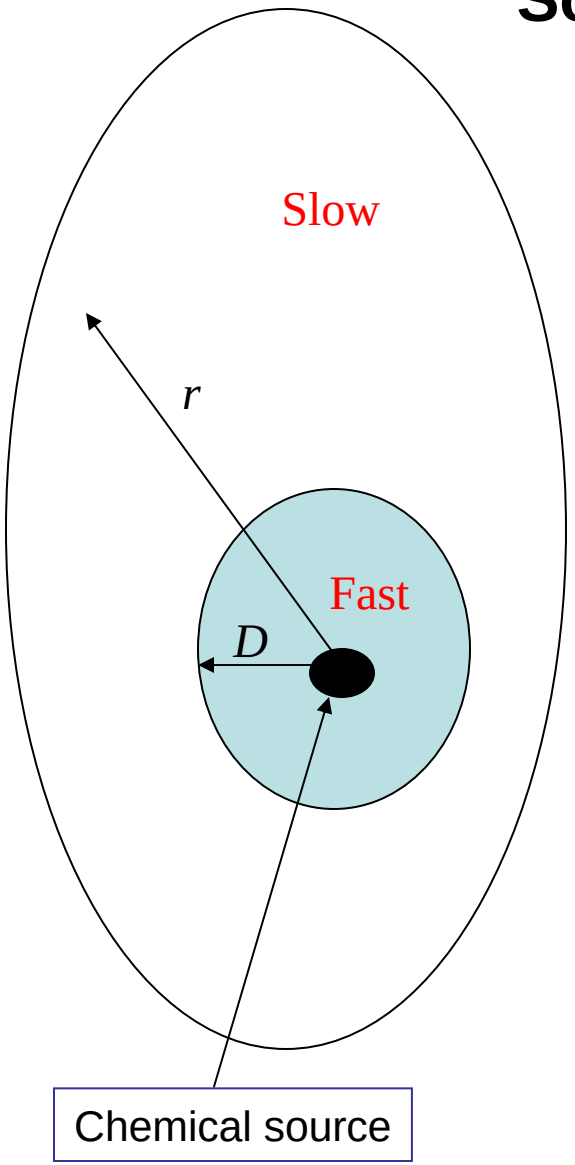
This allows to increase the resolution i.e. accuracy of numerical calculations and/or to speed up computational simulations

Basic Idea: Typical fast reactant density distribution



Our algorithm is inspired by the observation that atmospheric emissions have most of their fast reactants and their quickly decomposing reaction products localized near the emitter (Fast region), typically on the ground. Far from the emitter (Slow region), the fast reactants do not play a significant role.

Solution: Spatial Reduction



$$n \sim \exp(-r/D)$$ ← In the Slow region

$D \sim \sqrt{\kappa \tau_r}$ or $D \sim u \tau_r$

Fast Region – the species is fully accounted as a dependent variable in the system of transport equations
Slow Region – the species concentration n is found through extrapolation

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For the algorithm to be efficient:

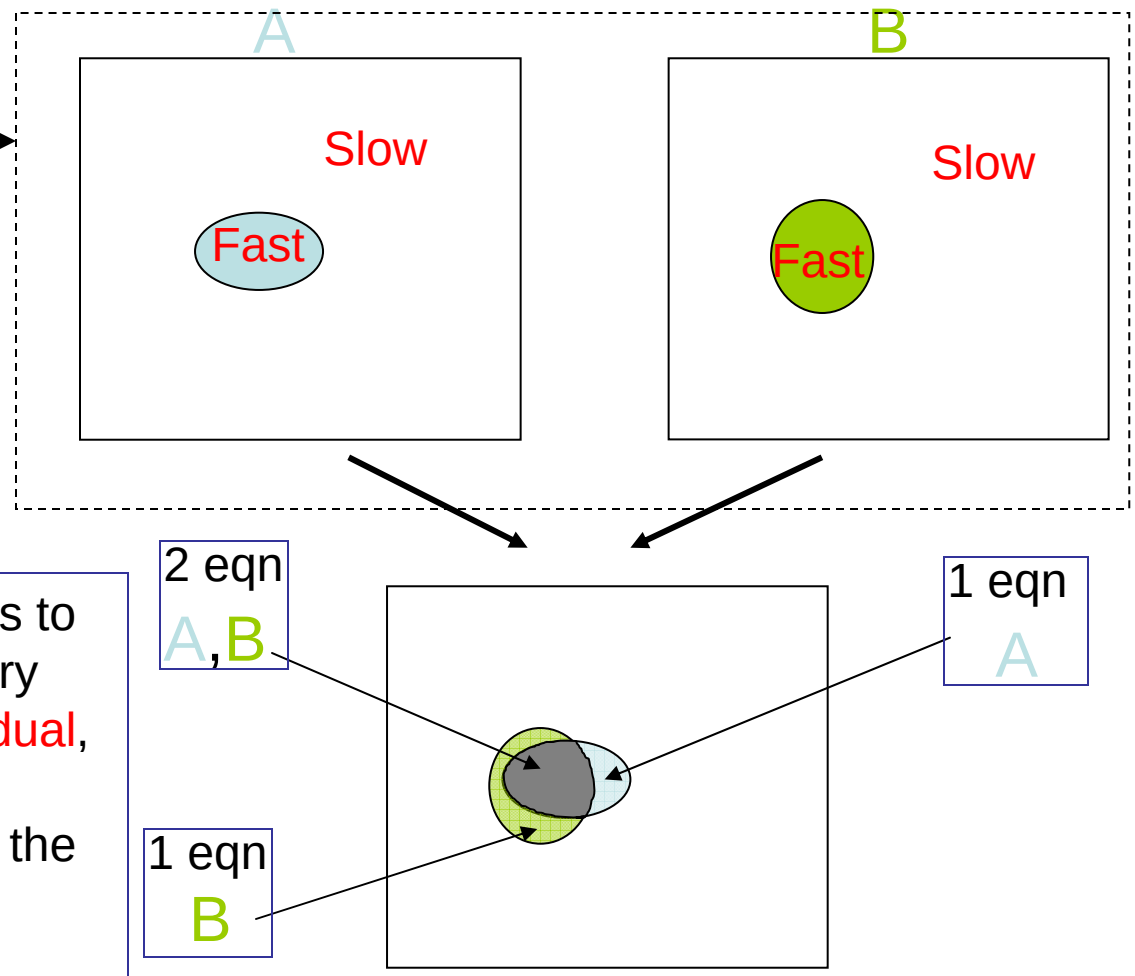
size Slow Region >> size Fast Region

comp. cost Slow Region << comp. cost Fast Region

<u>Gradual</u> Spatial Reduction

Consider a two species reaction system, comprised of chemicals *A* and *B*

Domain partitioning for A and B

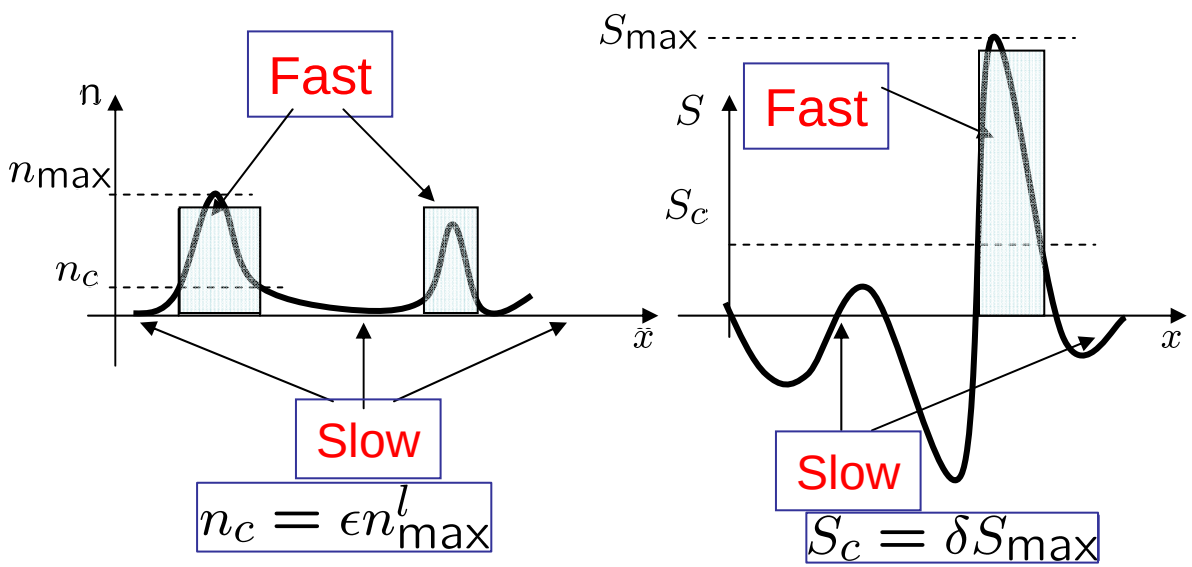


The central idea of our algorithm is to track a series of chemical boundary layers (CBL) within which the gradual, continuous spatial reduction is employed from the domain where the full mechanism is needed to the domain where the most simplified mechanism is sufficient.

Prerequisites for Spatial Reduction Numerical Method

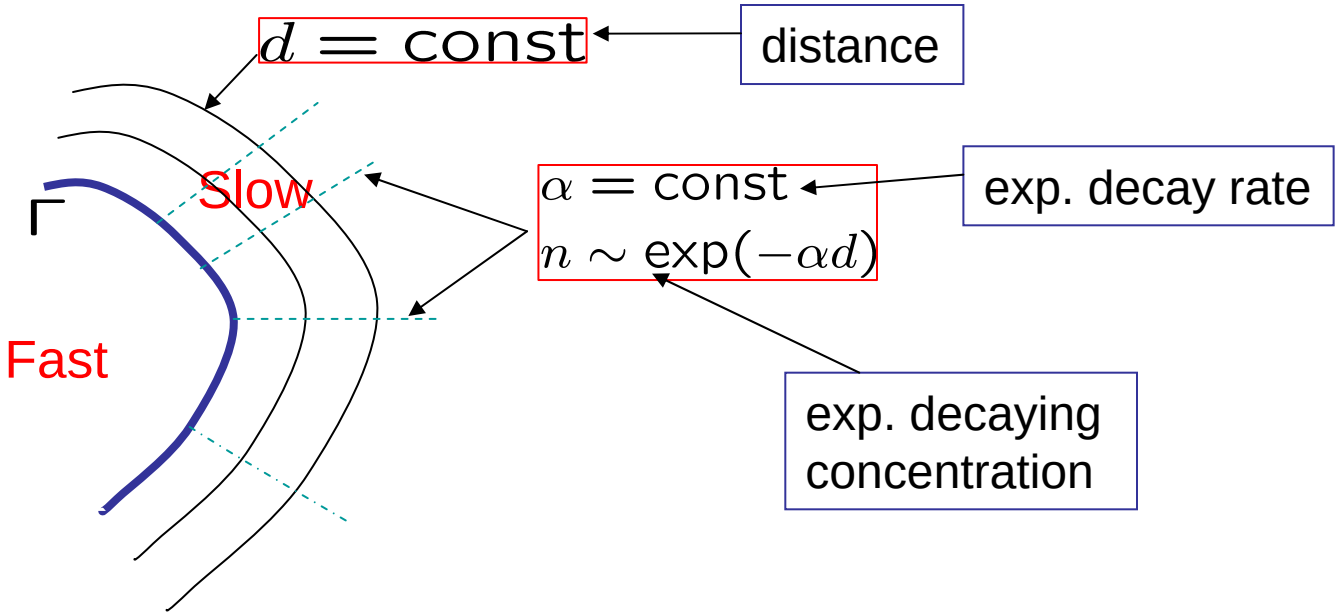
- Fast-Slow domain partitioning algorithm
- Algorithms for Reduced Model construction
- Matching procedure
- Efficient methodology for adaptation in time

Domain partitioning



Fast if $n > n_c \quad or \quad S > S_c$ Slow otherwise

Reduced model – exponential extrapolation into Slow region



Matching conditions

$$n_i^F = n_i^S$$
$$\nabla n_i^F = \nabla n_i^S$$

matching procedure for concentration values and mass fluxes ensures good mass conservation and continuity properties of the numerical scheme

<u>Adaptive</u> algorithm summary

1. Construct slow-fast domain partitioning for every species individually based on the current species density and source distributions;
2. Advance governing equations to obtain the solution at the next time steps inside the fast domains using the solution from the previous time steps initial condition;
3. Construct the species concentration in the slow domains through the exponential extrapolation;
4. Go back to step 1.

Computational Savings

Assume the chemical sheme contains N reacting species with N_s slow-reacting species, that the volume of the computational domain is V and that of the fast reacting domain is V_f.

Assume a constant mesh spacing, the computational cost of calculations with spatial reduction algorithm

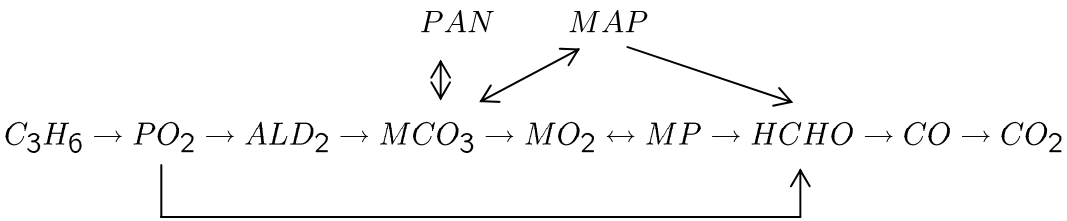
$$\boxed{\phi = V_\mathsf{f}/V + \left(\frac{N_\mathsf{s}}{N}\right)^2 (1 - V_\mathsf{f}/V)}$$

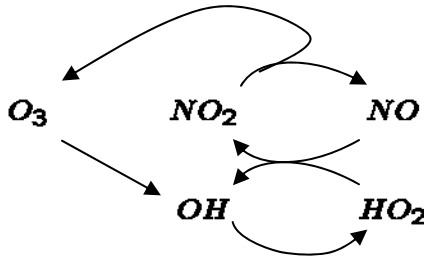
For GEOS-Chem mechanism $V_\mathsf{f}/V \sim 0.1$ and $N_\mathsf{s}/N \sim 0.1$, thus $\phi \sim 0.1$

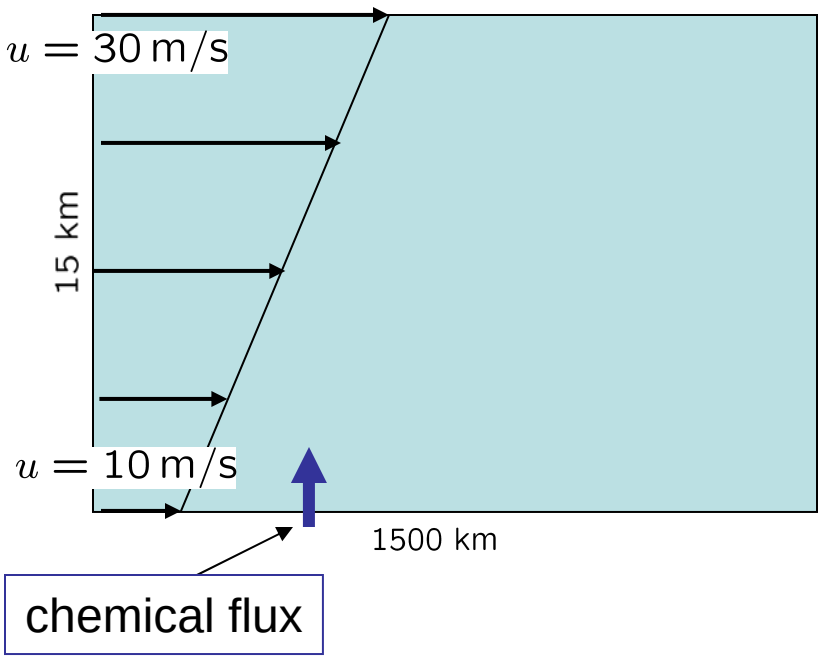
Chemical model

oxidation of a number of *C3H6* in an *OH* oxidizing atmosphere, with *NOx* serving as catalyst through the cycling of *HOx* radicals

15 chemical species and 24 reactions







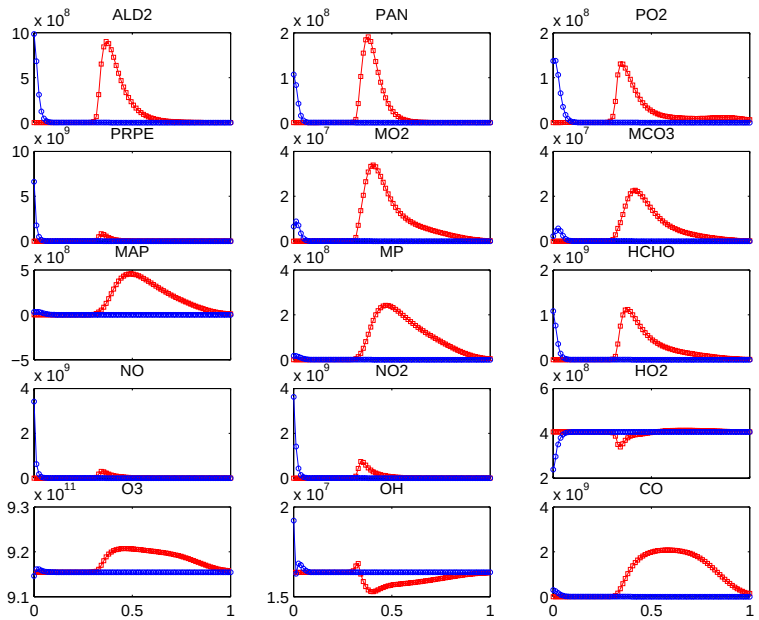
$P = \text{atm},\ T = 298\text{K}$

$\kappa = 3 \times 10^5\,\text{cm}^2/\text{s}$

$n_{\text{init}}(\text{O}_3) = 10^{12}\,\text{molecules/cm}^3$

$J(\text{C}_3\text{H}_6) = 10^{11}\,\text{molecules/s cm}^2$

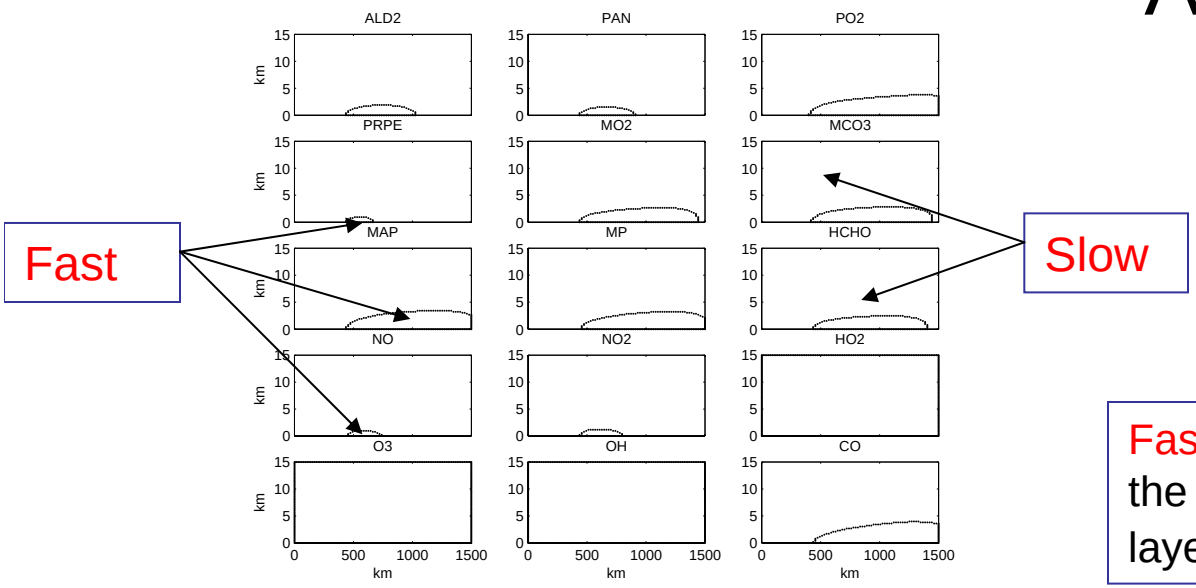
$J(\text{NO}) = 10^{11}\,\text{molecules/s cm}^2$



Comparison of species distribution obtained by the spatial reduction algorithm (spheres and cubes) and conventional method (solid line) depicted in blue and red colors at $x = 750$ km and at $y = 0.5625$ km correspondingly at time $t = 4 \times 10^4$ sec

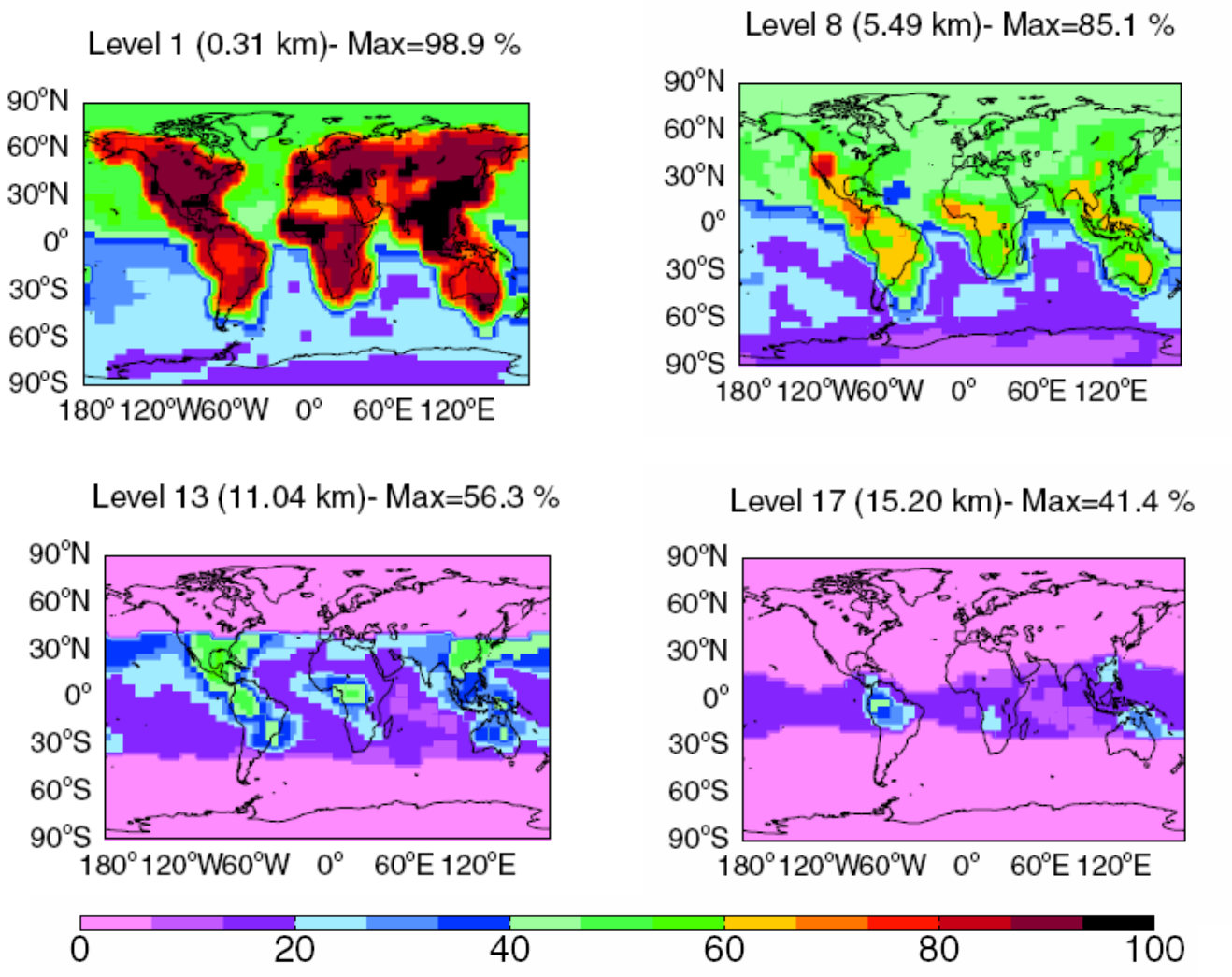
Max err = 2-3 %

Average err = 0.5 %



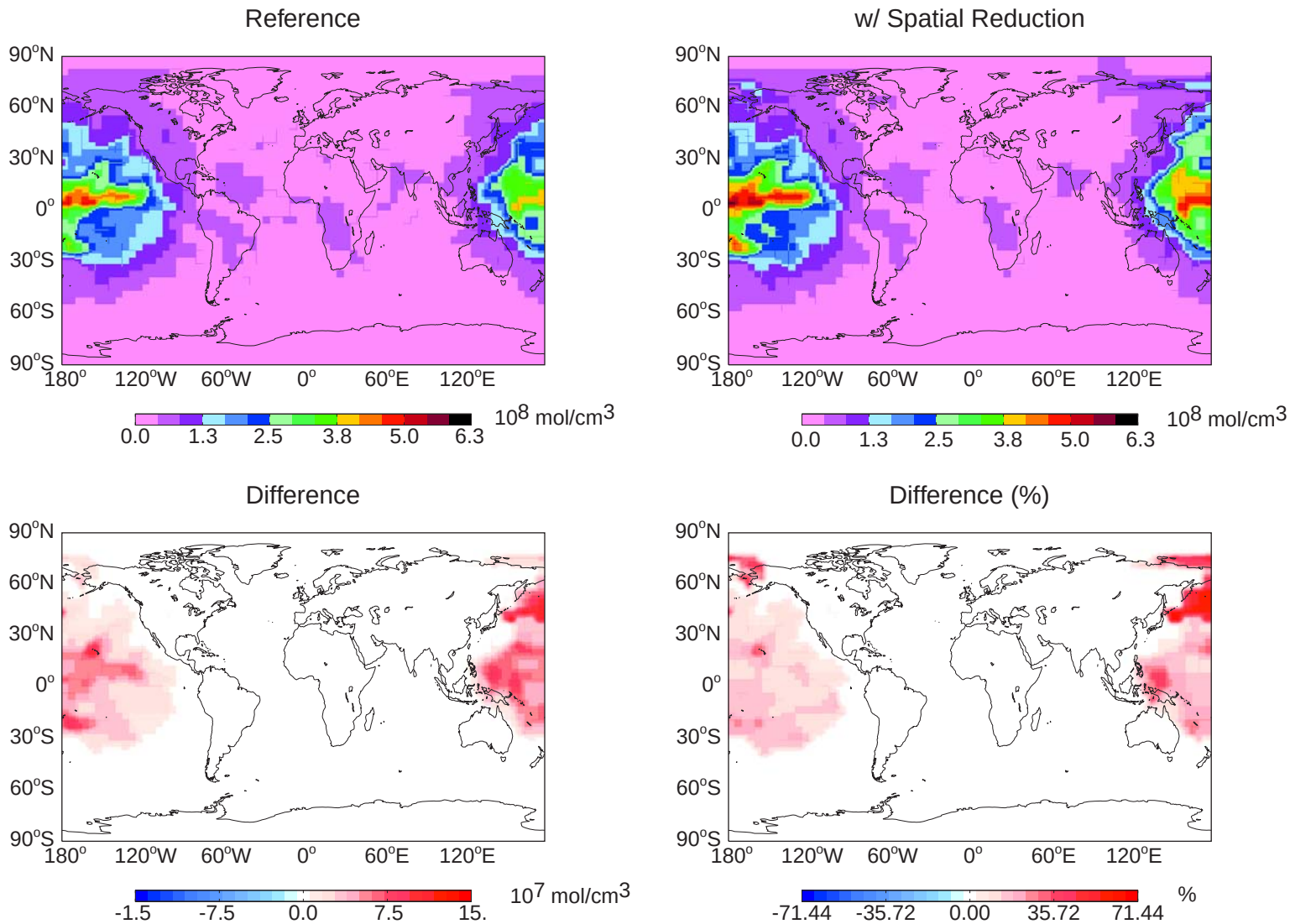
Fast – Slow domain partitioning for the atmosphere with horizontal shear layer flow at time

Three-dimensional calculations



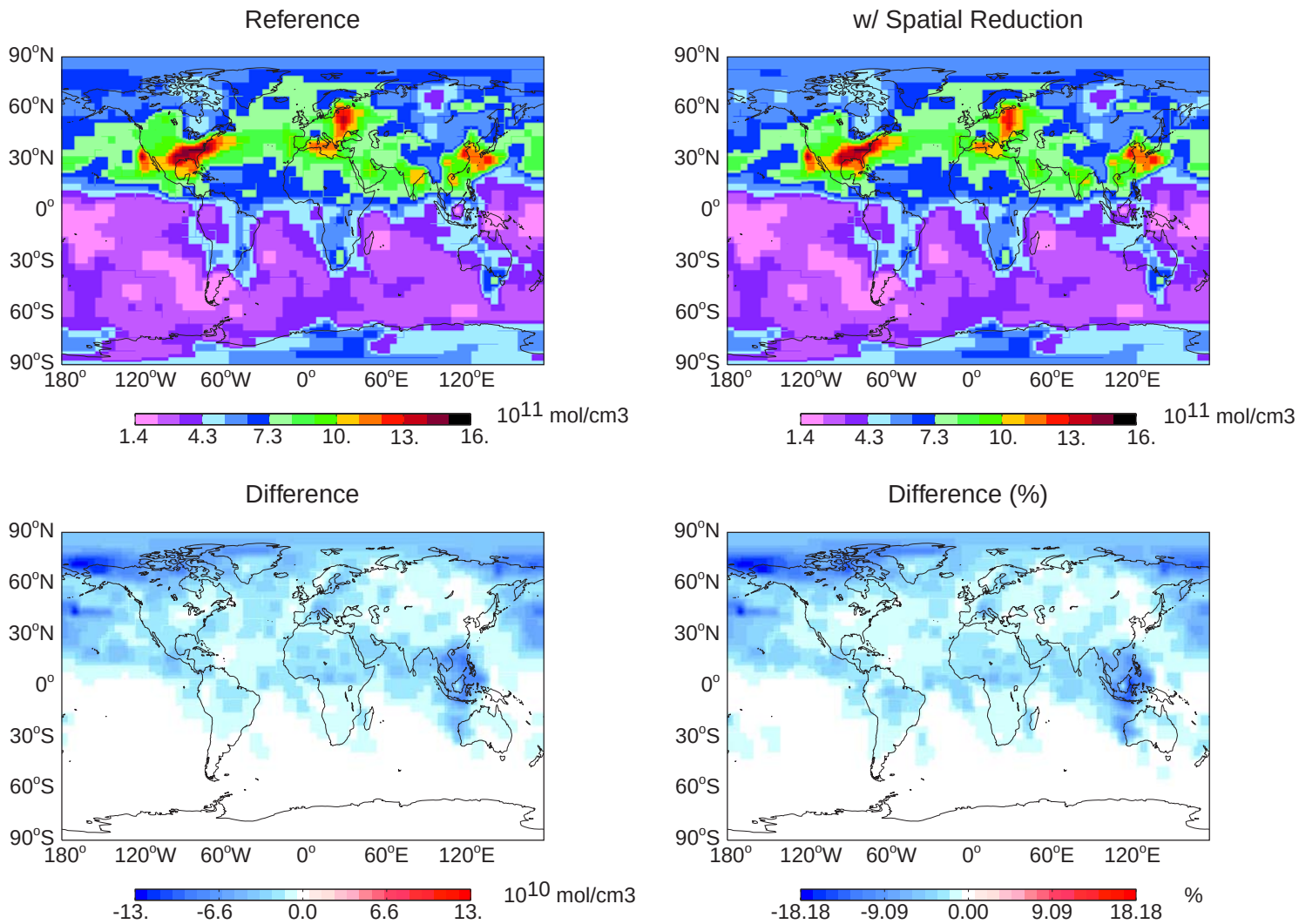
Number of equations integrated

MO2 - Level 6 (3.16 km) - RMS = 20.00 %



Short lived species : Max error close to the boundary separating Fast and Slow regions

O_3 - Level 1 (0.31 km) - RMS = 3.60 %



Short lived species : Max error close to the boundary separating Fast and Slow regions

Work in the progress …

1)Reduced model – exponential extrapolation implementation into the GEOS-Chem

- Substantially reduce the error in the slow region
- Noticeably reduce the size of the fast region

(currently average error ~ 7%)

2) Efficient implementation of sparse structure and related algorithms

- Substantial speed up

3) More efficient Fast-Slow domain partitioning criteria

- Discriminatory (selective) criteria
- Combined relative-absolute criteria

Some conclusions

- A *gradual continuous* spatial reduction computational method for Atmospheric chemistry has been developed.
- Unlike conventional time-scale separation methods, the spatial reduction algorithm allows to speed up not only a "chemical solver" but also advection-diffusion numerical integration.
- The method produced accurate results at an order of magnitude lower computational cost for the Atmospheric chemistry problems tested.
- Currently we are working on the algorithm implementation into GEOS-Chem three-dimensional solver.
- The algorithm could be utilized for numerical simulation of other multi-scale complex problems with isolated chemical reaction sources (stratosphere – troposphere chemical mechanisms matching, flames, detonation waves, thin reactive sheets, etc.)