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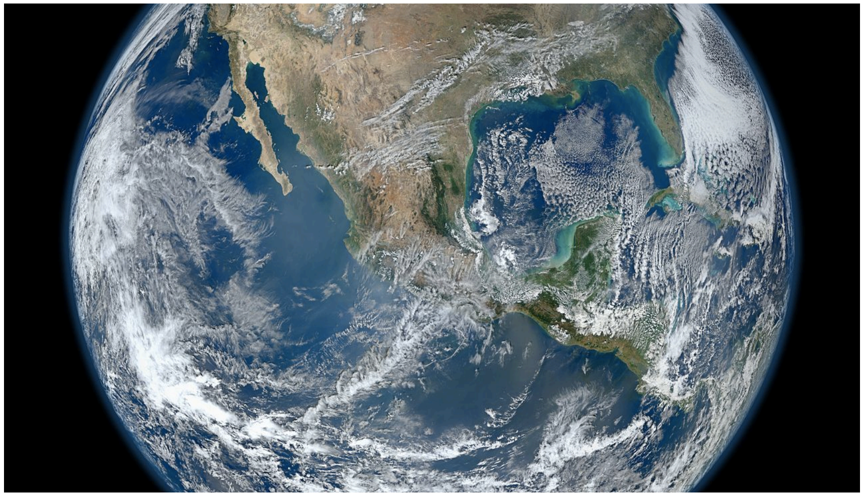
Desired Properties of Transport Schemes for Coupled Atmospheric-Chemistry Models



Peter Hjort Lauritzen

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Meteorology And Climate Modeling for Air Quality (MAC-MAQ)
Sacramento, September 16-18, 2015

Desired Properties of Transport Schemes for Coupled Atmospheric-Chemistry Models

AMP develops and maintains NCAR's global **Community Atmosphere Model (CAM)** which is a component of NCAR's Community Earth System Model (CESM)

I specialize in the resolved-scale fluid flow solver (a.k.a. the dynamical core) and its coupling to physics (sub-grid-scale parameterizations)

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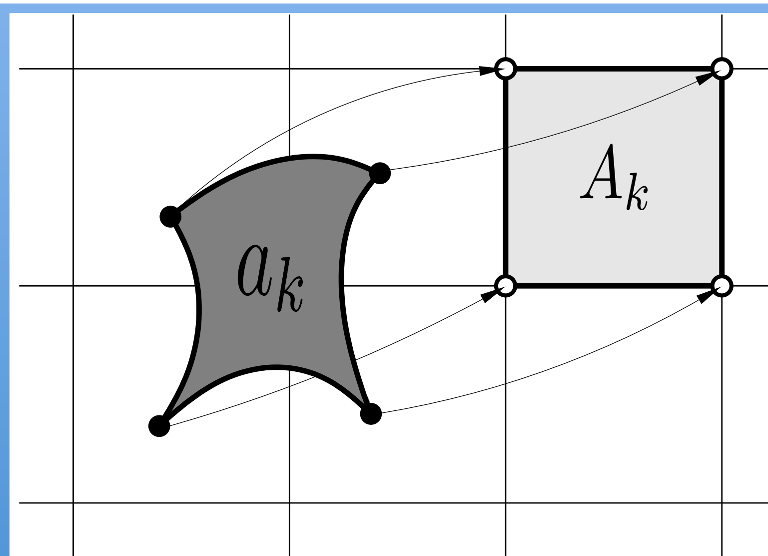
Desired Properties of Transport Schemes for Cou

A

Consider the finite-volume Lagrangian form of continuity equation for air (pressure level thickness, Δp), and tracer (mixing ratio, q):

$$\int_{A_k} \psi_k^{n+1}\, dA = \int_{a_k} \psi_k^{n}\, dA, \qquad \psi = \Delta p,\, \Delta p\, q, \tag{1}$$

where n time-level.



No sources/ sinks

Overall, tracer transport needs to be:

A. Efficient (on massively parallel computers):

Most atmospheric models solve at least a handful of continuity equations and, in most cases, many more:

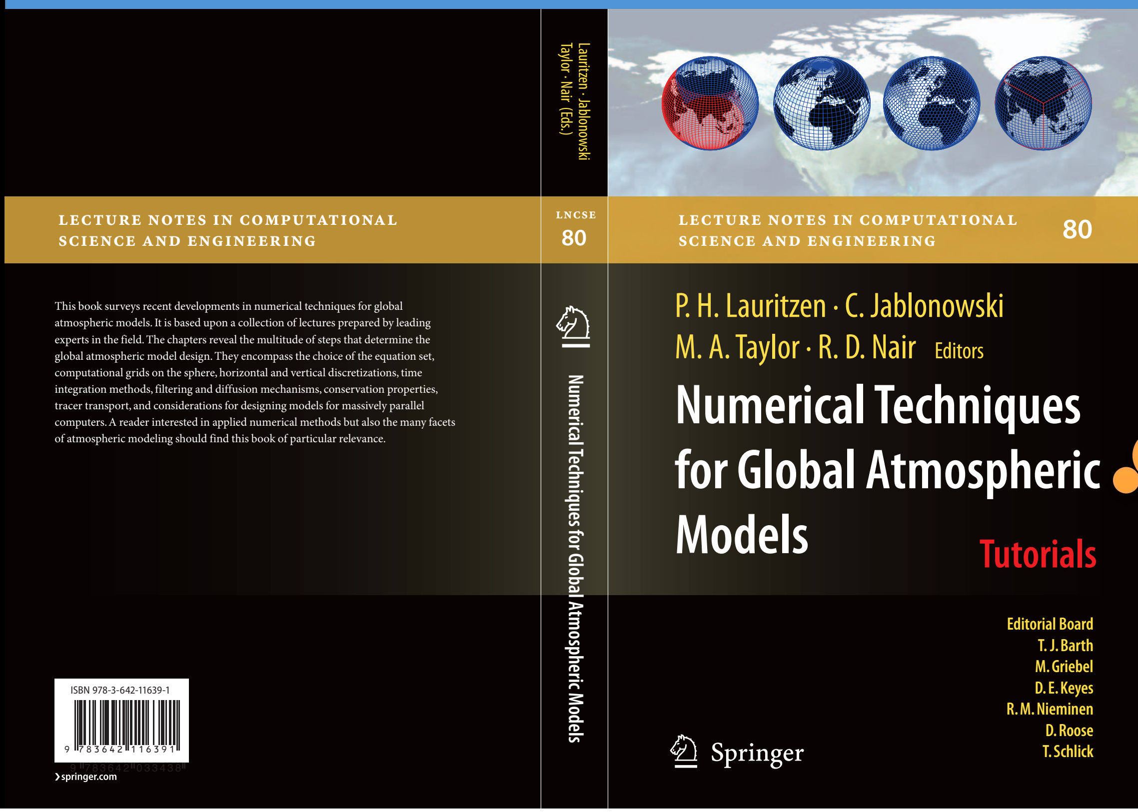
- Air (either dry or moist)
- Water species: water vapor, cloud liquid water and cloud ice water.
(rain, snow, hail, graupel, ...)
- Microphysics: aerosol mass and number concentration.
- Chemistry: 100+ tracers in chemistry version of CAM. E.g. ozone, chlorine compounds, bromine, ... (some highly reactive; some long lived)

Tracer transport is the most computationally costly part of a dynamical core!

Overall, tracer transport needs to be:

B. Accurate:

Accuracy requirements in the context climate/chemistry-climate applications are much more stringent than conventional root-mean-square error convergence for smooth problems …



See, e.g., Springer book for more detailed discussion

Requirements (desirable properties) for transport schemes intended for global climate/climate-chemistry applications:

1. Global (and local) Mass-conservation

If Δp is pressure-level thickness and q is mixing ratio, then the total mass

$$M(t) = \int_{\Omega} \Delta p \, q \, dA,$$

is invariant in time: $M(t) = M(t = 0)$ (no sources/sinks)

2. Shape-preservation

Scheme does not produce new extrema (in particular negatives) in q

3. Preservation of pre-existing functional relations between tracers

Transport scheme preserves $q_2 = f(q_1)$ (no sources/sinks)

4. Consistency

The continuity equations for air and tracers are coupled:

$$\int_{A_k} \Delta p_k^{n+1} \, dA = \int_{a_k} \delta p_k^n \, dA, \quad (2)$$

$$\int_{A_k} (\Delta p \, q)_k^{n+1} \, dA = \int_{a_k} (\delta p_k q)^n \, dA. \quad (3)$$

If $q = 1$ then (3) should reduce to (2).

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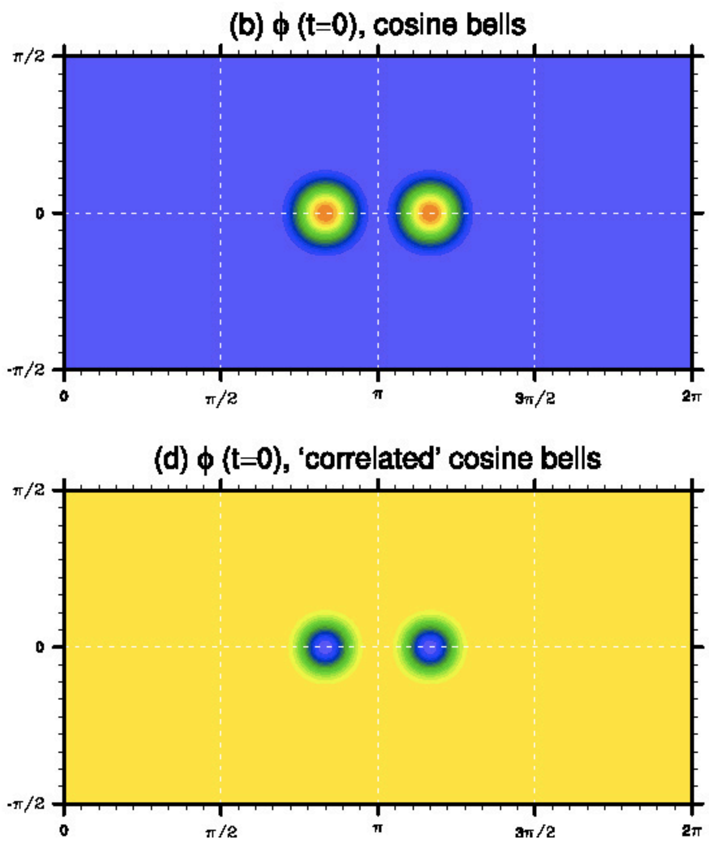
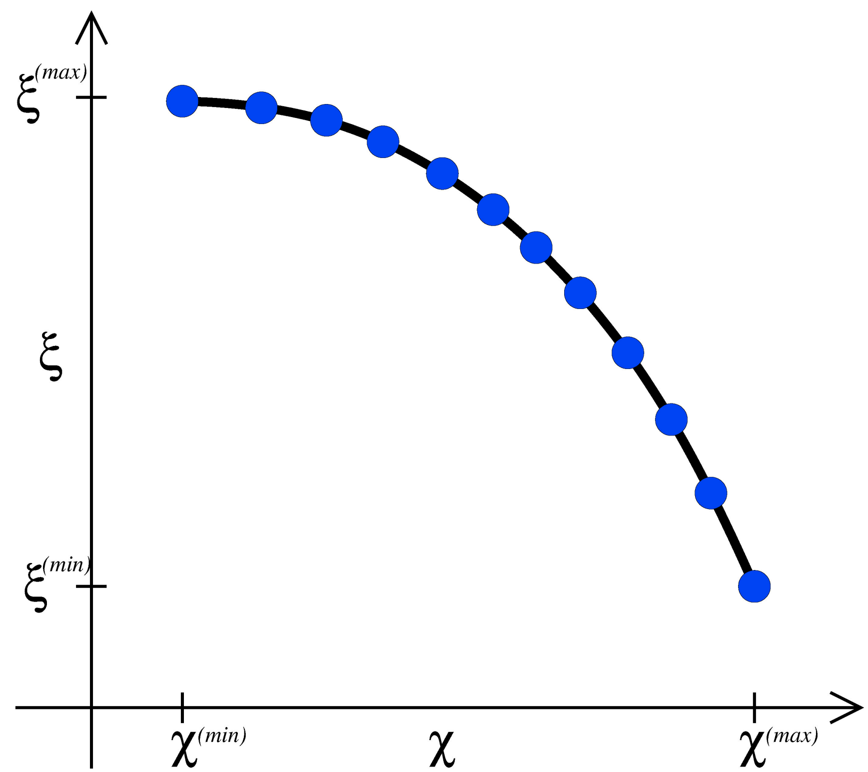
Preserving pre-existing functional relation between tracers under challenging flow conditions

Initial conditions

tracer 1: cosine bells   tracer 2: correlated cosine bells $\Psi(\chi)=a\chi^2+b$





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Lauritzen and Thuburn (2011,QRJMS)

Preserving pre-existing functional relation between tracers under challenging flow conditions

Initial conditions
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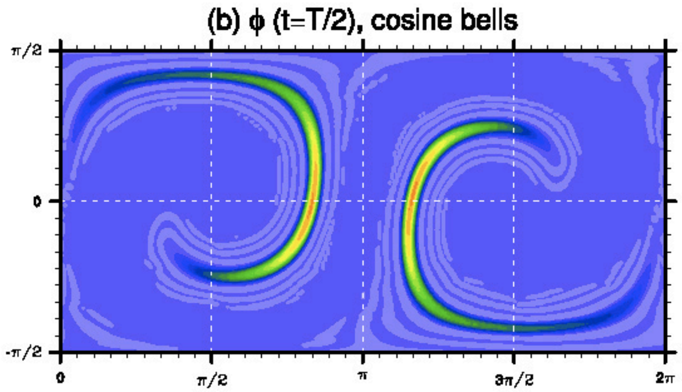

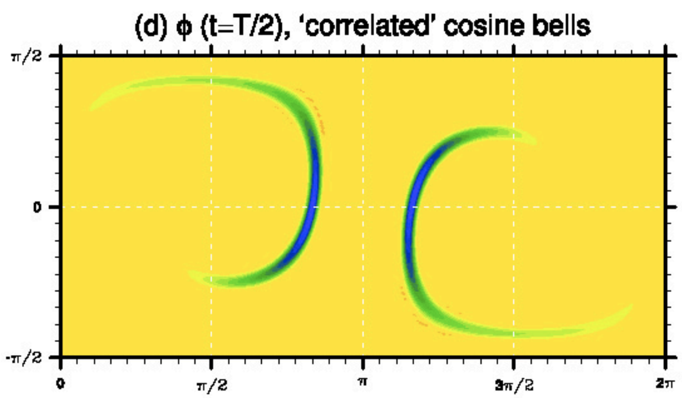

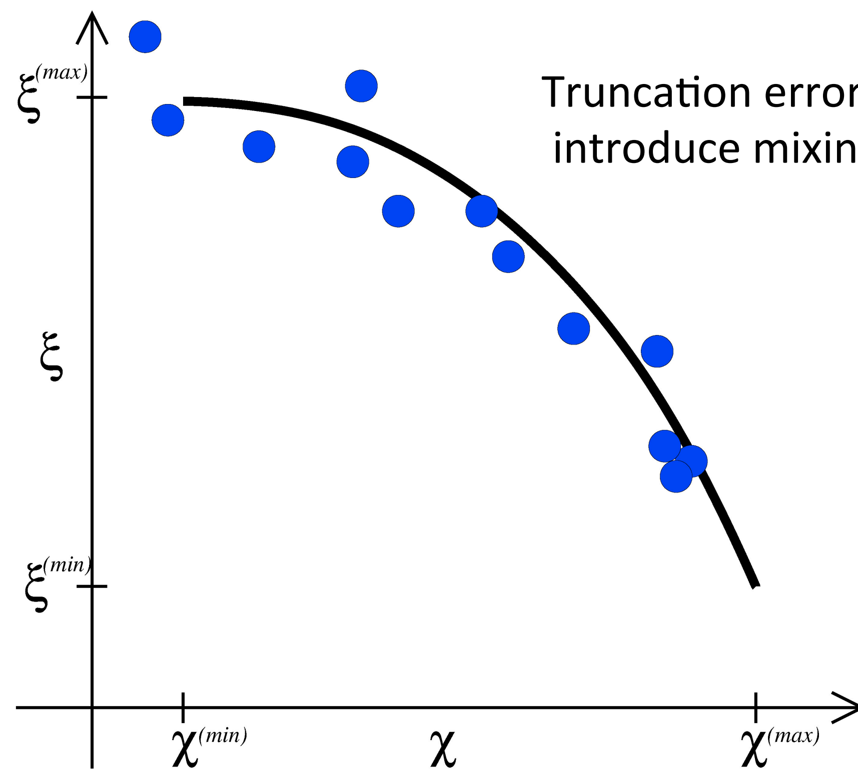

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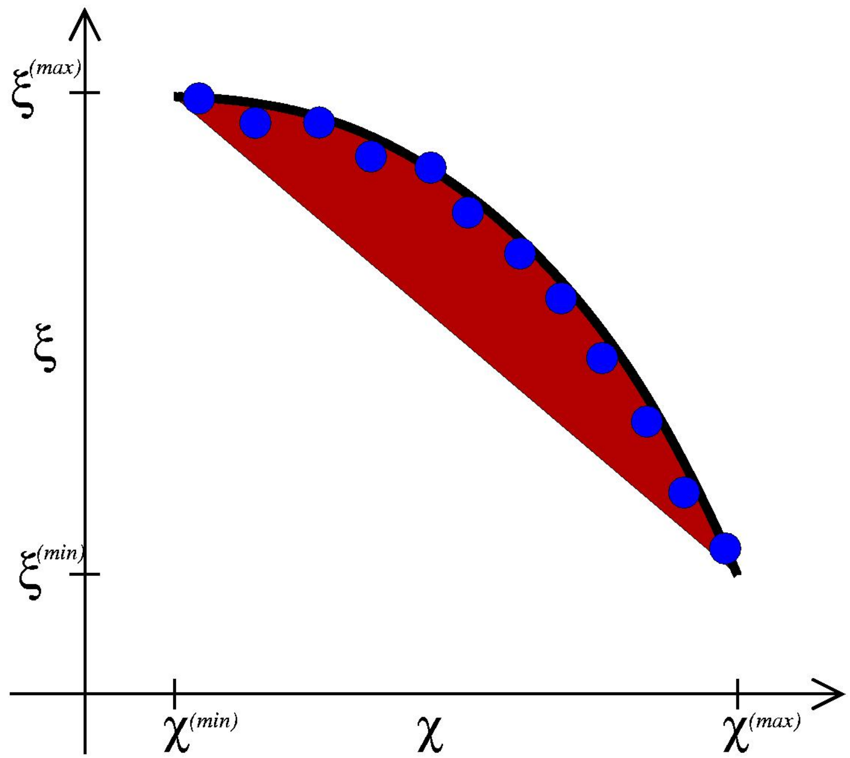
Classification of mixing on scatter plot:

a. Mixing that resembles `real' mixing – convex hull (red area)
b. Everything else is spurious unmixing



Thuburn and McIntyre (1997,JGR)

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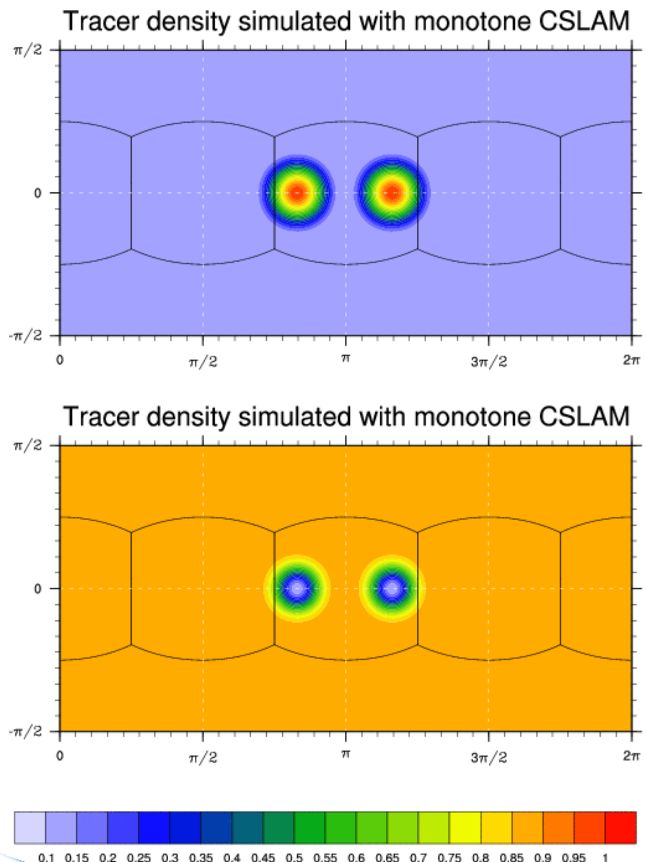
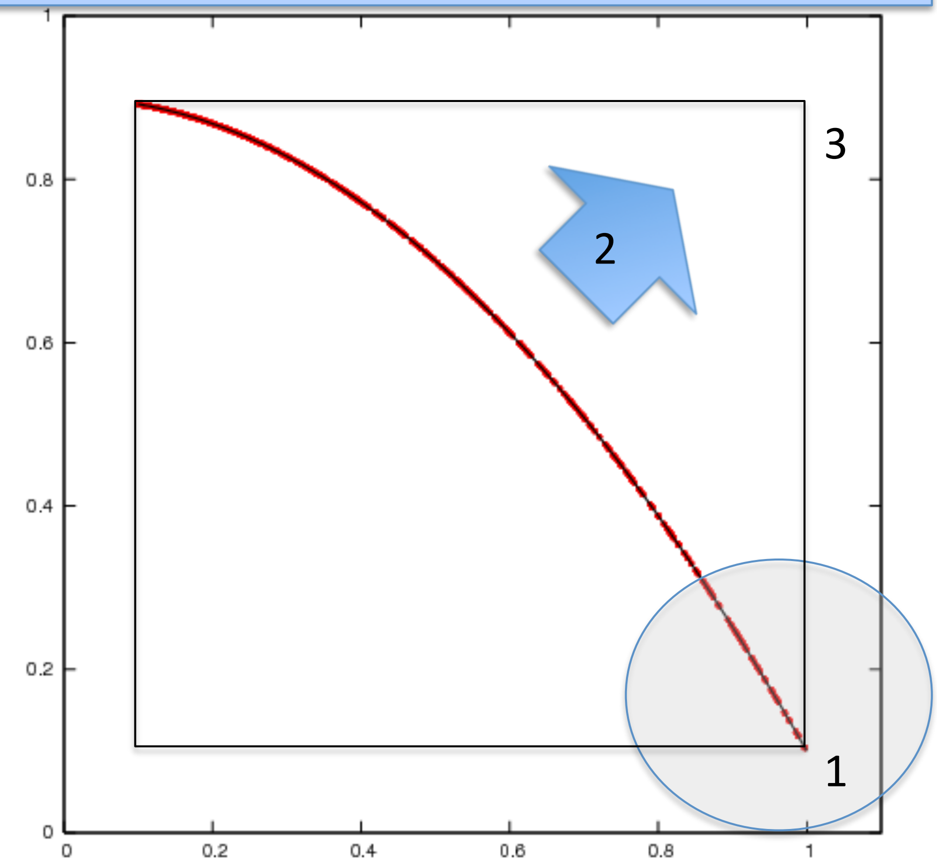
Preserving pre-existing functional relation between tracers under challenging flow conditions

Note: 1. Max value decrease, 2. Unmixing even if scheme is shape-preserving, 3. No expanding range unmixing





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A standard test case suite for two-dimensional linear transport on the sphere

P. H. Lauritzen[1], W. C. Skamarock[1], M. J. Prather[2], and M. A. Taylor[3]

[1]National Center for Atmospheric Research, Boulder, Colorado, USA
[2]Earth System Science Department, University of California, Irvine, California, USA
[3]Sandia National Laboratories, Albuquerque, New Mexico, USA

http://www.geosci-model-dev.net/5/887/2012/gmd-5-887-2012.pdf

A standard test case suite for two-dimensional linear transport on the sphere: results from a collection of state-of-the-art schemes

P. H. Lauritzen[1], P. A. Ullrich[11], C. Jablonowski[2], P. A. Bosler[2], D. Calhoun[3], A. J. Conley[1], T. Enomoto[4], L. Dong[5], S. Dubey[6], O. Guba[7], A. B. Hansen[14], E. Kaas[8], J. Kent[2], J.-F. Lamarque[1], M. J. Prather[9], D. Reinert[10], V. V. Shashkin[12,13], W. C. Skamarock[1], B. Sørensen[9], M. A. Taylor[7], and M. A. Tolstykh[12,13]

http://www.geosci-model-dev.net/7/105/2014/gmd-7-105-2014.html

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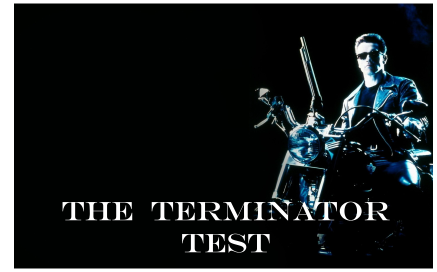
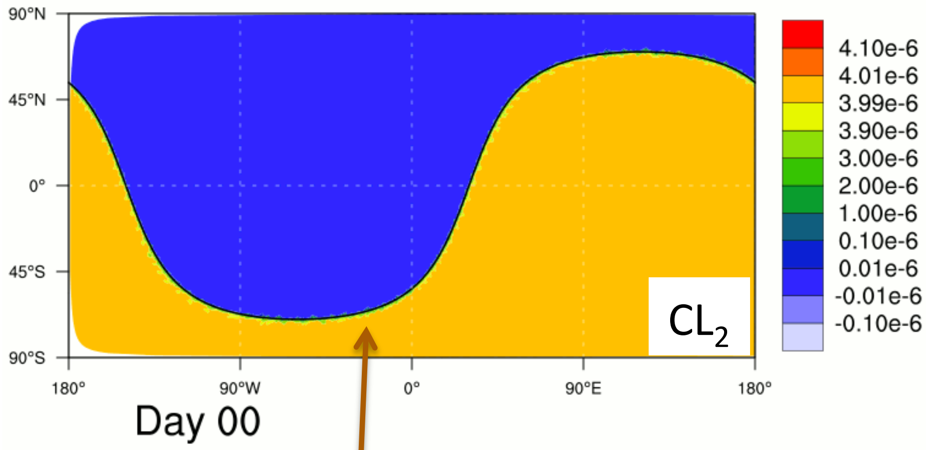
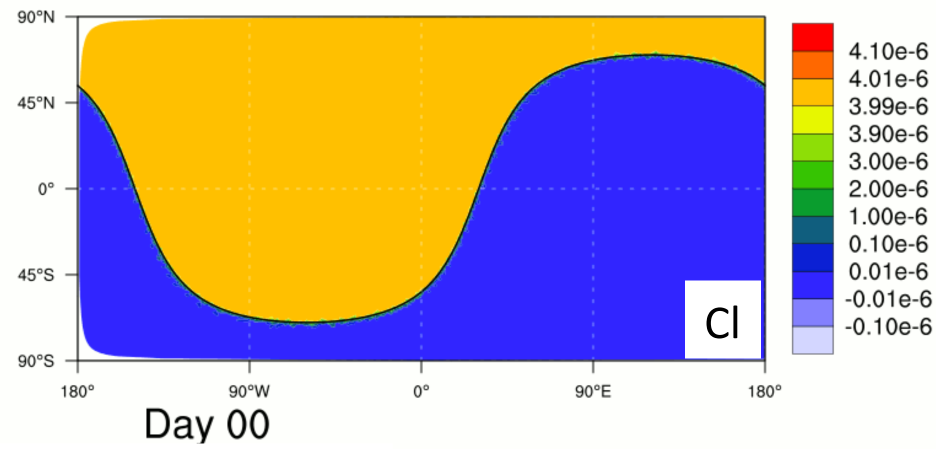
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015, GMD)

See: http://www.cgd.ucar.edu/cms/pel/terminator.html







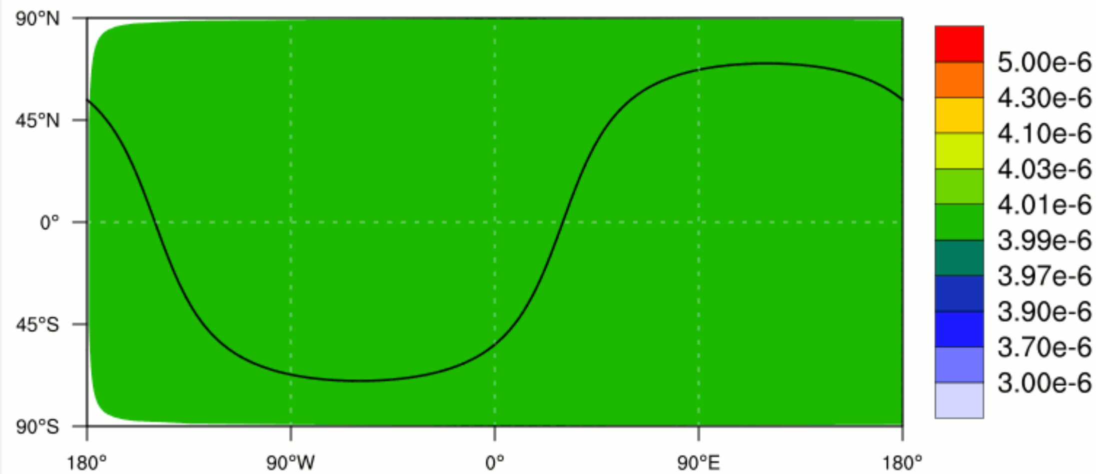
Non-linear Terminator 'toy' chemistry:

$$Cl_2 \rightarrow Cl + Cl : k_1$$

$$Cl + Cl \rightarrow Cl_2 : k_2$$

Exact solution: $Cl+2*Cl_2$ = constant

$Cl+2*Cl_2$ = constant



Wind field: Nair and Lauritzen deformational flow

Errors are due to non-conservation of linear correlations usually caused by the limiter/filter and/or physics-dynamics coupling!

Requirements (desirable properties) for transport schemes intended for global climate/climate-chemistry applications:

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If Δp is pressure-level thickness and q is mixing ratio, then the total mass

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The continuity equations for air and tracers are coupled:

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If $q = 1$ then (3) should reduce to (2).

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Requirements (desirable properties) for transport schemes intended for gl…

Consistency is trivial if (2) and (3) are solved with the same numerical method, however, that is not always the case:

- "Off-line" chemistry: prescribed wind and mass fields from , e.g., re-analysis.
- "Online" applications where (3) is solved with a different numerical method than (2)

3. Preser… functional relations between tracers

Transpor… preserves $q_2 = f(q_1)$ (no sources/sinks)

4. Consistency

The continuity equations for air and tracers are coupled:

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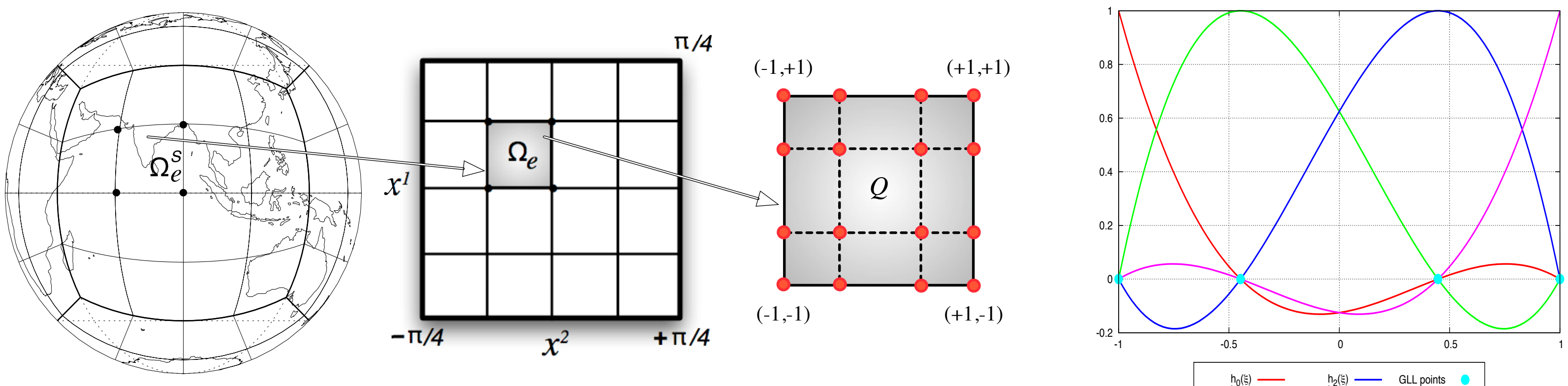
CAM-SE: NCAR Community Atmosphere Model with Spectral Elements dynamical core

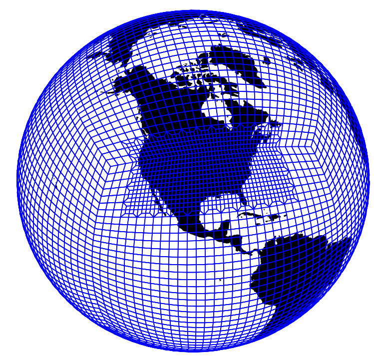
Continuous Galerkin finite-element method (Taylor et al., 1997) on a cubed-sphere:

Nair et al., 2011



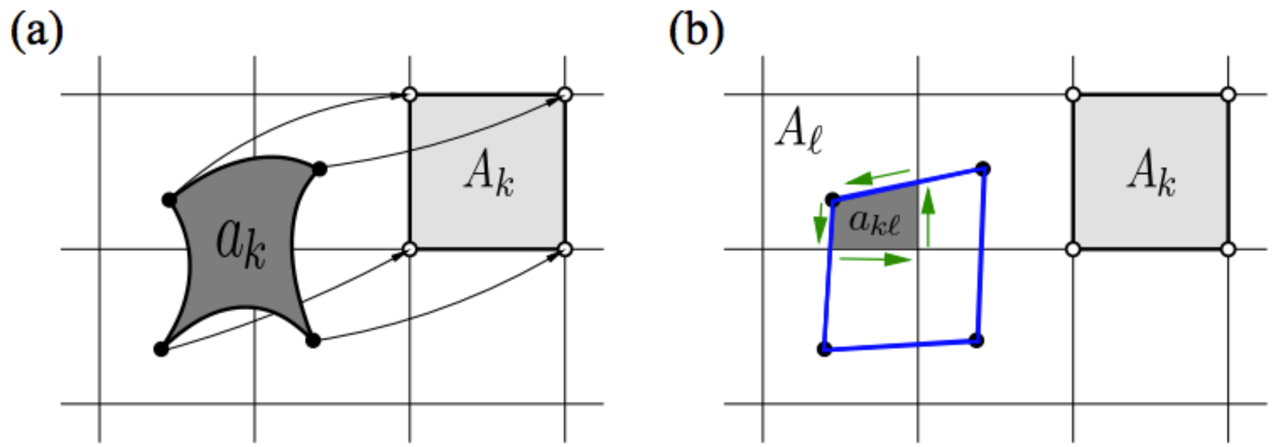
Physical Domain | Computational Domain | GLL Quadrature Grid

- Discretization is mimetic => mass-conservation & total energy conservation
- Conserves axial angular momentum very well (Lauritzen et al., 2014)
- Support static mesh-refinement and retains formal order of accuracy!
- Highly scalable to at least O(100K) processors (Dennis et al., 2012)
- Competitive "AMIP-climate" (Evans et al., 2012)
- **Lower computational throughput for many-tracer applications**



A way to accelerate tracer transport:

CSLaM scheme (Conservative Semi-Lagrangian Multi-tracer)



Finite-volume Lagrangian form of continuity equation for $\psi = \rho, \rho\,\phi$:

$$\int_{A_k} \psi_k^{n+1}\, dx\, dy = \int_{a_k} \psi_k^n\, dx\, dy \quad = \quad \sum_{\ell=1}^{L_k} \left[\sum_{i+j\leqslant 2} c_\ell^{(i,j)} w_{k\ell}^{(i,j)} \right],$$

where weights $w_{k\ell}^{(i,j)}$ are functions of the coordinates of the vertices of $a_{k\ell}$.

- $w_{k\ell}^{(i,j)}$ can be re-used for each additional tracer (Dukowicz and Baumgardner, 2000)
- computational cost for each additional tracer is the reconstruction and limiting/filtering.
- CSLAM is stable for long time-steps (CFL>1)

Lauritzen, Nair and Ullrich (*J. Comput. Phys.*, 2010)

Coupling finite-volume semi-Lagrangian transport with spectral element dynamics

4. Consistency

The continuity equations for air and tracers are coupled:

$$\int_{A_k} \Delta p_k^{n+1}\, dA = \int_{a_k} \delta p_k^n\, dA, \quad (2)$$

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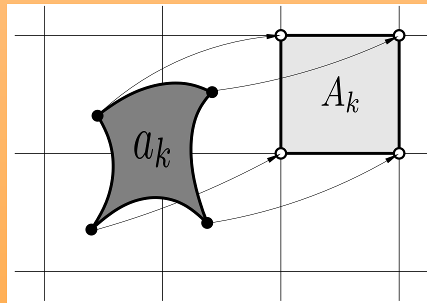
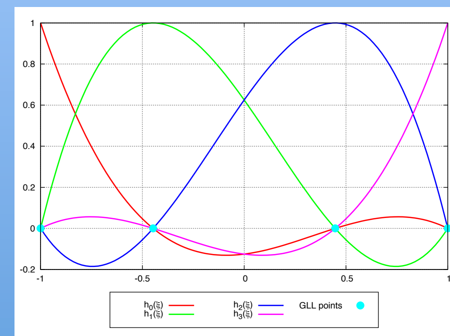
Coupling finite- ... an tra ... leme

Solved with semi-Lagrangian scheme (CSLAM)
(max Courant number < 1)



Solved with spectral-element Eulerian advection operator
(max Courant number < 0.3)



The continuity equ ... for air and tracers ... coupled:

$$\int_{A_k} \Delta p_k^{n+1}\, dA = \int_{a_k} \delta p_k^n\, dA, \qquad (2)$$

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If $q = 1$ then (3) should reduce to (2).

We need to couple without violating mass-conservation, shape-preservation, and consistency

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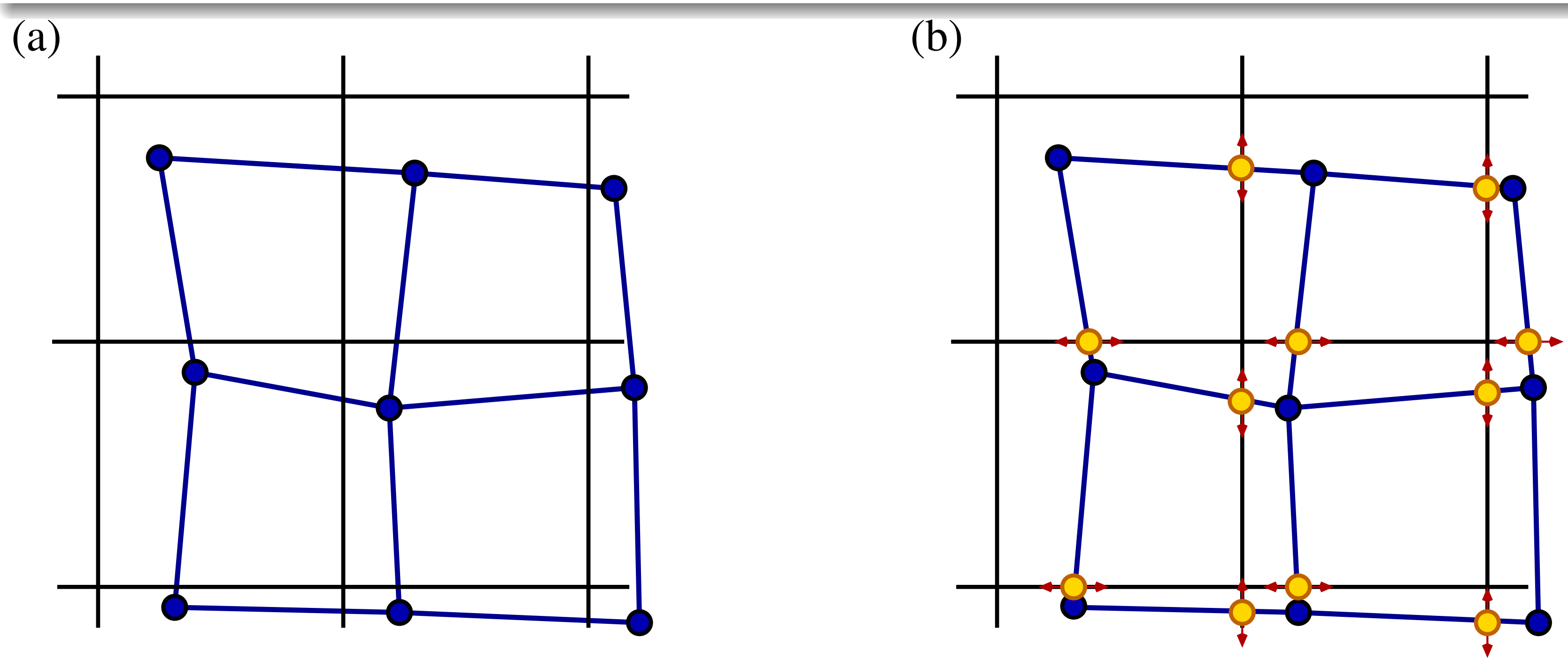
4. Consistency

Find upstream area, a_k, so that CSLAM predicted mass field is equal to CAM-SE predicted mass field:

$$\Delta p_k^{n+1}(\text{CAM-SE}) = \frac{1}{\Delta A}\int_{a_k} \delta p_k^n \, dA \; (\text{CSLAM}) \; ,. \qquad (4)$$

Many details of algorithm (well-posedness, ...) are left out here ...



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Lauritzen, Taylor, Overfelt, Ullrich and Goldhaber (2015, IN PREP)

CAM-SE-CSLAM

A new model configuration based on CAM-SE:

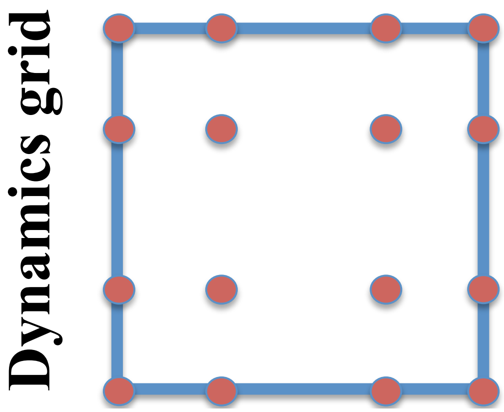
- **SE**: Spectral-element dynamical core solving for $\vec{v}$, T, p_s

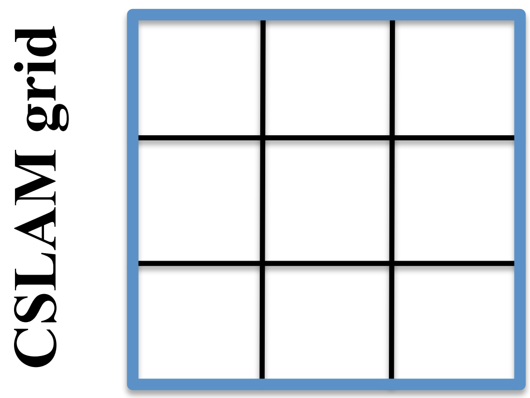
  (Dennis et al., 2012; Evans et al., 2012; Taylor and Fournier, 2010; Taylor et al., 1997)

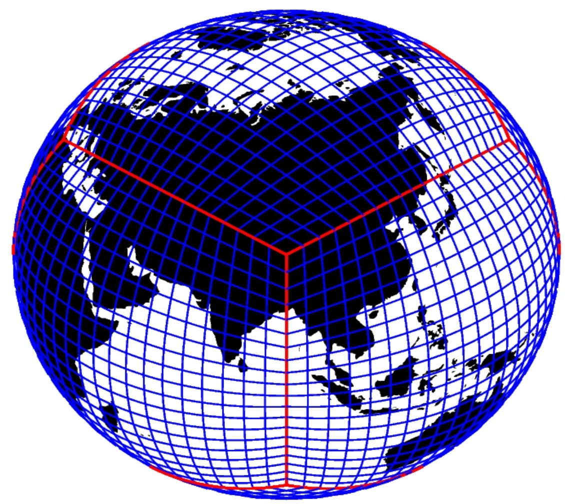
- **CSLAM**: Semi-Lagrangian finite-volume transport scheme for tracers

  (Lauritzen et al., 2010; Erath et al., 2013, 2012; Harris et al., 2010)

- **Phys-grid**: Separating physics and dynamics grids, i.e. ability to compute physics tendencies based on cell-averaged values within each element instead of quadrature points







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Lauritzen, Taylor, Overfelt, Ullrich and Goldhaber (2015, IN PREP)

Idealized baroclinic wave

No sub-grid-scale forcing, dry.
Jablonowski and Williamson (2006) and Lauritzen et al. (2010).

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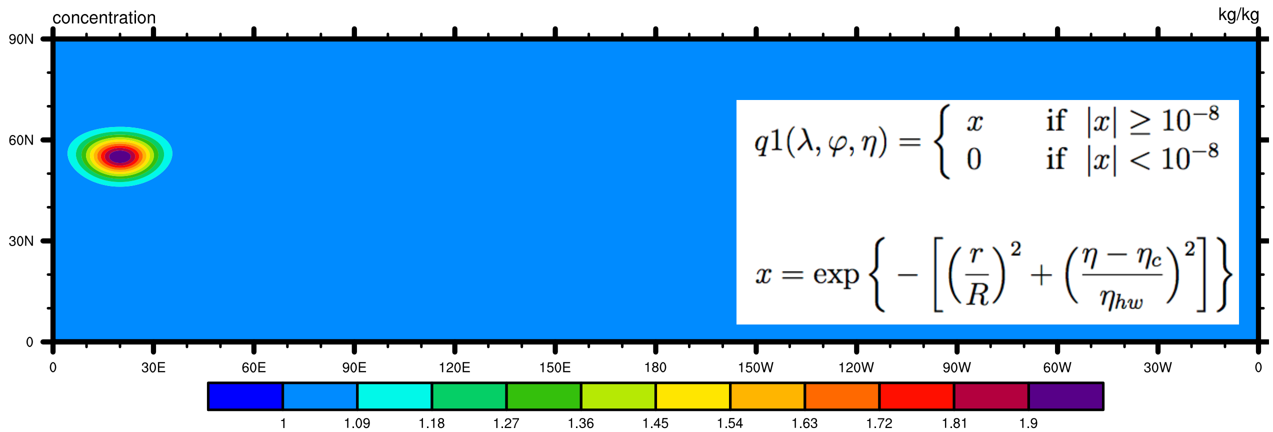
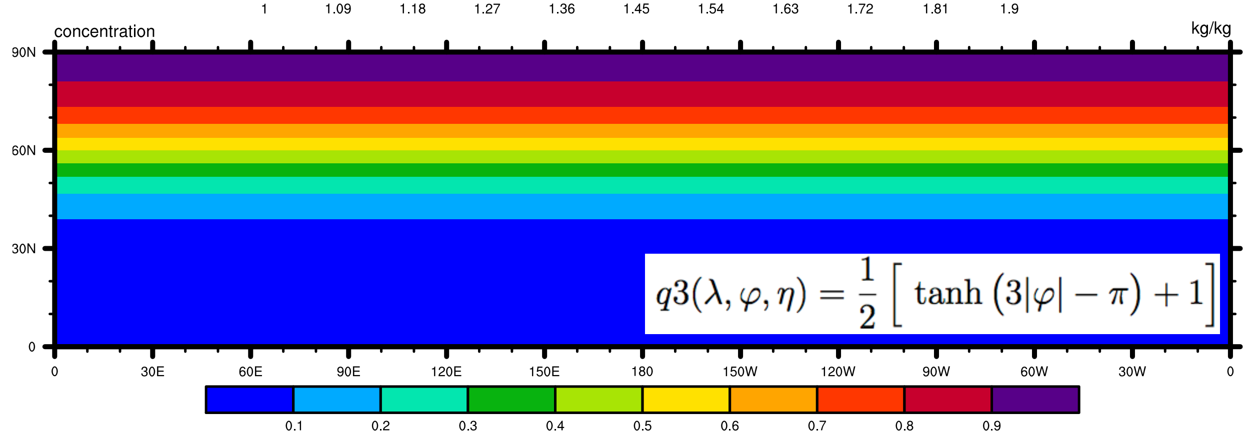
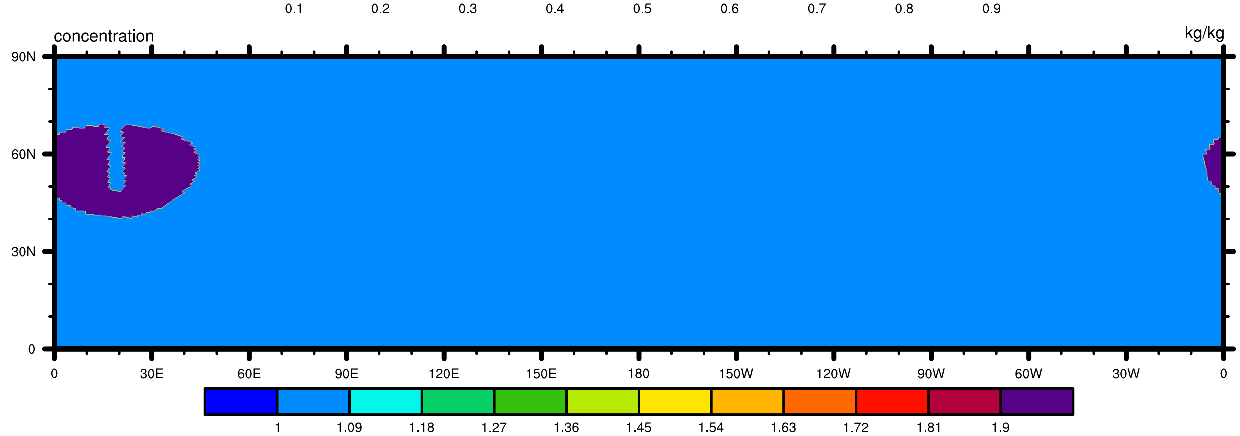
3 tracers: initial conditions



Gaussian “ball”



Zonally symmetric (smooth)



Slotted cylinder

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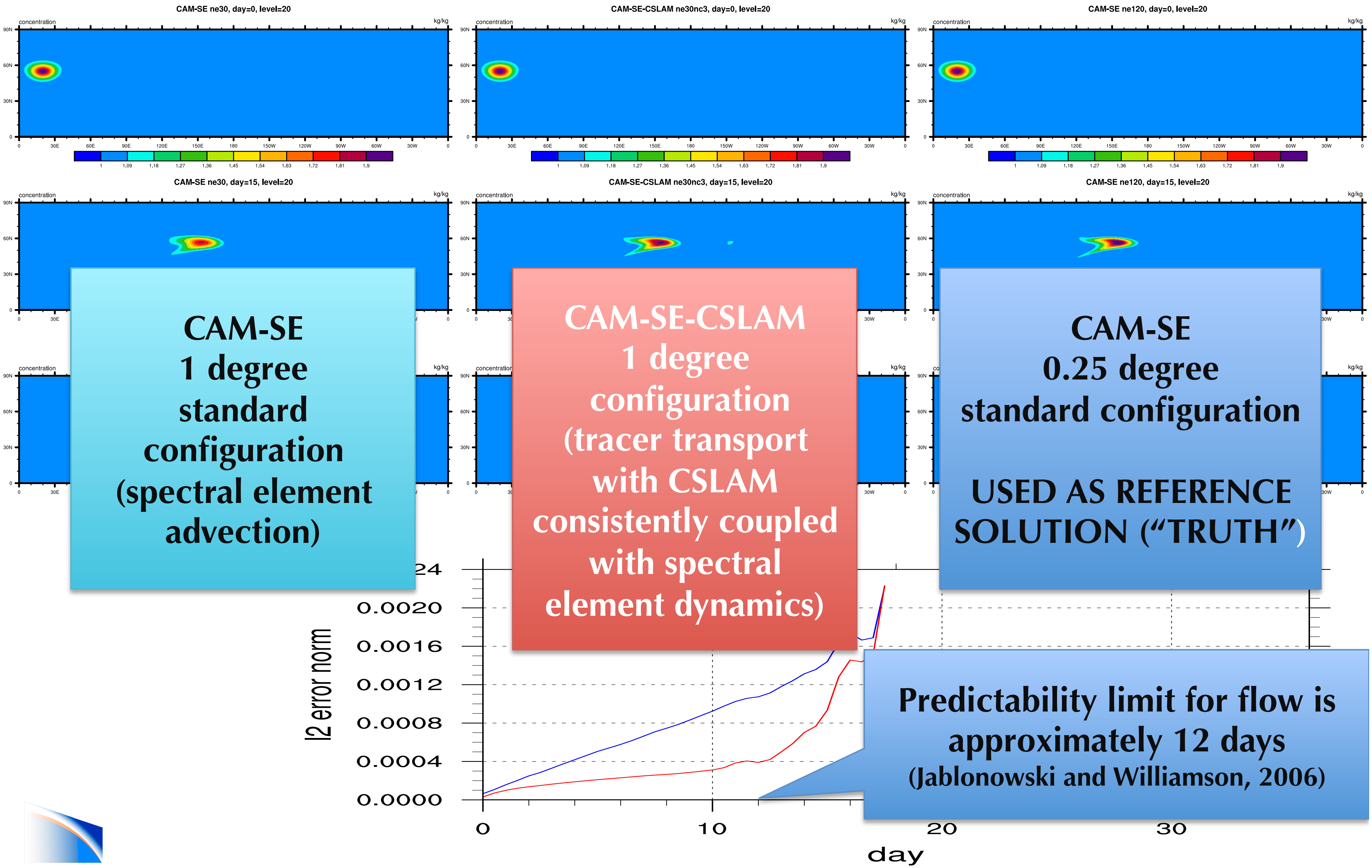

CAM-SE
1 degree
standard configuration
(spectral element advection)

CAM-SE-CSLAM
1 degree configuration
(tracer transport with CSLAM consistently coupled with spectral element dynamics)

CAM-SE
0.25 degree
standard configuration

USED AS REFERENCE SOLUTION ("TRUTH")

Predictability limit for flow is approximately 12 days
(Jablonowski and Williamson, 2006)

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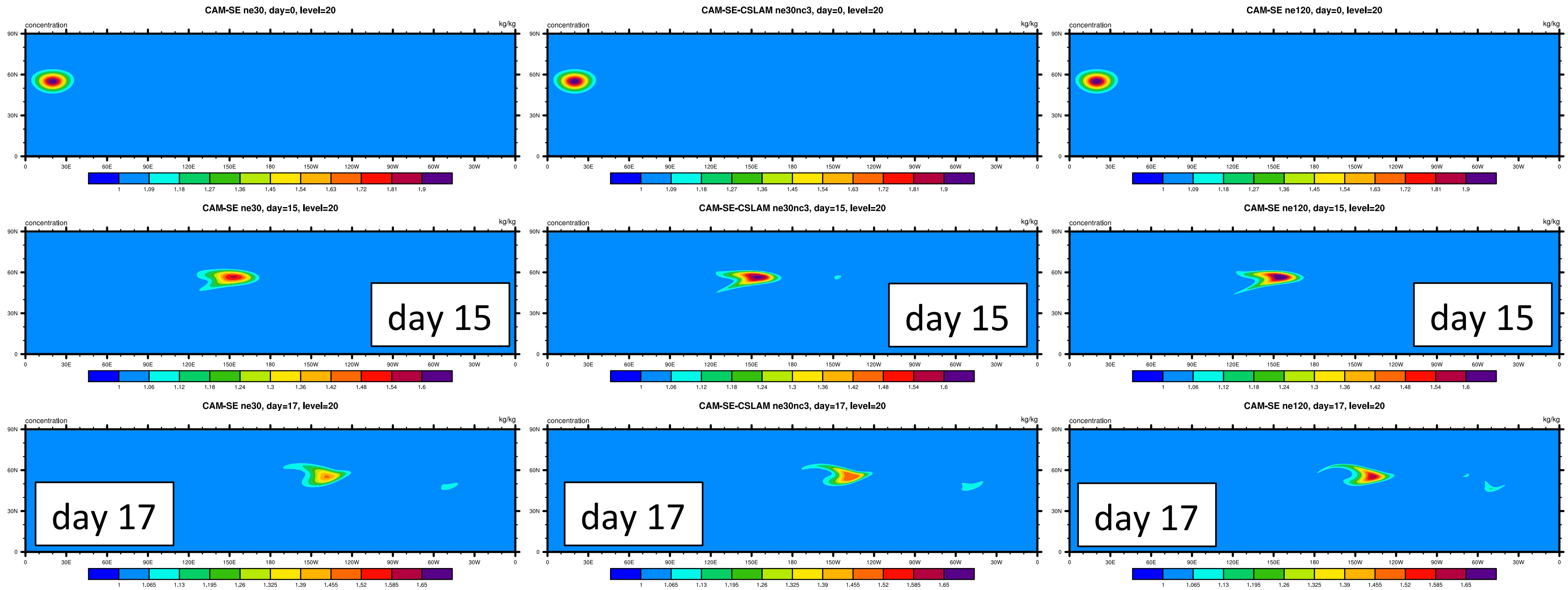
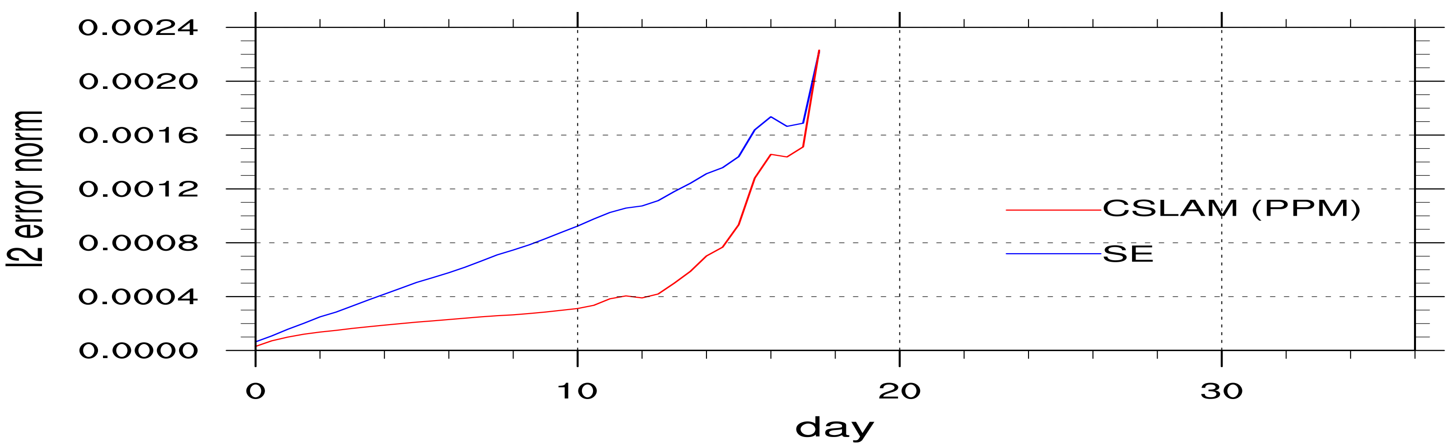
CAM-SE | CAM-SE-CSLAM | CAM-SE reference





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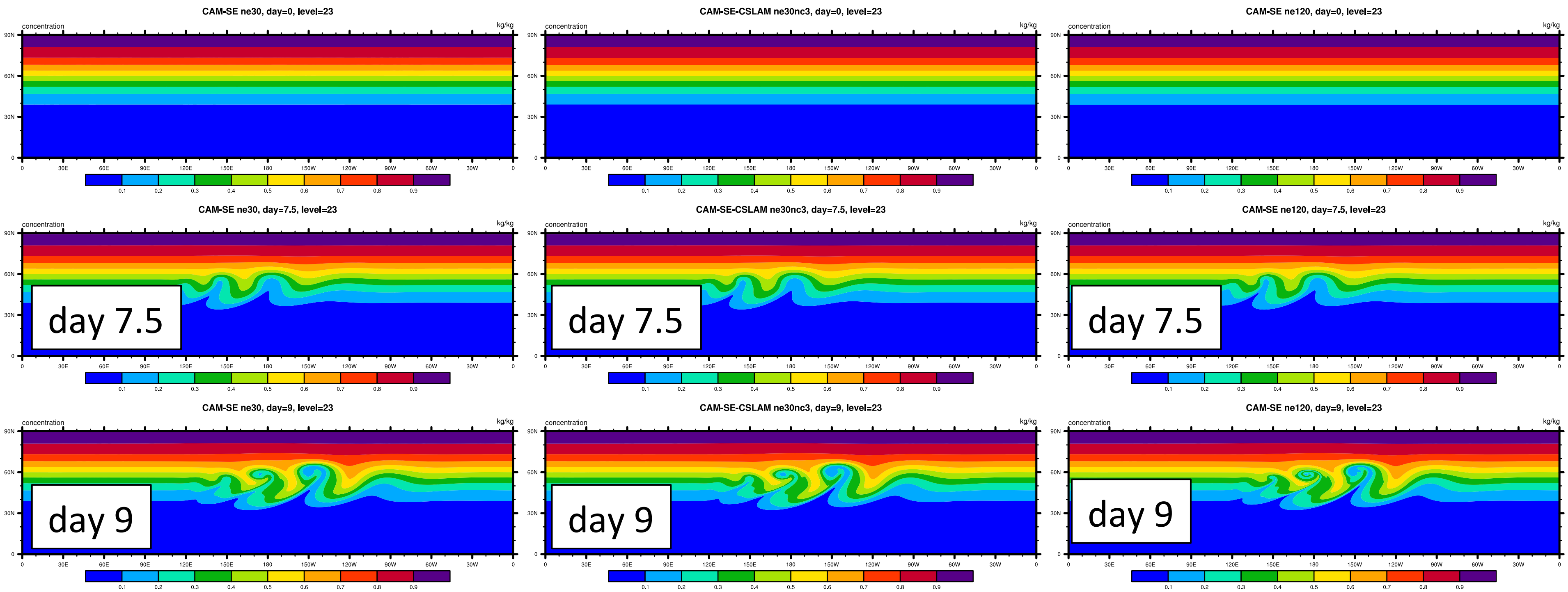
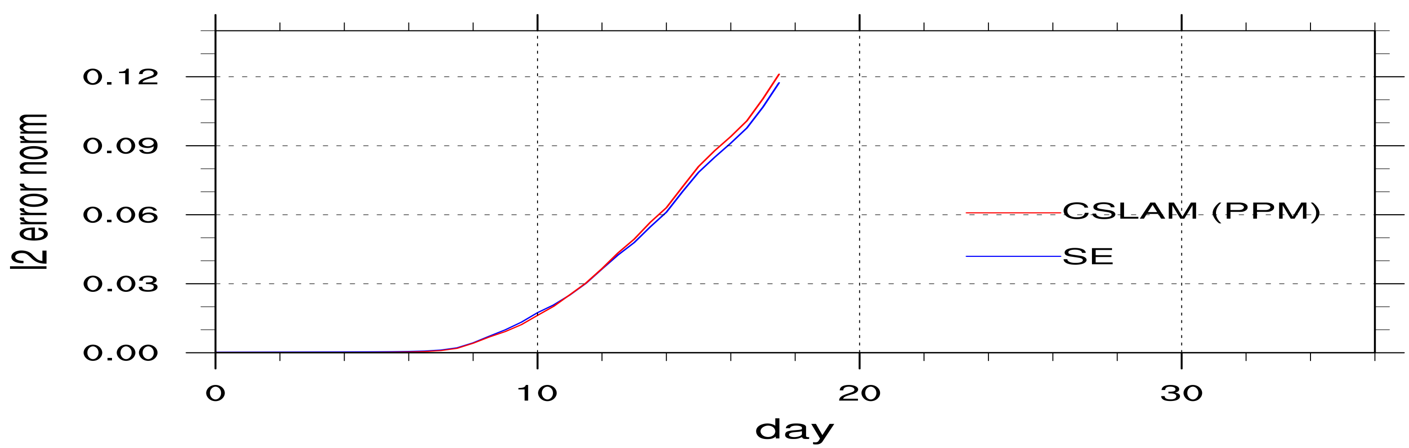
CAM-SE | CAM-SE-CSLAM | CAM-SE reference





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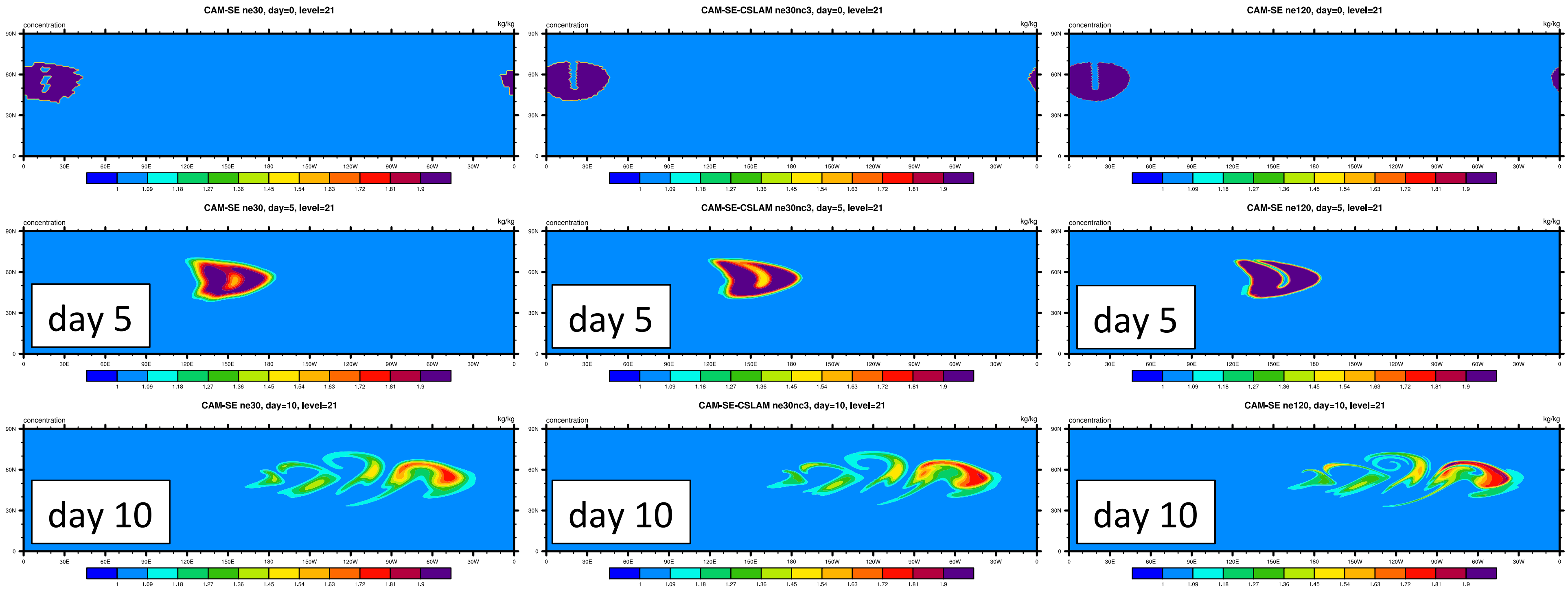
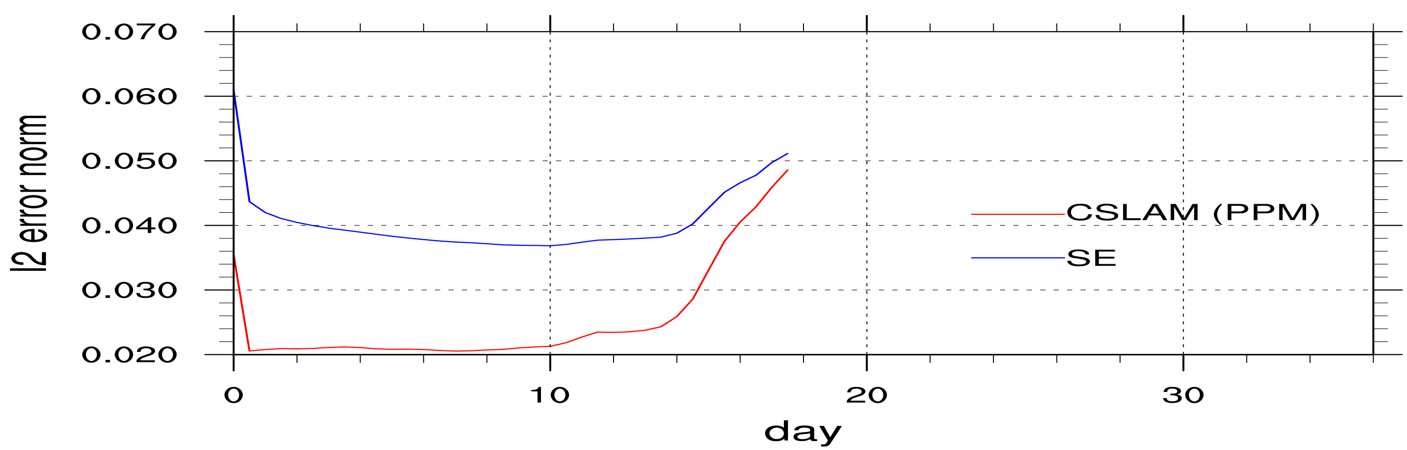
CAM-SE | **CAM-SE-CSLAM** | **CAM-SE reference**





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