



Desirable properties of transport schemes

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**Dynamical Core Model Intercomparison Project (DCMIP) 2016
June 6-17, 2016
NCAR, Boulder, Colorado**

Accuracy?

The degree to which the result of a measurement, calculation, or specification conforms to the correct value or a standard.



Until fairly recently the most widely used idealized test case to assess transport accuracy in global models was:

A Standard Test Set for Numerical Approximations to the Shallow Water Equations in Spherical Geometry

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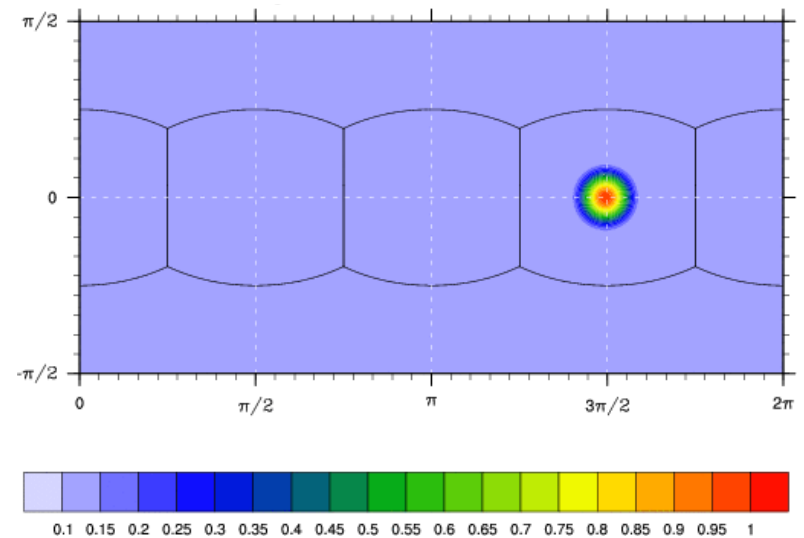
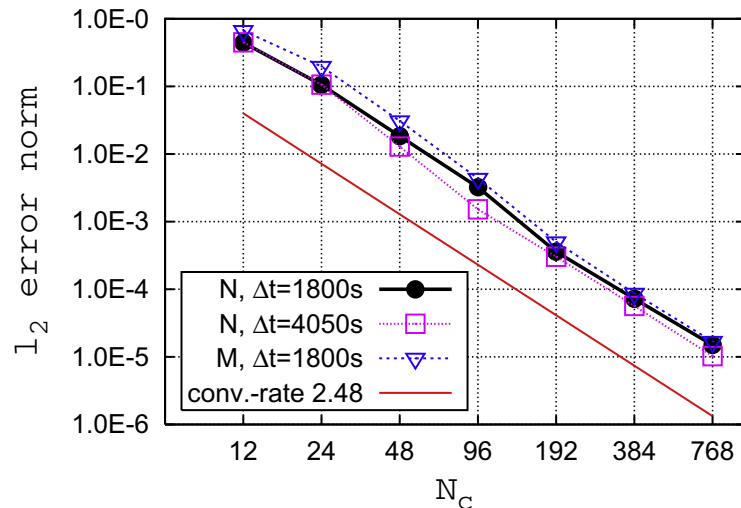
AND

JAMES J. HACK, RÜDIGER JAKOB, AND PAUL N. SWARZTRAUER

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Received June 17, 1991

Test 1: Solid-body advection



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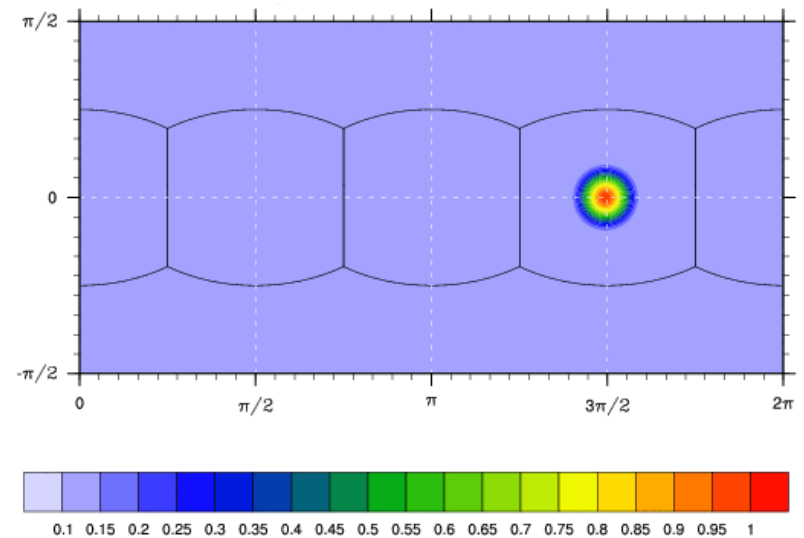
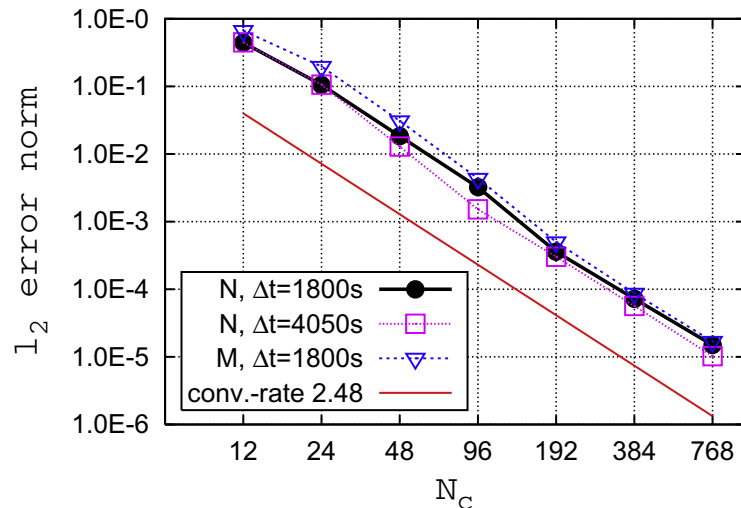


Test 1: Solid-body advection

Until fairly recently the most widely used idealized test case to assess transport accuracy in global models was:

- No deformation only translation:
 - > Flow does not force tracer features to collapse to the grid scale (as it does in nature)
- Parcel trajectories are trivial
- No divergence/convergence

1: Solid-body
rotation



Beyond standard error norms:

Standard error measures

If $\phi = \phi(\lambda, \theta, t)$ is the transported mixing ratio field, then global normalized standard errors are defined by Williamson et al. (1992):

$$\ell_2 = \left[\frac{I[(\phi - \phi_T)^2]}{I[(\phi_T)^2]} \right]^{1/2},$$

$$\ell_\infty = \frac{\max_{\forall \lambda, \theta} |\phi - \phi_T|}{\max_{\forall \lambda, \theta} |\phi_T|},$$

$$\phi_{\max} = \frac{\max_{\forall \lambda, \theta} (\phi) - \max_{\forall \lambda, \theta} (\phi_T)}{\Delta \phi_0},$$

$$\phi_{\min} = \frac{\min_{\forall \lambda, \theta} (\phi) - \min_{\forall \lambda, \theta} (\phi_T)}{\Delta \phi_0},$$

where ϕ_T and ϕ_0 are, respectively, the exact/analytical solution, and its initial value, $\Delta \phi_0$, is the difference between

Conservation of mass

Consider the continuity equation for X (e.g., water vapor, cloud ice, cloud liquid, chemical species, ...)

$$\frac{\partial}{\partial t} (m_x \rho_d) + \nabla \cdot (m_x \rho_d \mathbf{v}) = \rho_d S^{m_x}, \quad (1)$$

where S^{m_x} is the source of X and/or sub-grid-scale transport term.

Integrate (1) over entire atmosphere Ω_{tot}

$$\frac{\partial}{\partial t} \iiint_{\Omega_{tot}} (m_x \rho_d) dV = \iiint_{\Omega_{tot}} \rho_d S^{m_x} dV.$$

Note: sub-grid-scale transport integrates to zero! Global mass only changes due to sources/sinks S^{m_x} .

Global conservation of mass

Globally the change in mass is exactly balanced by the source/sink terms!

The resolved-scale tracer transport must not be a spurious source or sink of mass

Why is that a problem?

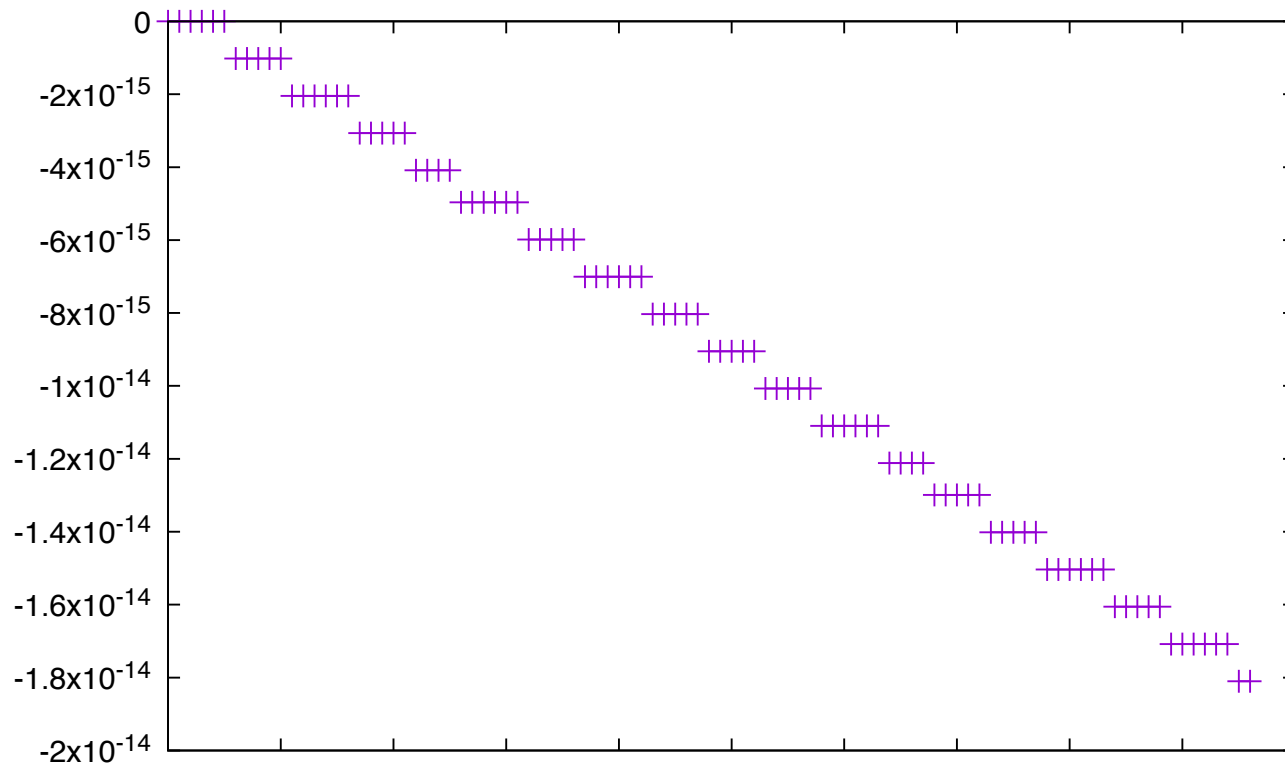
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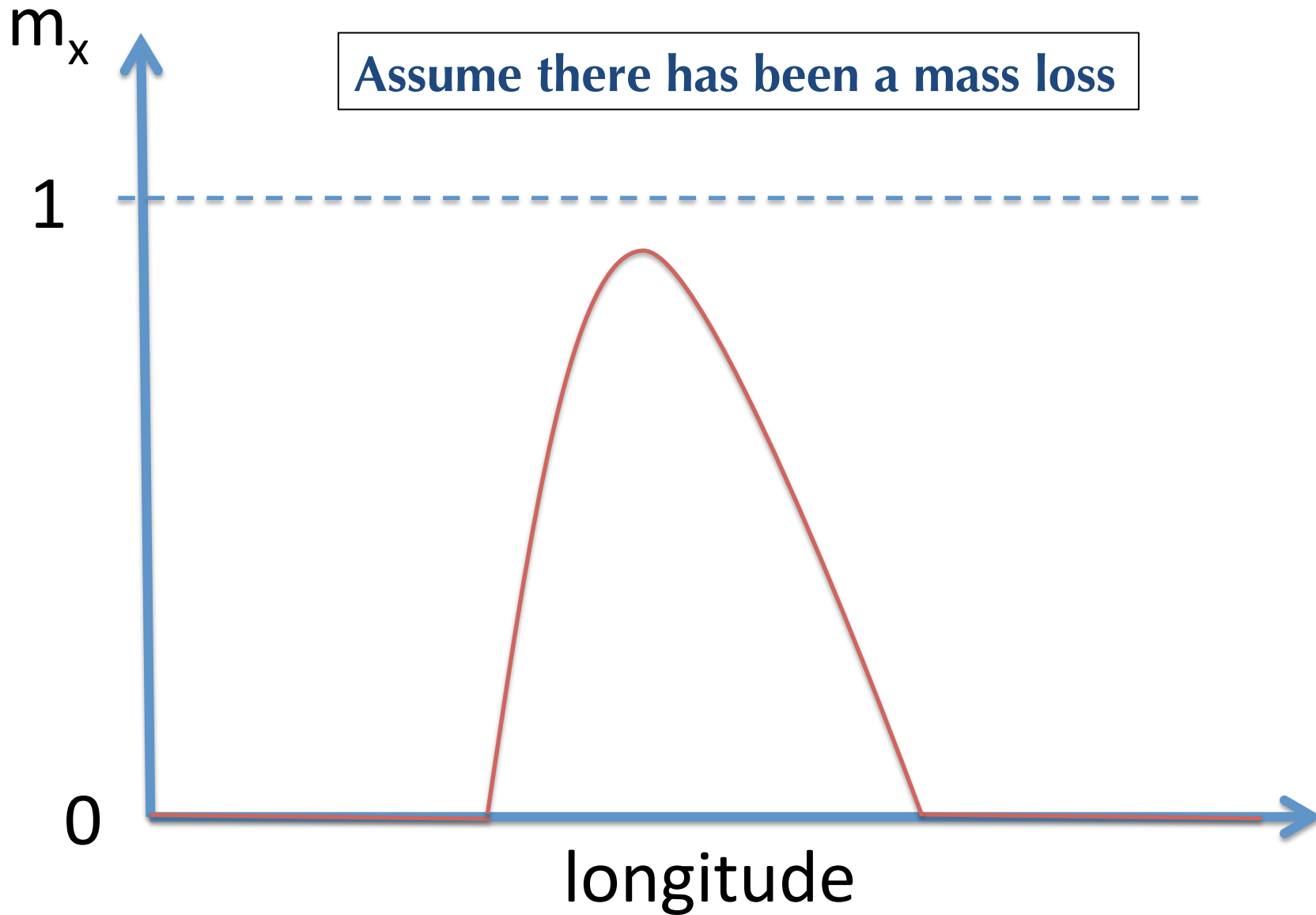
Accumulation of error

Relative dry mass change: $[M(t)-M(t=0)]/M(t=0)$

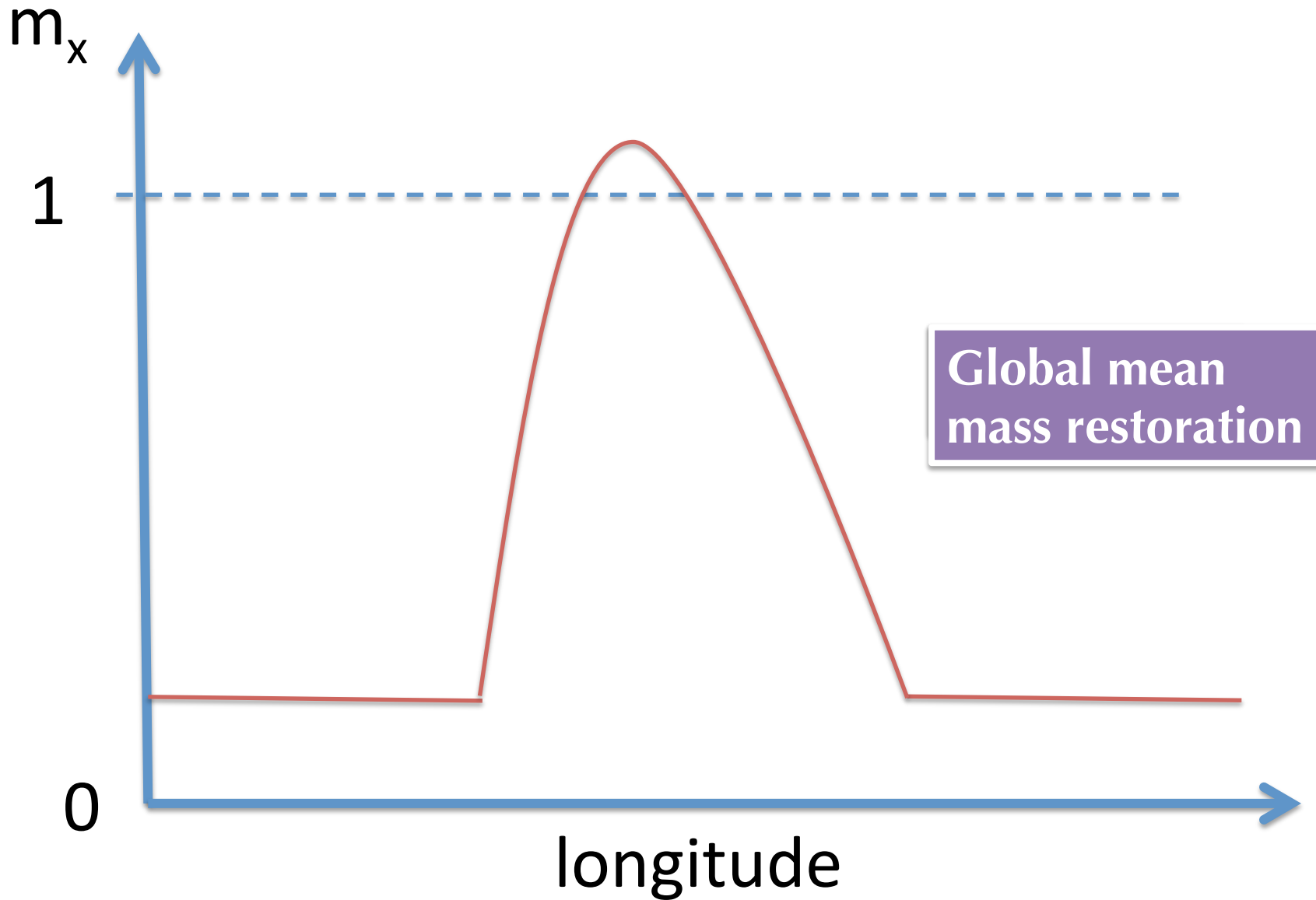


1000 year simulation $\approx O(10^7)$ 30 minute time-steps

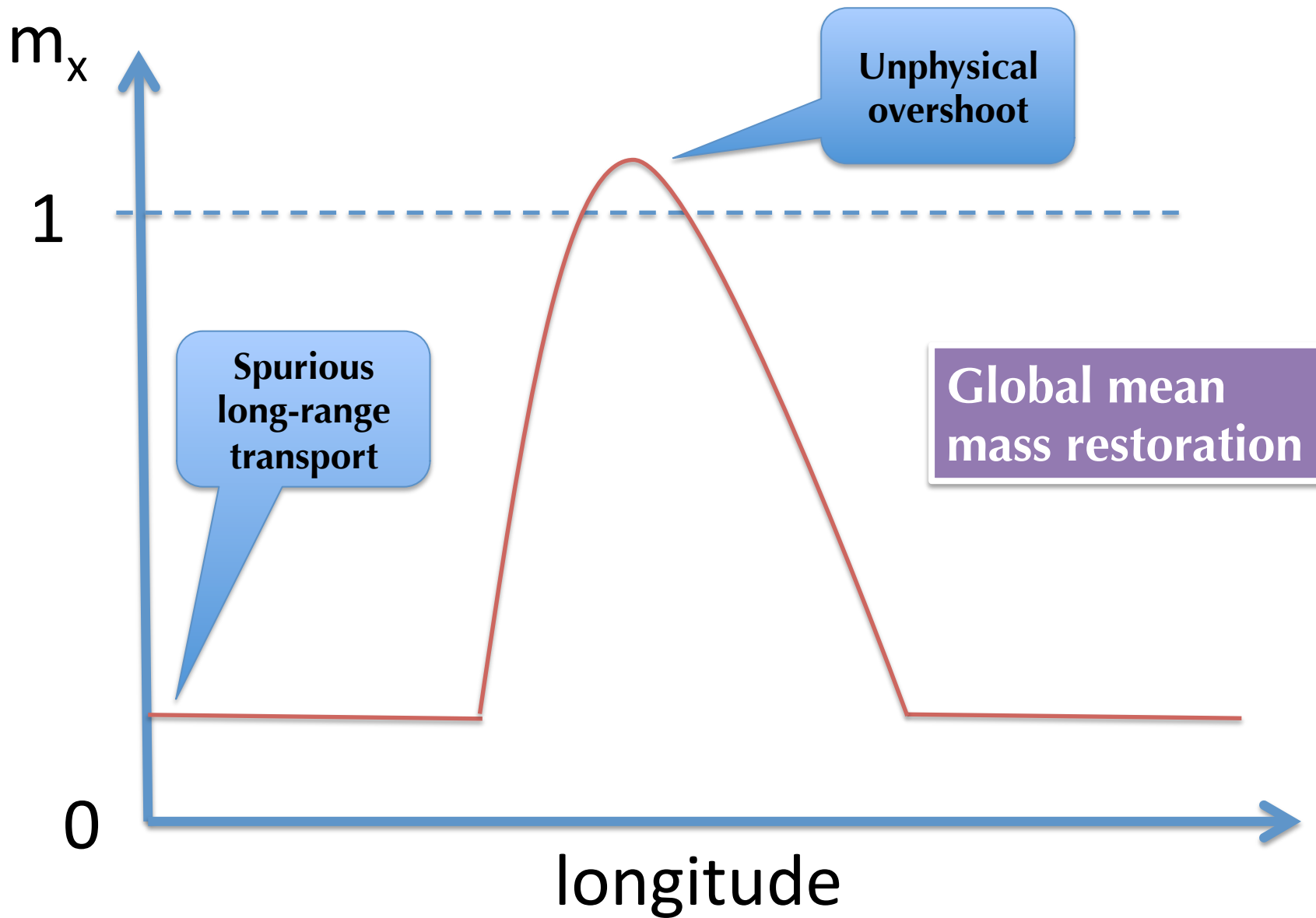
Ad hoc mass fixers are inherently problematic



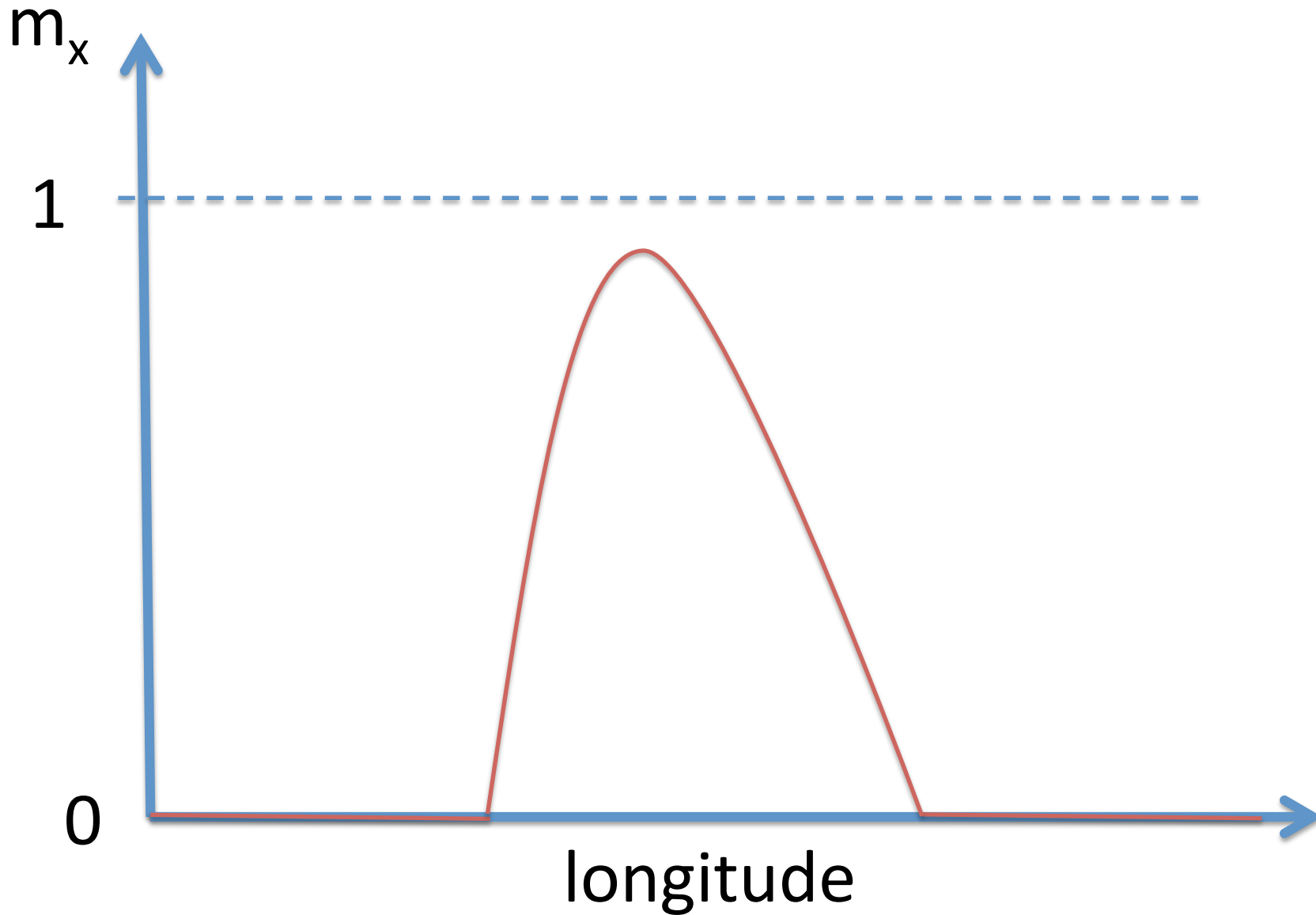
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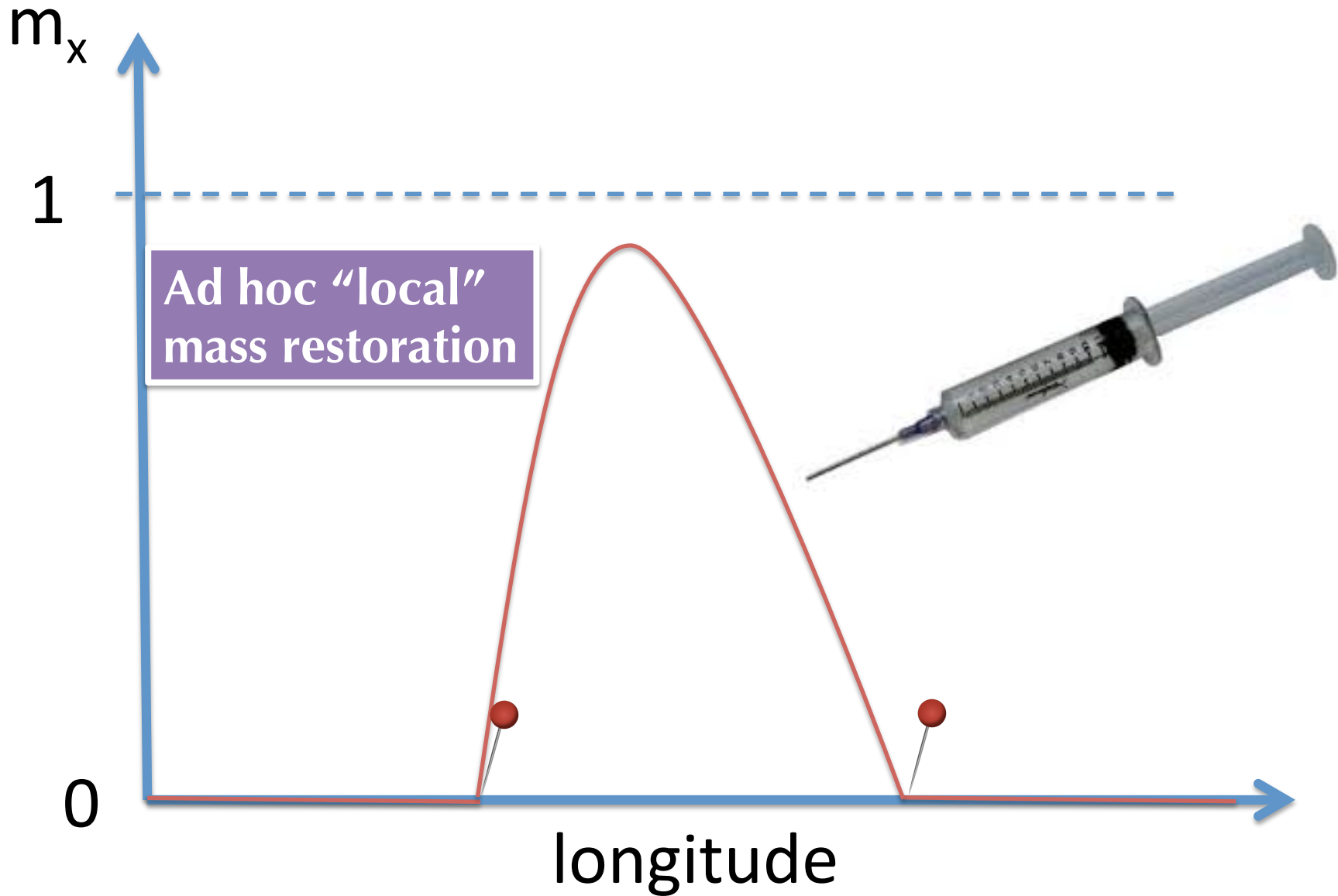
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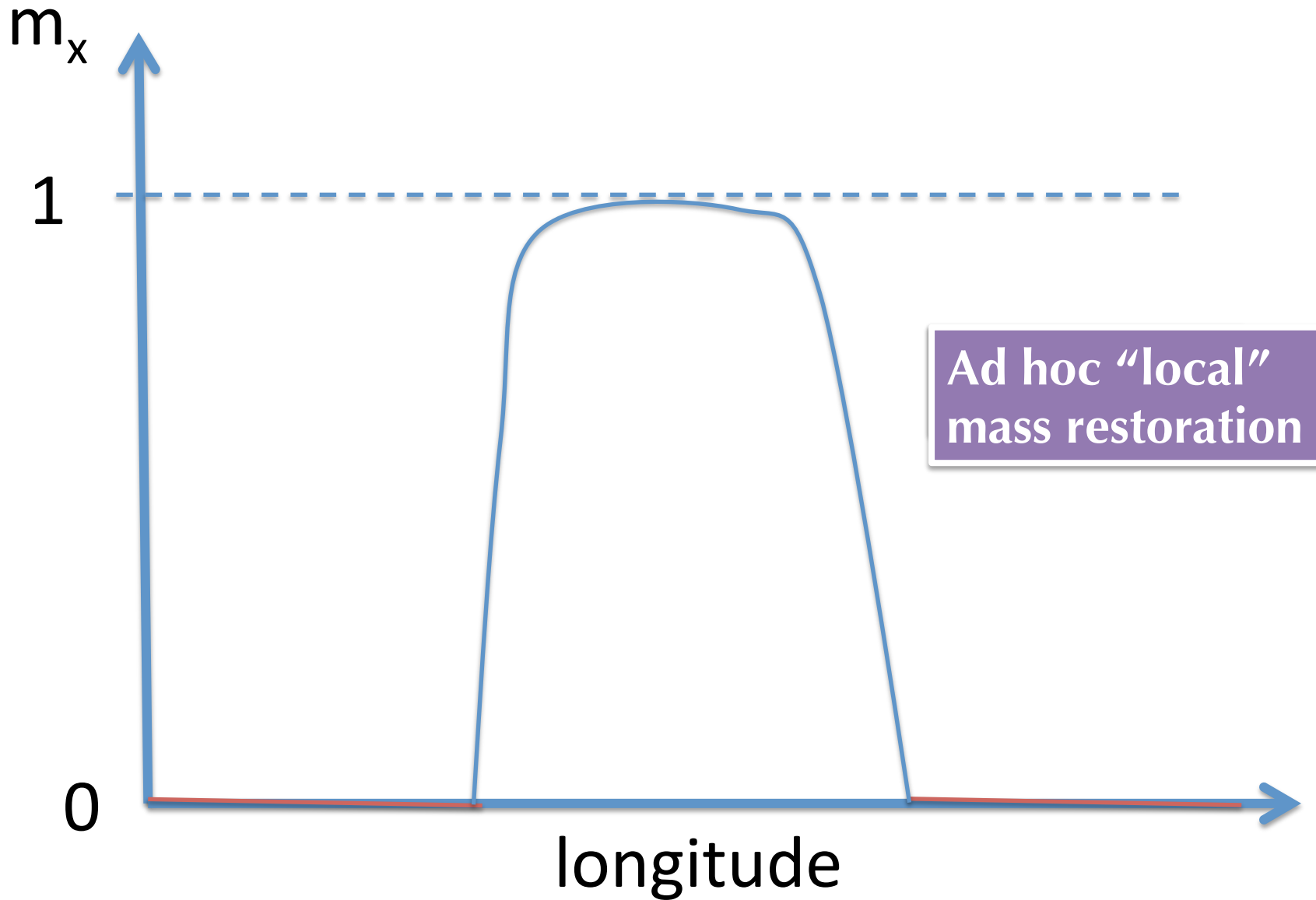
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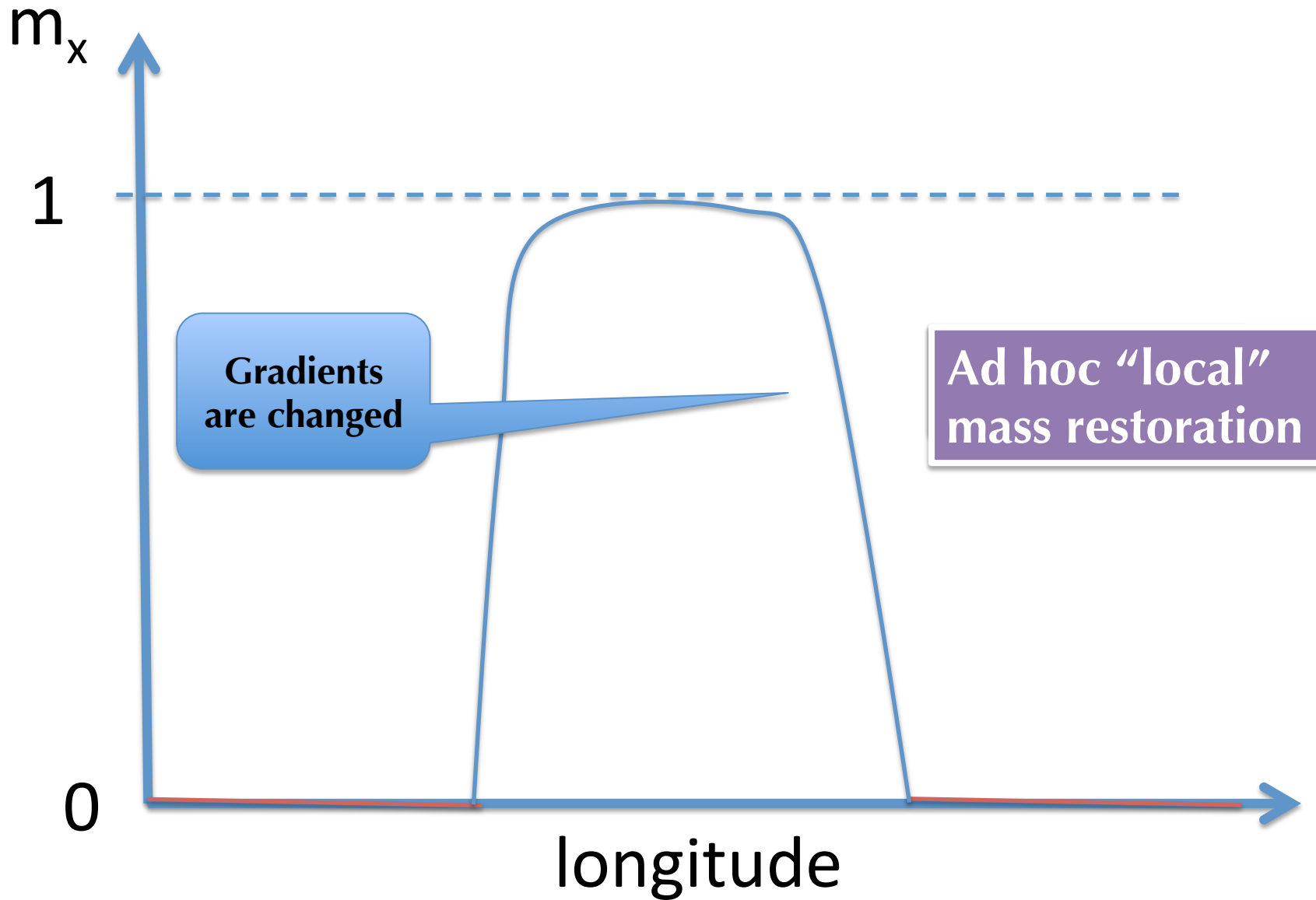
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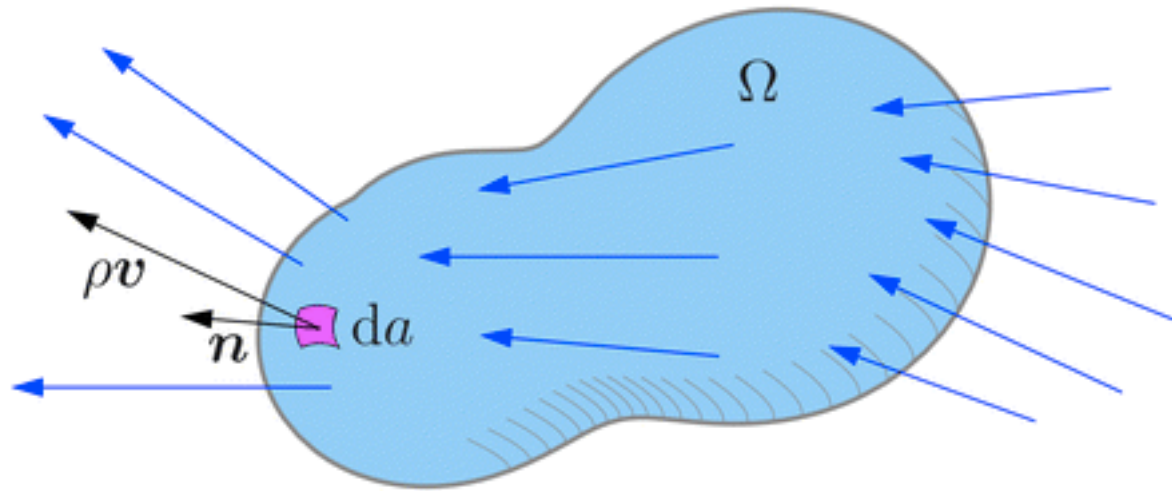
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Ad hoc mass fixers are inherently problematic



Inherent local mass-conservation is desirable



- ▶ The continuity equation is a conservation law for mass:

$$\begin{aligned} \frac{\partial}{\partial t} \iiint_{\Omega} \rho_d dV &= - \iiint_{\Omega} \nabla \cdot (\rho_d \mathbf{v}) dV, \\ &= - \iint_{\partial\Omega} (\rho_d \mathbf{v}) \cdot \mathbf{n} dS \end{aligned}$$

Conservation of m_X along parcel trajectories

Consider the continuity equation for dry air and X

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (2)$$

$$\frac{\partial}{\partial t} (m_X \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = \rho_d S^{m_X}, \quad (3)$$

respectively. Applying the chain rule to (3), re-arranging and substituting (2) implies

$$\frac{Dm_X}{Dt} = S^{m_X},$$

where $D/Dt = \frac{\partial}{\partial t} + \vec{v}\nabla$ is the total (material) derivative.

Conservation of m_X along parcel trajectories

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$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \vec{v}) = 0 \quad (2)$$
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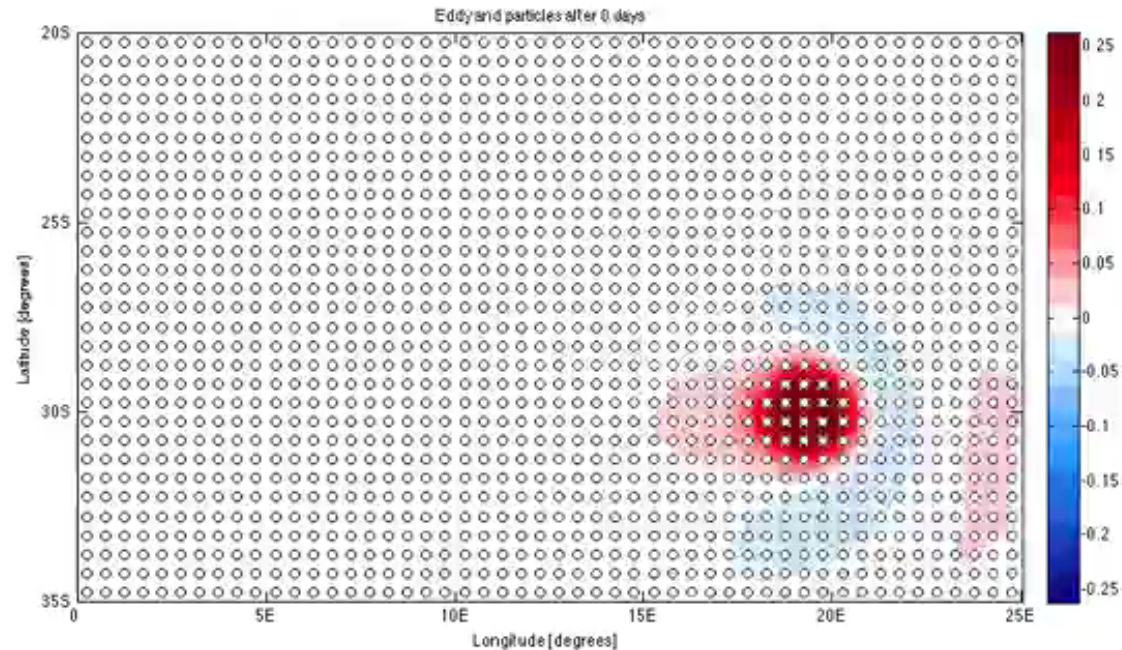
respectively. Applying the chain rule and substituting (2) implies

If the discretization scheme is based on the advective form of the continuity equation (.e.g, grid-point semi-Lagrangian schemes) then inherent mass-conservation is not guaranteed

$$\frac{Dm_X}{Dt} = S^{m_X},$$

where $D/Dt = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla$ is the total (material) derivative.

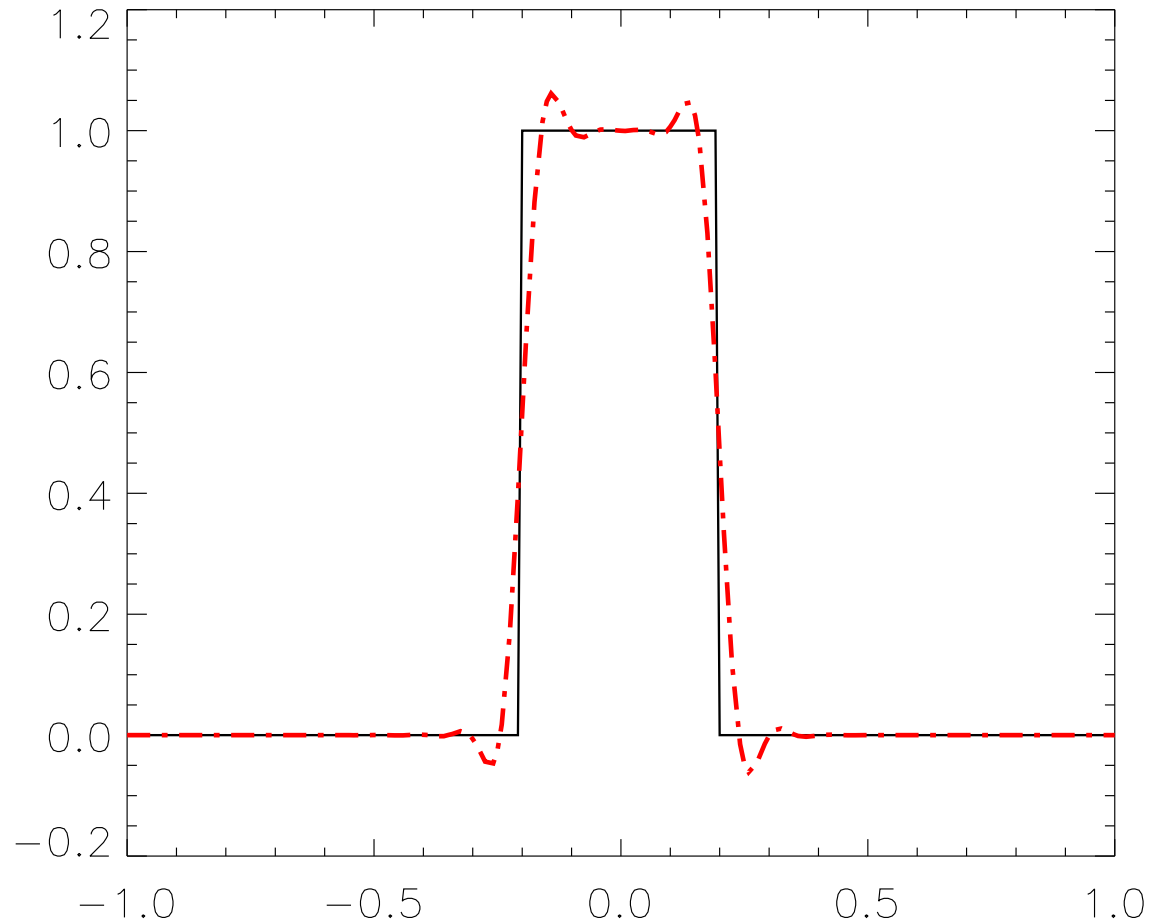
Conservation of m_x along parcel trajectories (if no sources/sinks of m_x)



- if $m_x(x,y,t=0)=\text{constant}$ then $m_x(x,y,t)=\text{constant}$
- $\text{MIN}[m_x(x,y,t=0)] \leq m_x(x,y,t) \leq \text{MAX}[m_x(x,y,t=0)]$

Source: <https://www.youtube.com/watch?v=tEHQH7Uly-8>

Conservation of m_x along parcel trajectories (if no sources/sinks of m_x)



Nair et al., (2011)

Conservation of m_x along parcel trajectories

Atmospheric modelers tend to be a bit loose with the term ‘monotone’!

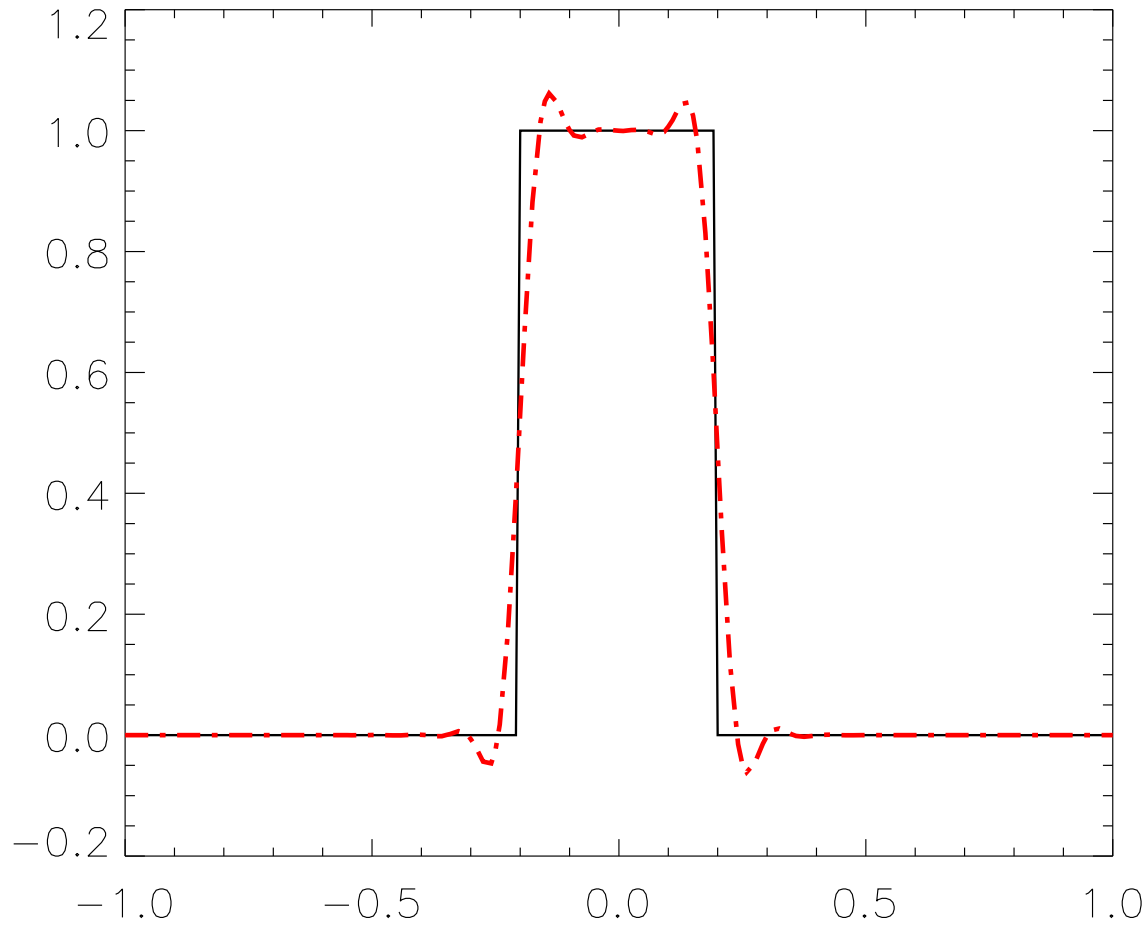
When modelers refer to “non-oscillatory”, “shape-preserving”, “physical realizable” or “monotone” they usually refer to the **monotonicity property** as defined by Harten (1983):

1. No new local extrema in m_x may be created
2. The value of a local minima/(maxima) is nondecreasing/(nonincreasing)

There are “stricter” characterizations such as total variation diminishing (TVD), however, they are probably too strong for our applications

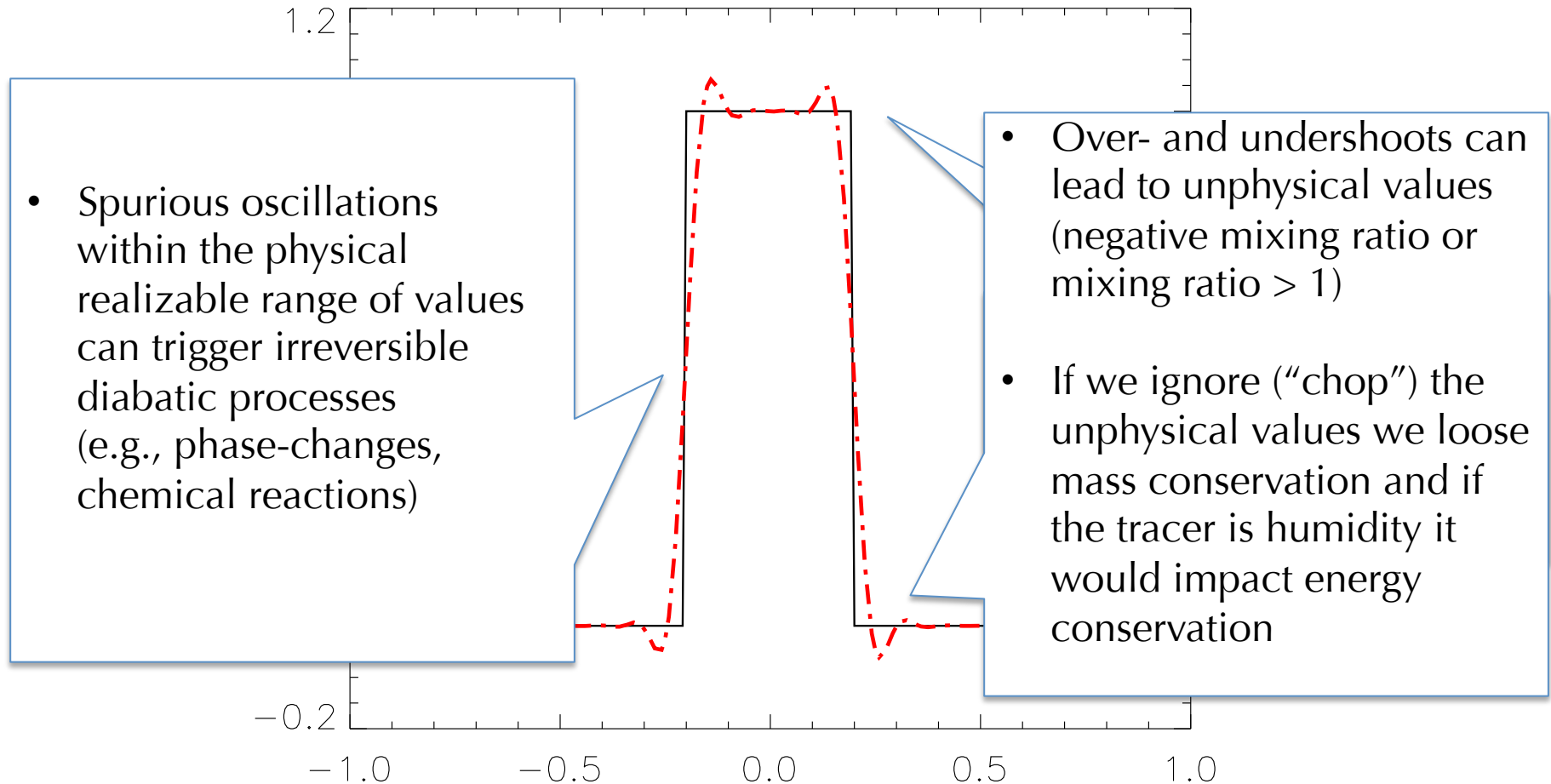
=> the monotonicity property applies to mixing ratio m_x and not tracer mass!

Why is the monotonicity property so important



Nair et al., (2011)

Why is the monotonicity property so important



Nair et al., (2011)

Conservation of mass along parcel trajectories

Note that

$$\frac{D\rho_d}{Dt} \neq 0,$$

but

$$\frac{D\rho_d}{Dt} = -\rho_d \nabla \cdot \vec{v}.$$

If we integrate ρ_d over a Lagrangian volume Ω_L then

$$\frac{\partial}{\partial t} \iiint_{\Omega_L} \rho_d dV = 0.$$

Lagrangian volumes are rapidly distorting

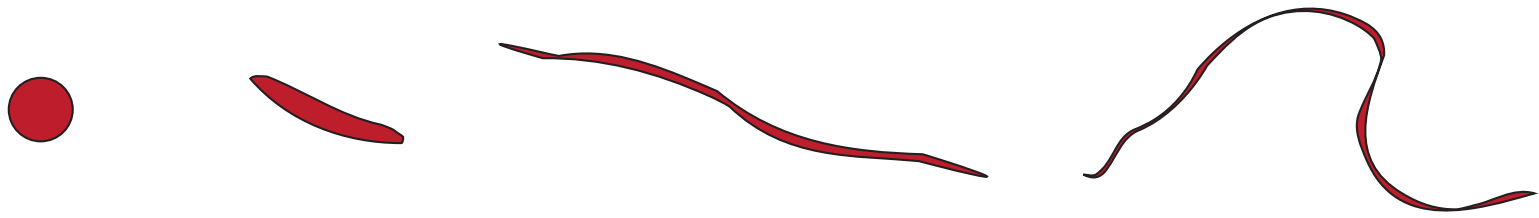
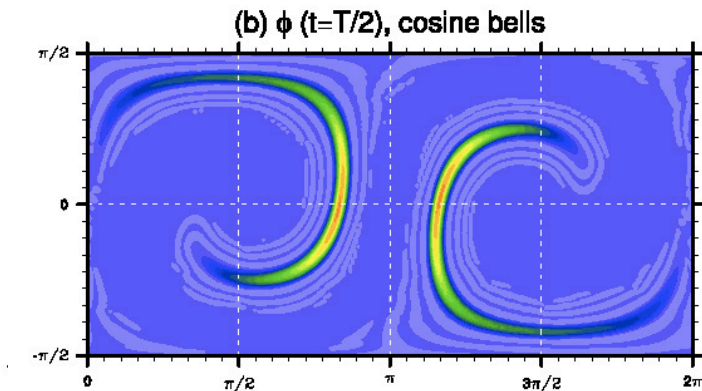
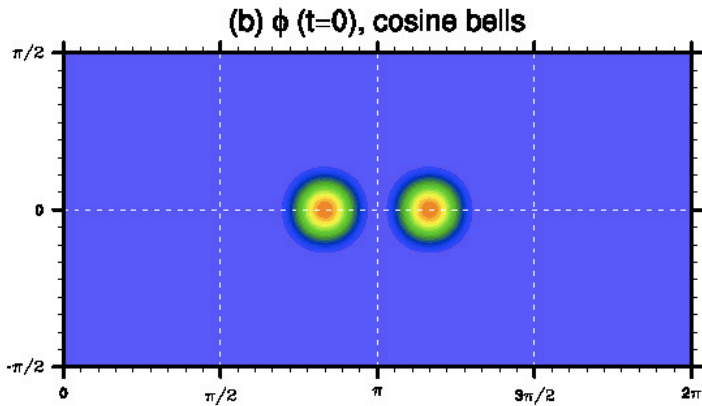


Fig. 2: In the highly nonlinear flows that characterize fluid motion in the atmosphere and ocean, Lagrangian control volumes are rapidly distorted due the presence of strong shear, rotation and dilation. The rapid distortion of Lagrangian control volumes makes the formulation of numerical models within the Lagrangian reference frame an extremely difficult challenge.

Ringler (2011)

Filament diagnostic (M. Prather, UCI)



The “filament” preservation diagnostic is formulated as follows. Define $A(\tau, t)$ as the spherical area for which the spatial distribution of the tracer $\phi(\lambda, \theta)$ satisfies

$$\phi(\lambda, \theta) \geq \tau, \quad (27)$$

at time t , where τ is the threshold value. For a non-divergent flow field and a passive and inert tracer ϕ , the area $A(\tau, t)$ is invariant in time.

The discrete definition of $A(\tau, t)$ is

$$A(\tau, t) = \sum_{k \in \mathcal{G}} \Delta A_k, \quad (28)$$

where ΔA_k is the spherical area for which ϕ_k is representative, K is the number of grid cells, and \mathcal{G} is the set of indices

$$\mathcal{G} = \{k \in (1, \dots, K) | \phi_k \geq \tau\}. \quad (29)$$

For Eulerian finite-volume schemes ΔA_k is the area of the k -th control volume. For Eulerian grid-point schemes a control volume for which the grid-point value is representative must be defined. Similarly for fully Lagrangian schemes based on point values (parcels) control volumes for which the point values are representative must be defined. Note that the “control volumes” should span the entire domain without overlaps or “cracks” between them.

Define the filament preservation diagnostic

$$\ell_f(\tau, t) = \begin{cases} 100.0 \times \frac{A(\tau, t)}{A(\tau, t=0)} & \text{if } A(\tau, t=0) \neq 0, \\ 0.0, & \text{otherwise.} \end{cases} \quad (30)$$

For infinite resolution (continuous case) and a non-divergent flow, $\ell_f(\tau, t)$ is invariant in time: $\ell_f(\tau, t=0) = \ell_f(\tau, t) = 100$ for all τ . At finite resolution, however, the filament

This diagnostic does not rely on an analytical solution!

Lauritzen et al. (2012)

Filament diagnostic

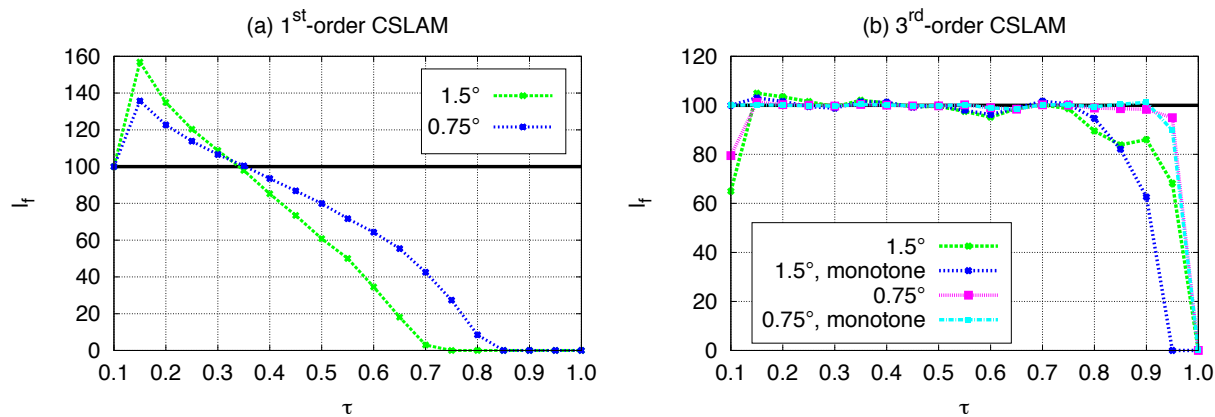


Fig. 6. Filament diagnostics $\ell_f(t = T/2)$ as a function of threshold value τ for different configurations of the CSLAM scheme with Courant number 5.5. (a) 1st-order version of CSLAM at $\Delta\lambda = 1.5^\circ$ and $\Delta\lambda = 0.75^\circ$, and (b) 3rd-order version of CSLAM with and without monotone/shape-preserving filter at resolutions $\Delta\lambda = 1.5^\circ$ and $\Delta\lambda = 0.75^\circ$.

Tracer mass and air mass consistency

Consider the continuity equation for dry air and X (no sources/sinks)

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (4)$$

$$\frac{\partial}{\partial t} (m_x \rho_d) + \nabla \cdot (m_x \rho_d \mathbf{v}) = 0, \quad (5)$$

respectively.

Note that if m_x is 1 then (5) reduces to (4).

A scheme satisfying this is referred to as “free-stream preserving”

Examples of tracer mass and air mass consistency violation

Consider the continuity equation for dry air and X (no

S Prescribed wind and mass fields from , e.g., re-analysis.

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (4)$$

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Note that if m_x is 1 then (5) reduces to (4).

Solve (4) and (5) with different numerical methods, on different grids and/or different time-steps

A scheme satisfying this is referred to as “free-stream preserving”

Examples of tracer mass and air mass consistency violation

Consider the continuity equation for dry air and X (no sources/sinks)

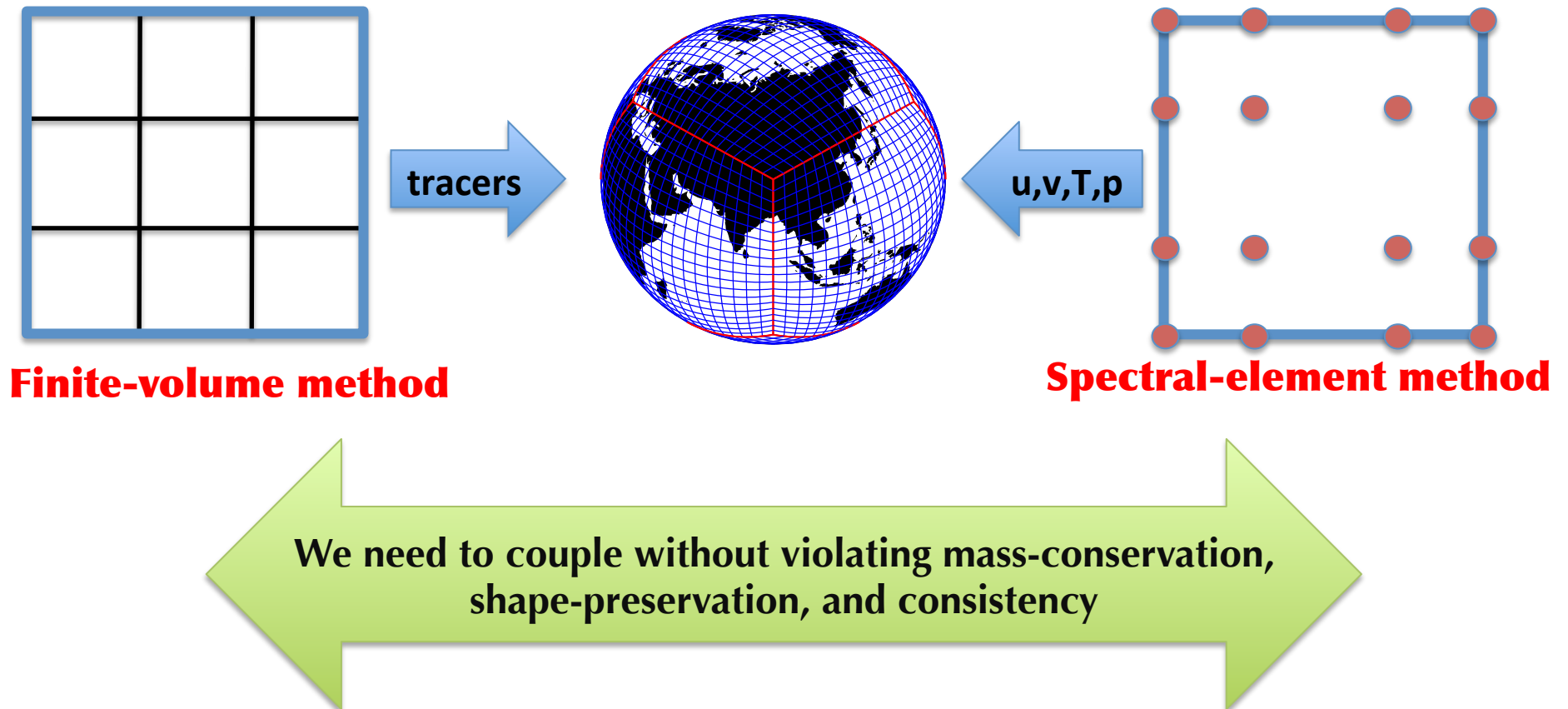
$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (4)$$

$$\frac{\partial}{\partial t} (m_X \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = 0, \quad (5)$$

If consistency is violated:

- **monotonicity preservation may be violated**
- **tracer mass-conservation may be violated**
- **(5) may start evolving independently of (4)**

Example: Separating transport and dynamics grids/methods in CAM-SE



Examples of tracer mass and air mass consistency violation

Assume we are solving (4) and (5) with the same finite-volume method:

(5) can be solved with a longer time-step than (4) – “free-stream preservation” can relatively easily be enforced.

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \quad (4)$$

$$\frac{\partial}{\partial t} (m_x \rho_d) + \nabla \cdot (m_x \rho_d \mathbf{v}) = 0, \quad (5)$$

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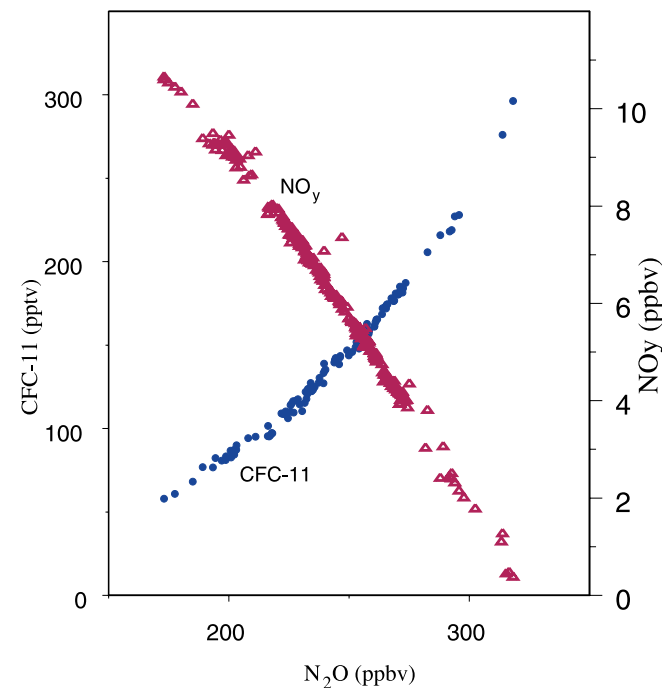
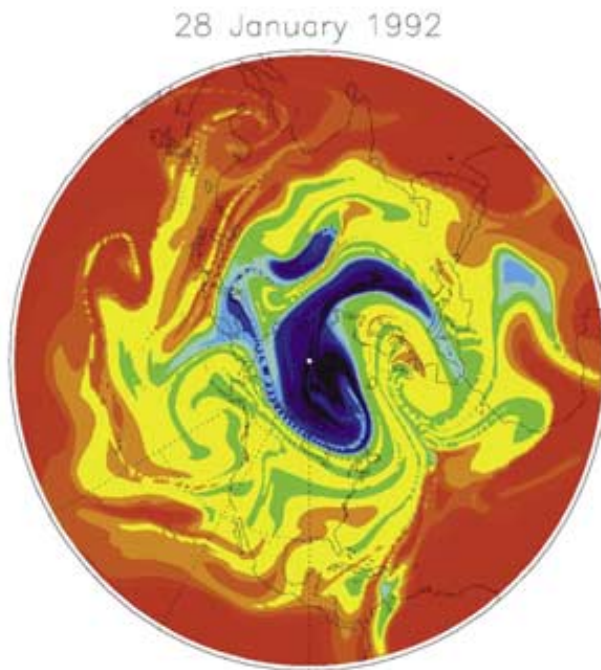
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Correlations between long-lived species in the stratosphere

Relationships between long-lived stratospheric tracers, manifested in similar spatial structures on scales ranging from a few to several thousand kilometers, are displayed most strikingly if the mixing ratio of one is plotted against another, when the data collapse onto remarkably compact curves. - Plumb (2007)

E.g., nitrous oxide (N_2O) against 'total odd nitrogen' (NO_y) or chlorofluorocarbon (CFC's)



Figures from Plumb (2007).

Correlations between long-lived species in the stratosphere

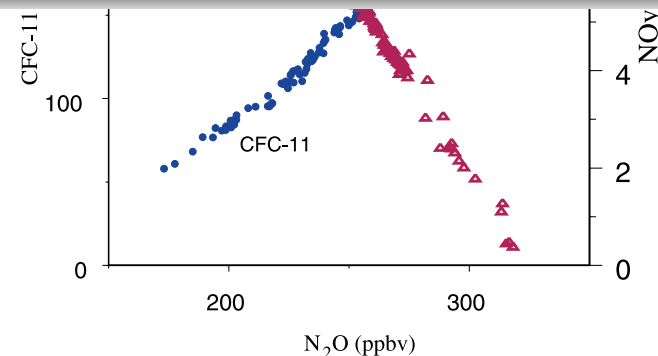
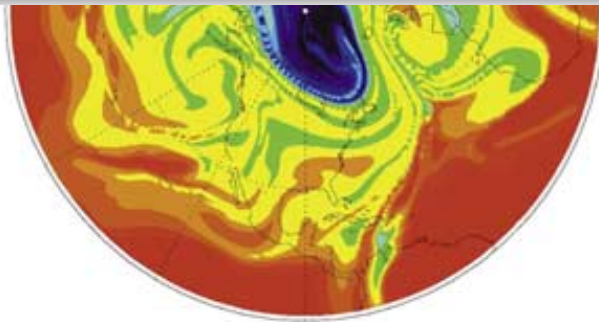
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Similarly:

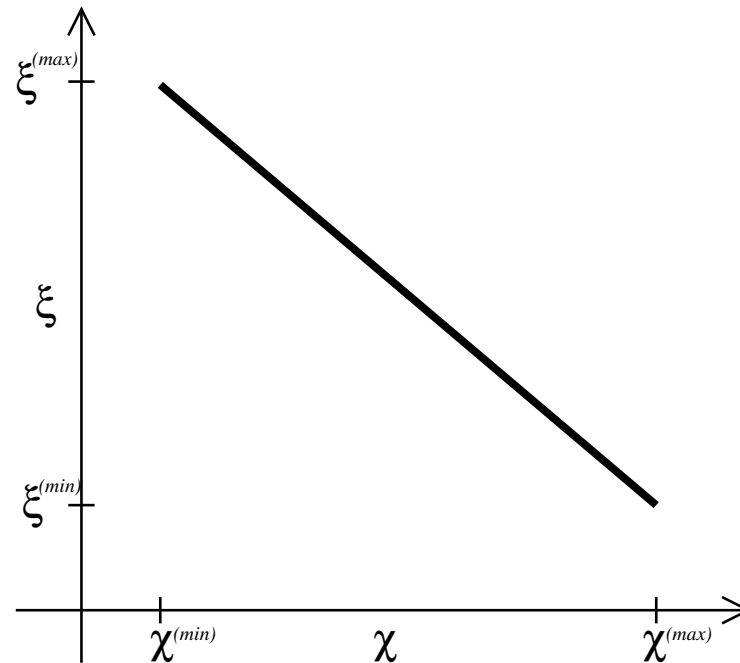
- The total of chemical species within some chemical family may be preserved following an air parcel although the individual species have a complicated relation to each other and may be transformed into each other through chemical reactions (e.g., total chlorine)
- Aerosol-cloud interactions (Ovtchinnikov and Easter, 2009)

The transport operator should ideally not perturb pre-existing functional relationships



Figures from Plumb (2007).

Analyzing scatter plots

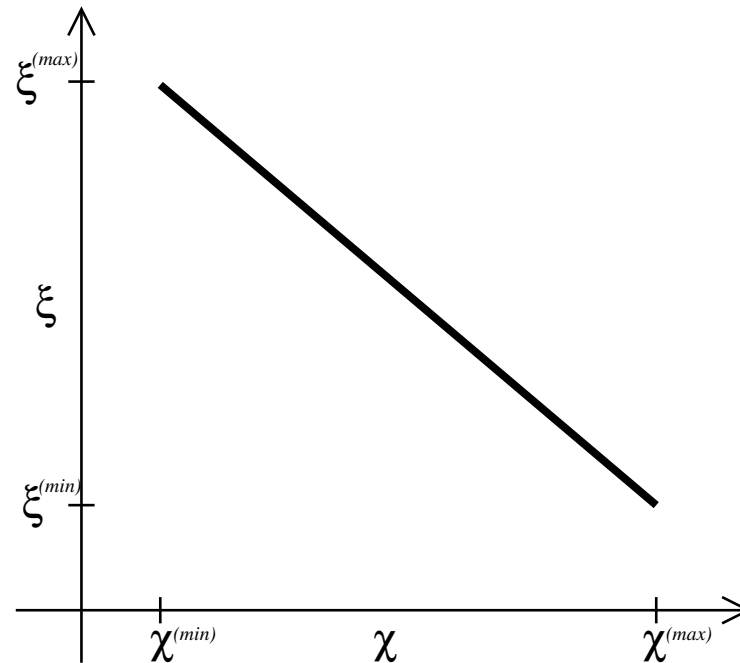


Analytical pre-existing functional relationship curve ψ (linear)

$$\xi = \psi(\chi) = a \cdot \chi + b, \quad \chi \in [\chi^{(min)}, \chi^{(max)}],$$

where a and b are constants, and χ and ξ are the mixing ratios of the two tracers

Analyzing scatter plots

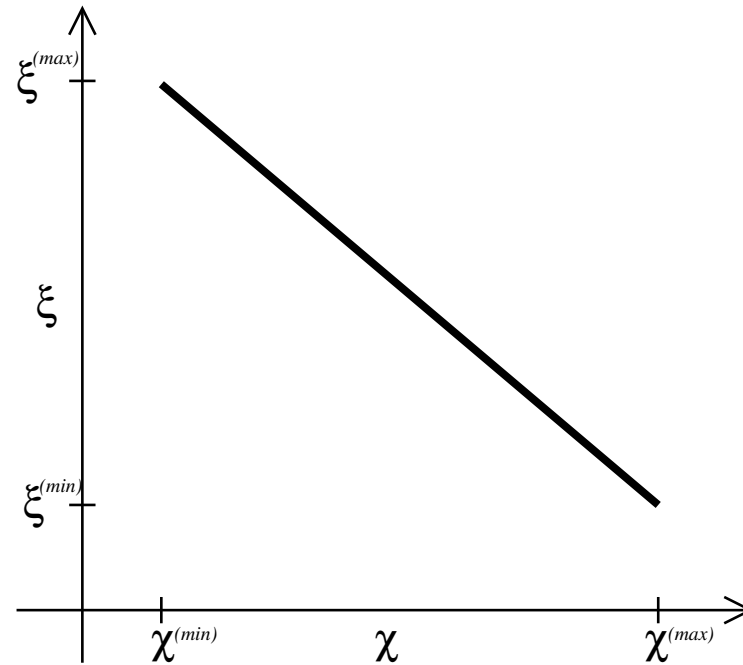


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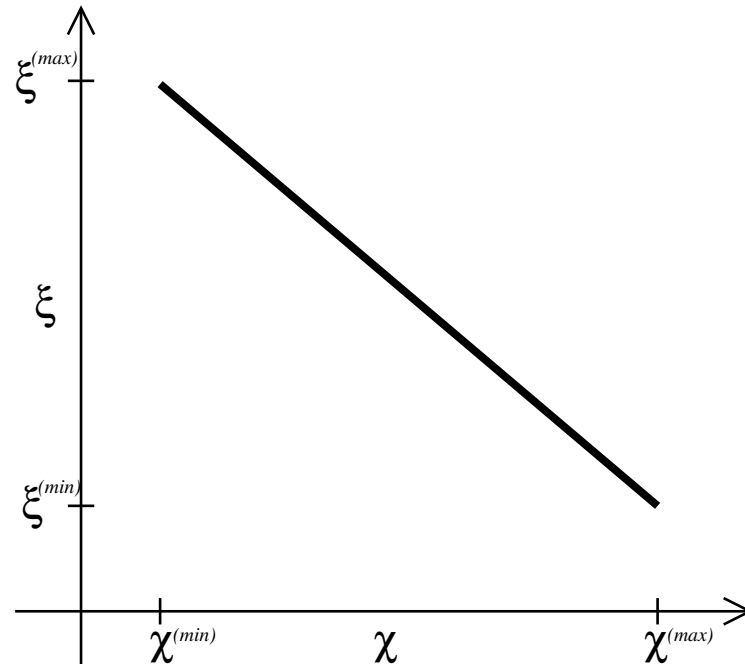
χ and ξ are transported separately by the transport scheme

$$\chi_k^{n+1} = \mathcal{T}(\chi_j^n), \quad j \in \mathcal{H},$$

$$\xi_k^{n+1} = \mathcal{T}(\xi_j^n), \quad j \in \mathcal{H},$$

where \mathcal{T} is the transport operator and \mathcal{H} the set of indices defining the 'halo' for \mathcal{T} .

Analyzing scatter plots



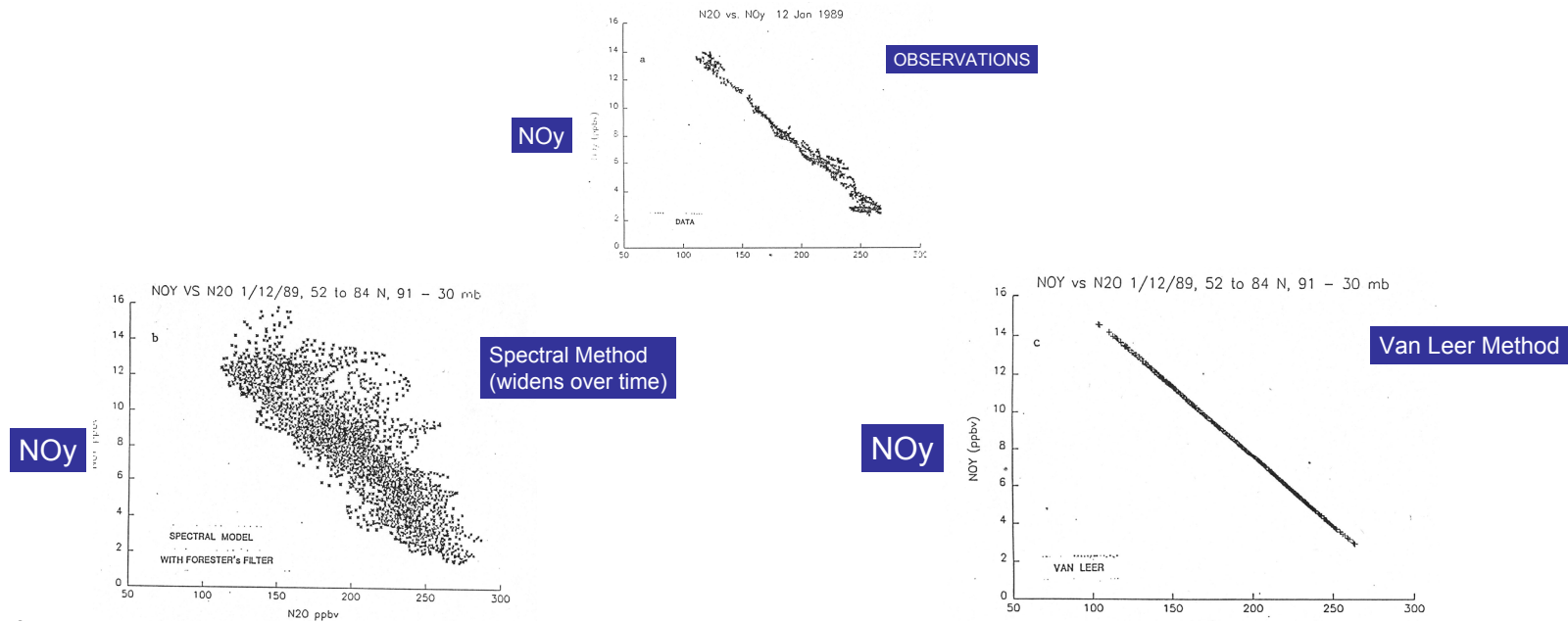
Analytical pre-existing functional relationship curve ψ (linear)

If \mathcal{T} is 'semi-linear' then linear pre-existing functional relations are preserved:

$$\xi_k^{n+1} = \mathcal{T}(\xi_j^n) = \mathcal{T}(a\chi_j^n + b) = a\mathcal{T}(\chi_j^n) + b\mathcal{T}(1) = a\mathcal{T}(\chi_j^n) + b = a\chi_k^{n+1} + b.$$

→ If transport operator is non-linear the relationship might be violated.

Analyzing scatter plots



Figures from R.Rood's talk at the 2008 NCAR ASP colloquium

Analytical pre-existing functional relationship curve ψ (linear)

→ carefully designed finite-volume schemes are 'semi-linear' even with limiters/filters!
(Thuburn and McIntyre, 1997; Lin and Rood, 1996)

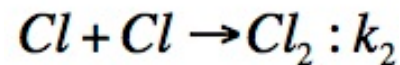
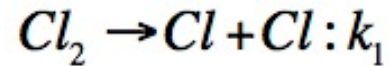
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

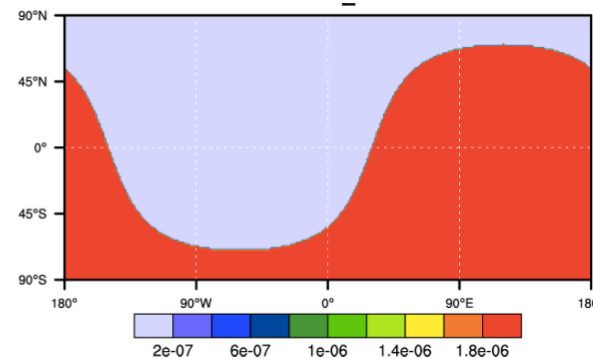
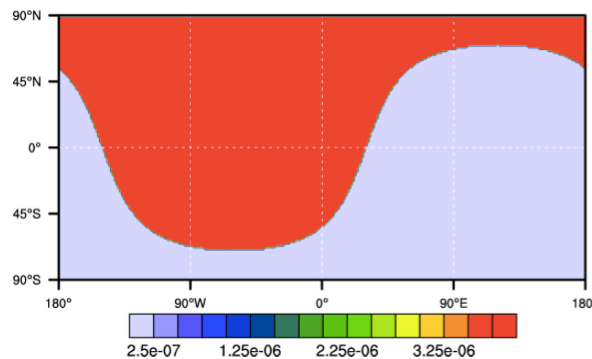
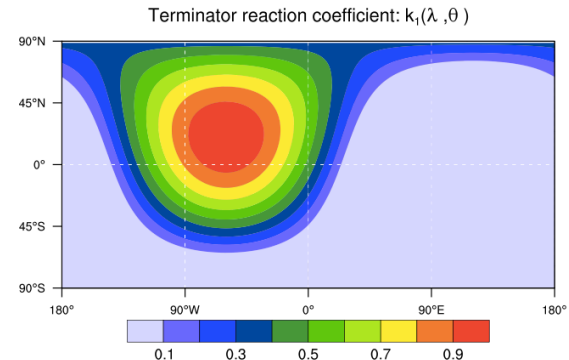
See: <http://www.cgd.ucar.edu/cms/pel/terminator.html>



- Consider 2 reactive chemical species, Cl and Cl₂ :



- Steady-state solution (no flow):

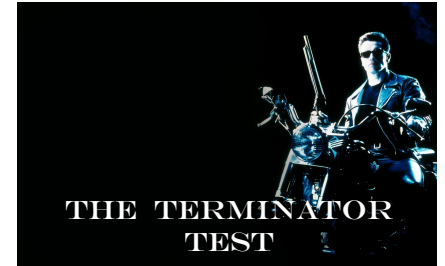


- In any flow-field $\text{Cl}_y = \text{Cl} + 2 * \text{Cl}_2$ should be constant at all times (correlation preservation)

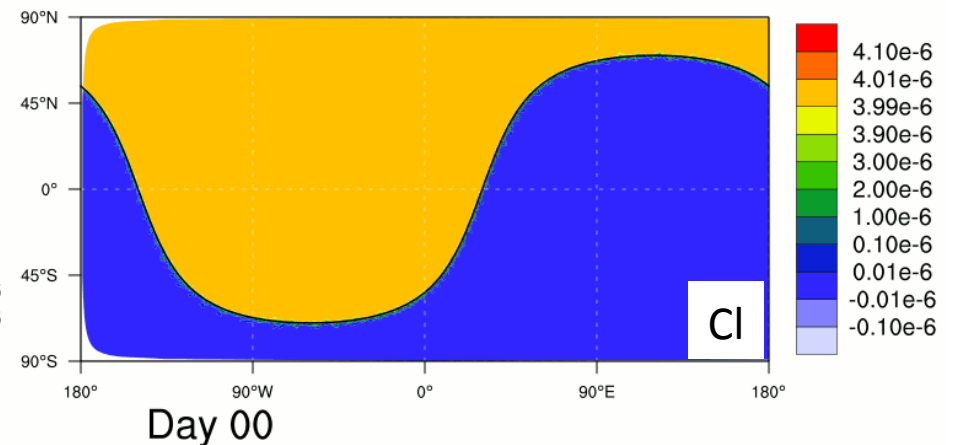
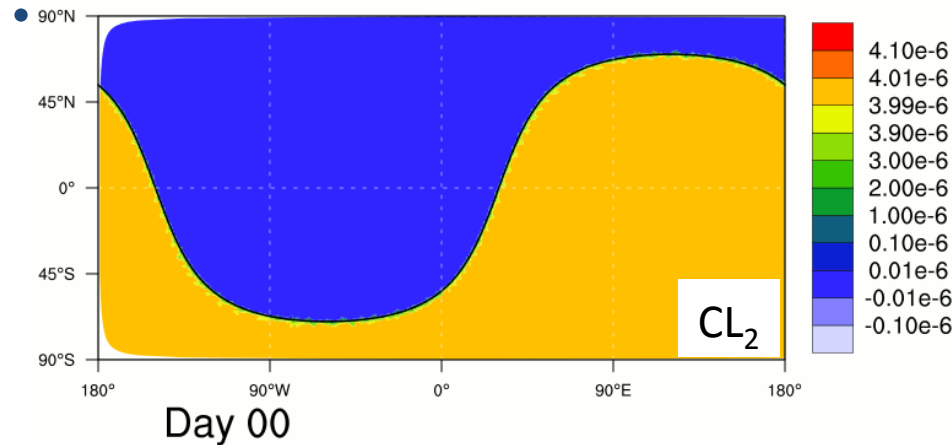
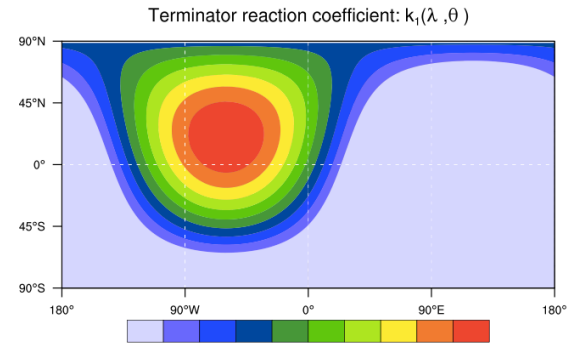
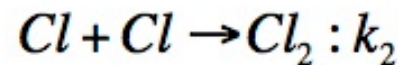
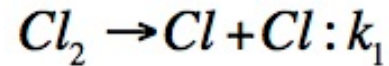
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See: <http://www.cgd.ucar.edu/cms/pel/terminator.html>



- Consider 2 reactive chemical species, Cl and Cl₂ :

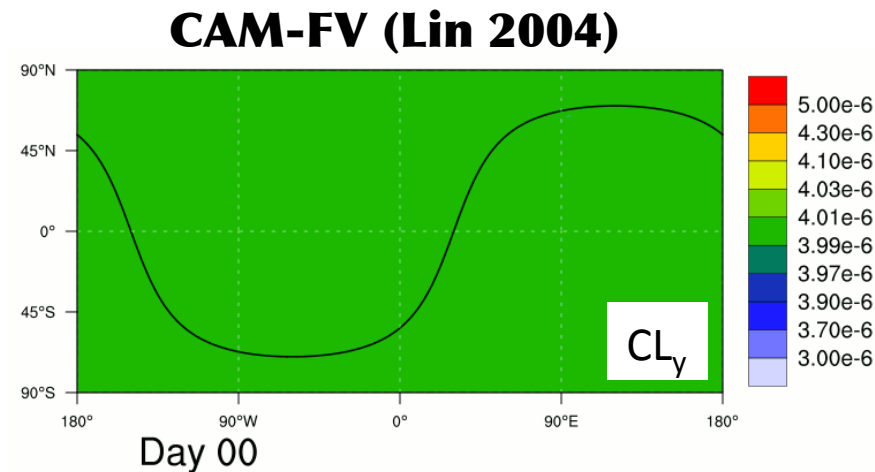
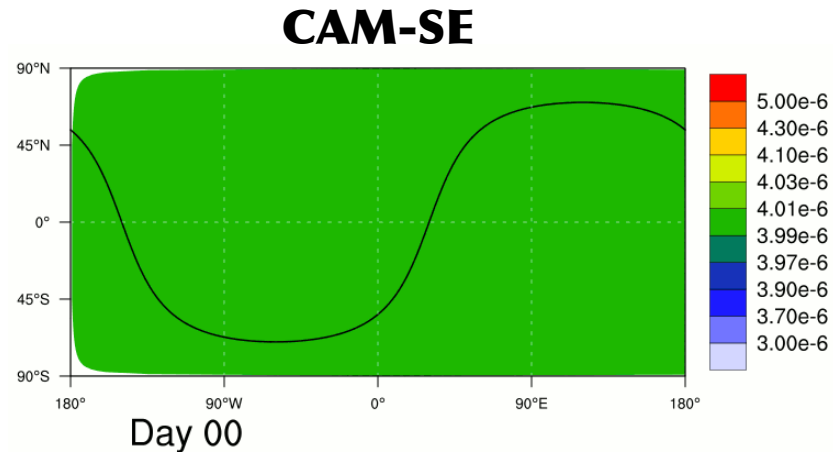
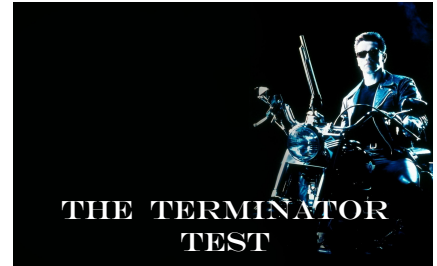


- In any flow-field $\text{Cl}_y = \text{Cl} + 2 * \text{Cl}_2$ should be constant at all times (linear correlation preservation).

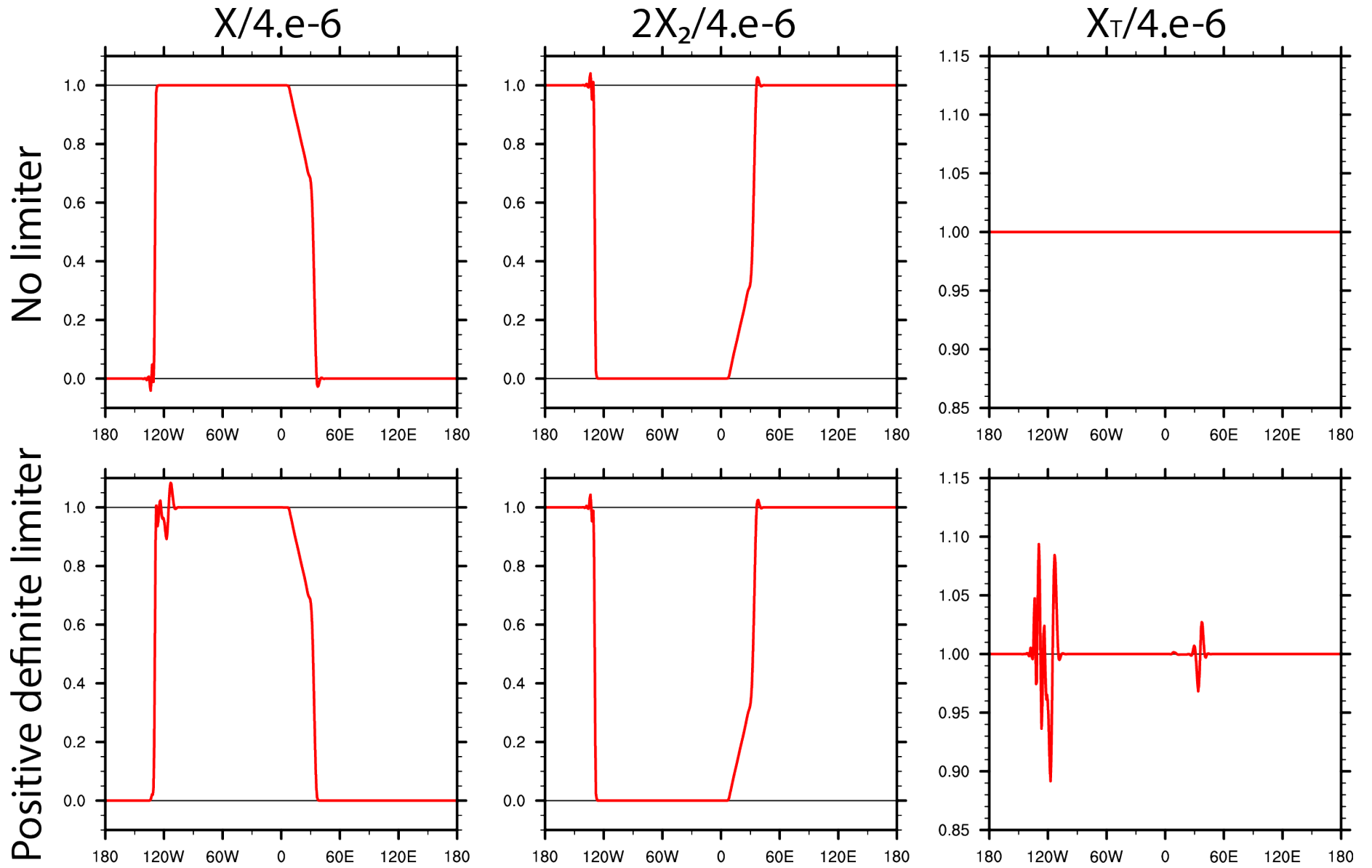
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

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

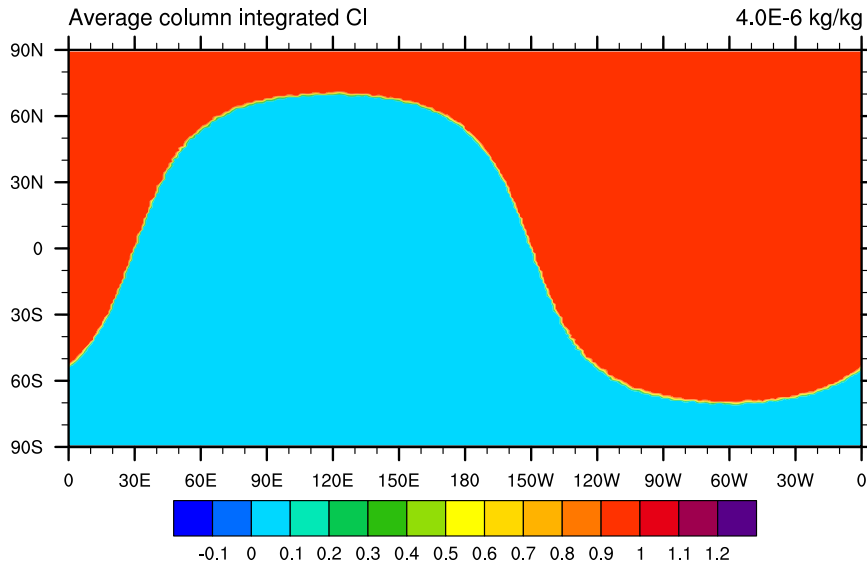


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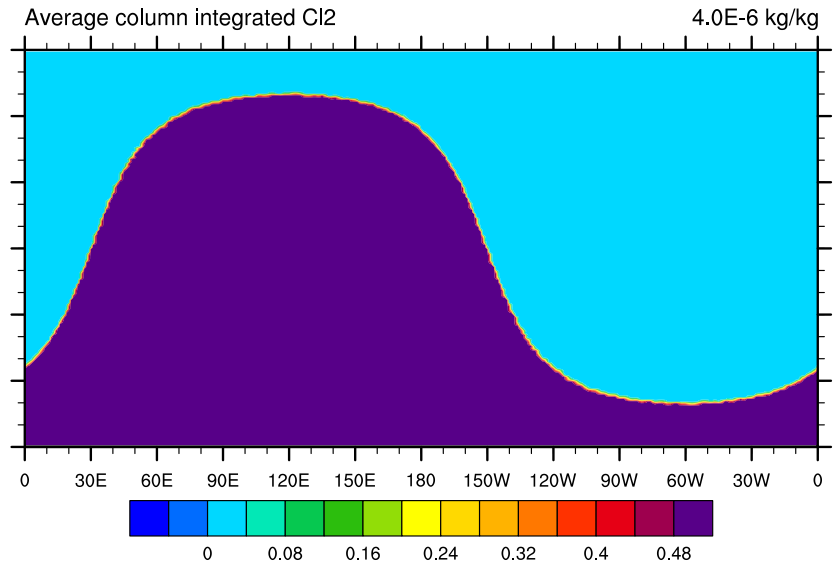


3D version: Initial condition

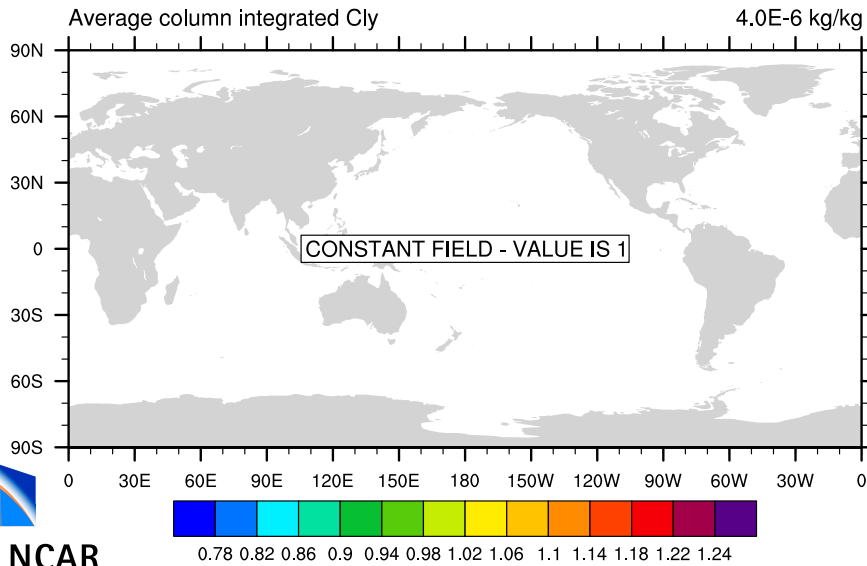
day 0



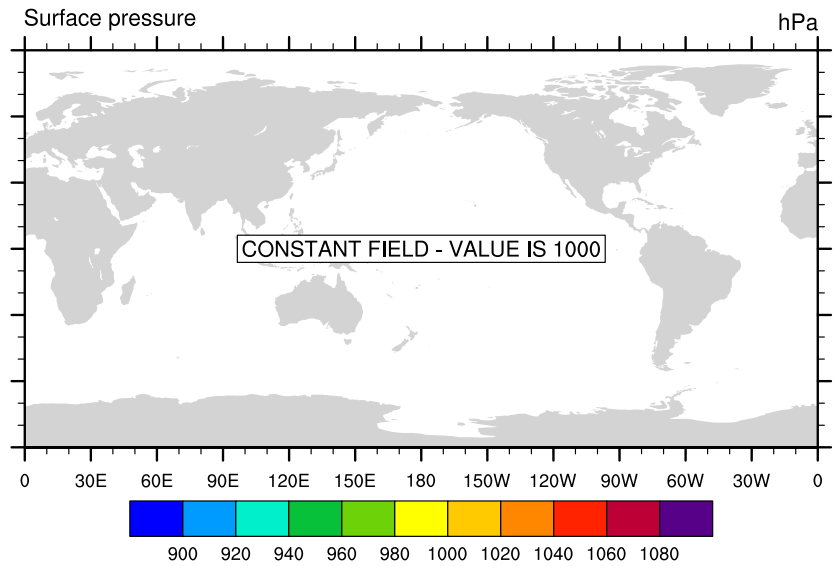
day 0



day 0

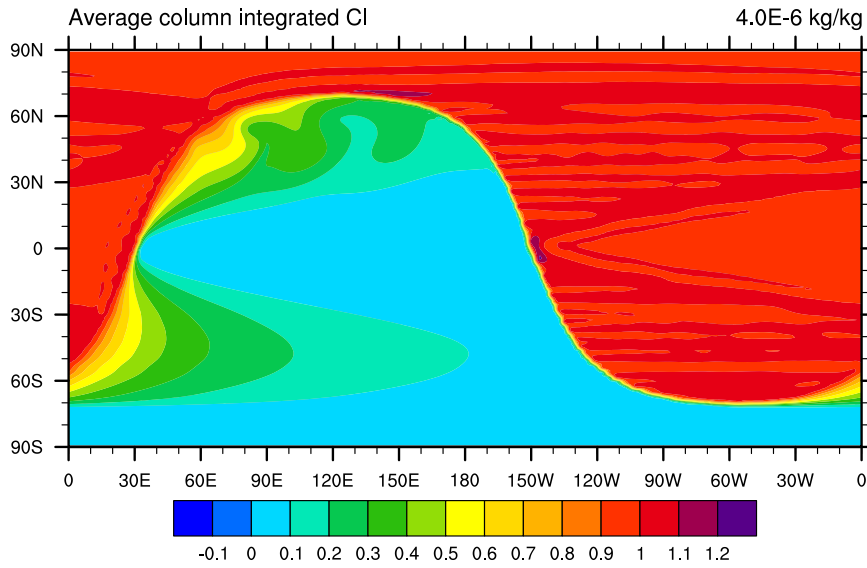


day 0

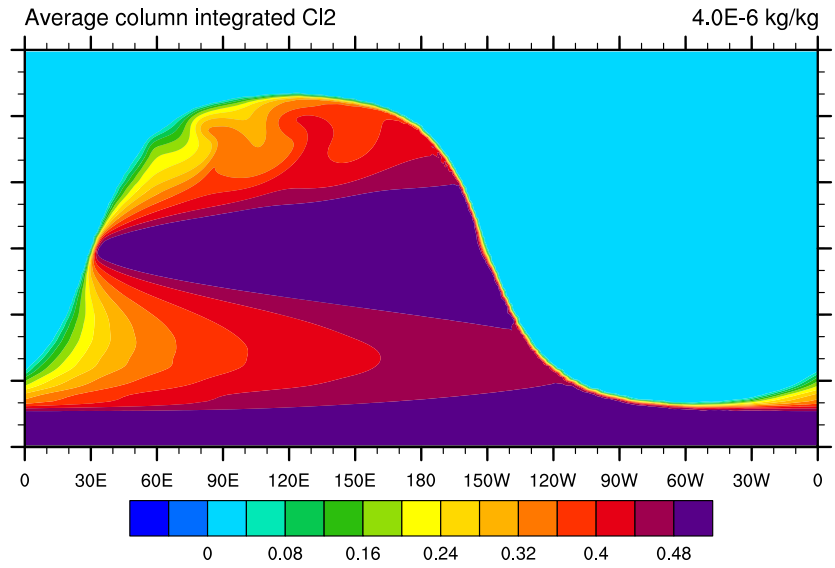


CAM-SE

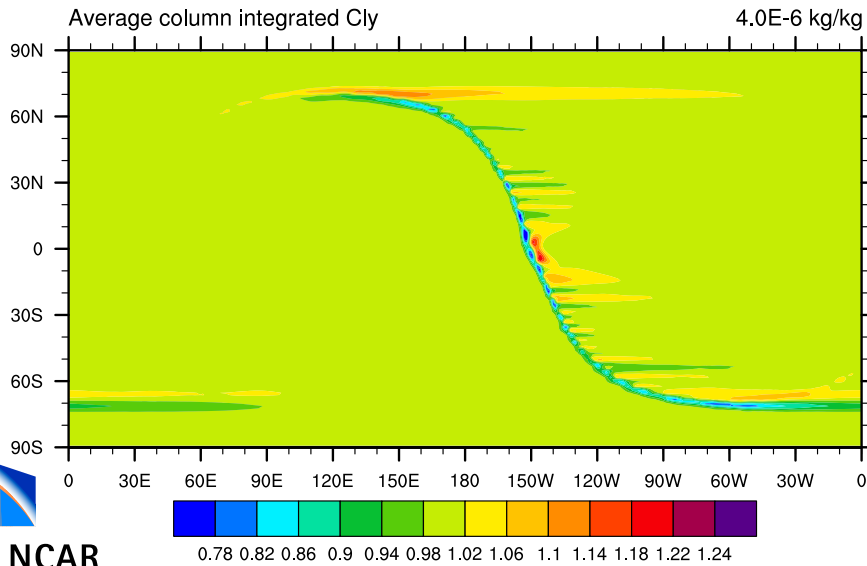
day 9



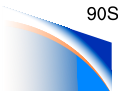
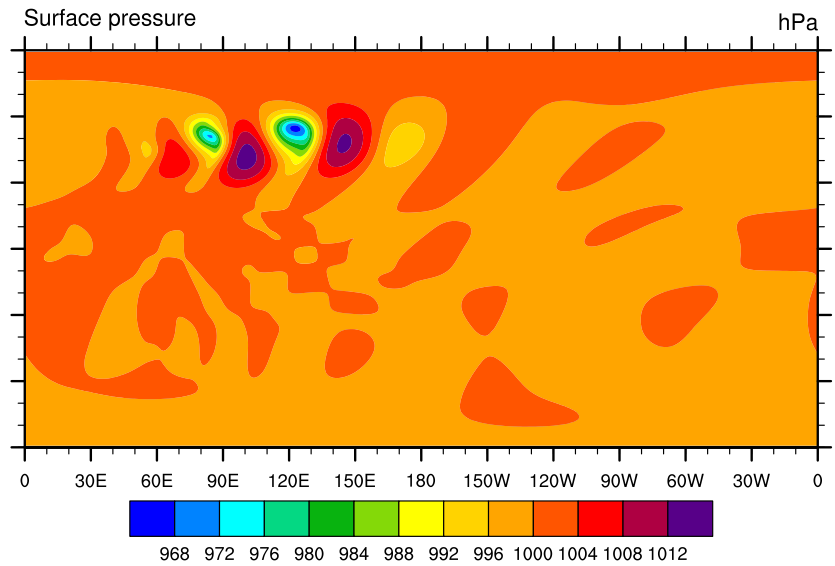
day 9



day 9

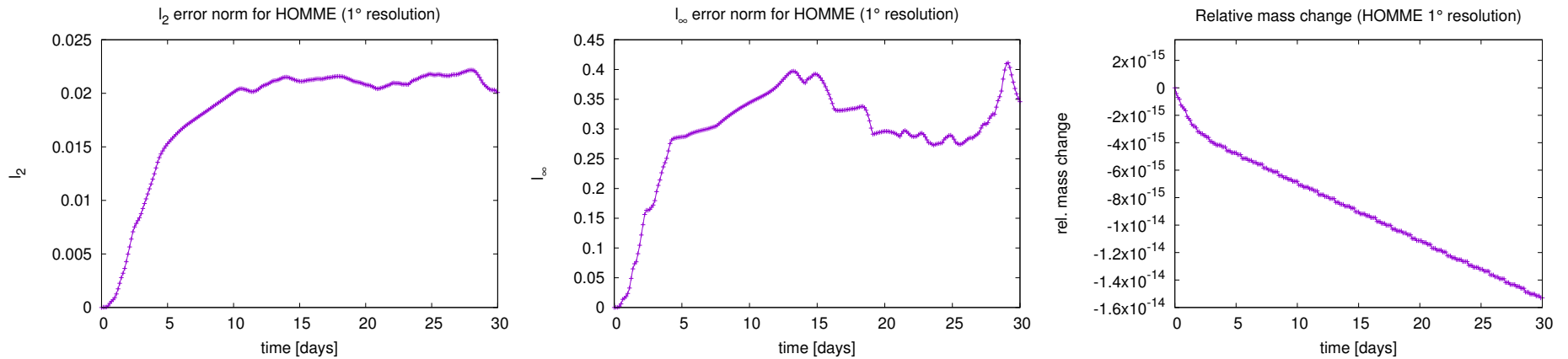


day 9

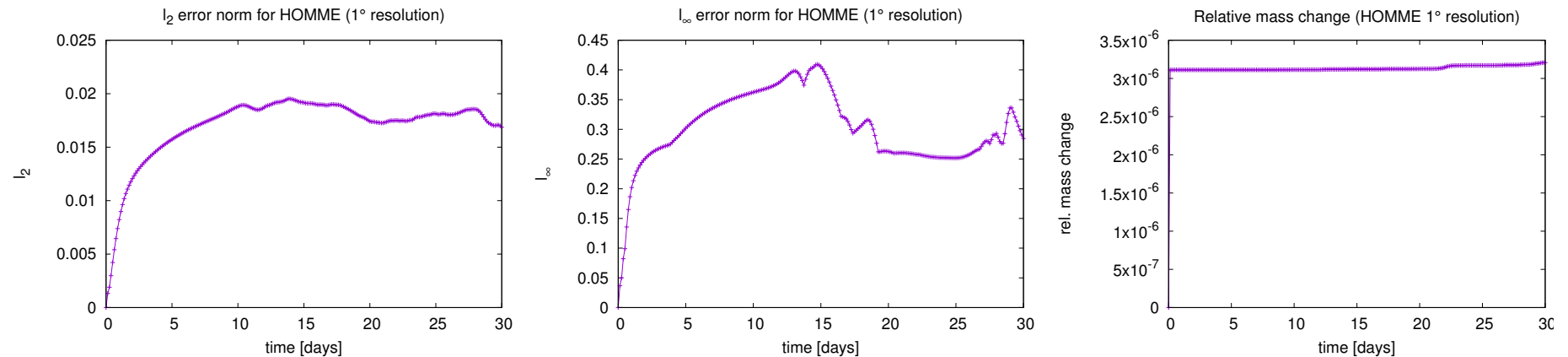


NCAR

Diagnostics for terminator test: chemistry time-step = 900s



Diagnostics for terminator test: chemistry time-step = 1800s



Conserving sum of “families” of species

Chlorine (in CAM-chemistry)

Total Organic Chlorine (set at the surface)

$$T_{Cl}^{ORG} = CH_3Cl + 3CFCl_3 + 2CF_2Cl_2 + 3ClCl_2FC Cl F_2 + HCF_2Cl + 4CCl_4 + 3CH_3CCl_3.$$

Total Inorganic Chlorine (created from break down of T_{Cl}^{ORG})

$$T_{Cl}^{INORG} = Cl + ClO + OClO + 2Cl_2 + 2Cl_2O_2 + HOCl + ClONO_2 + HCl,$$

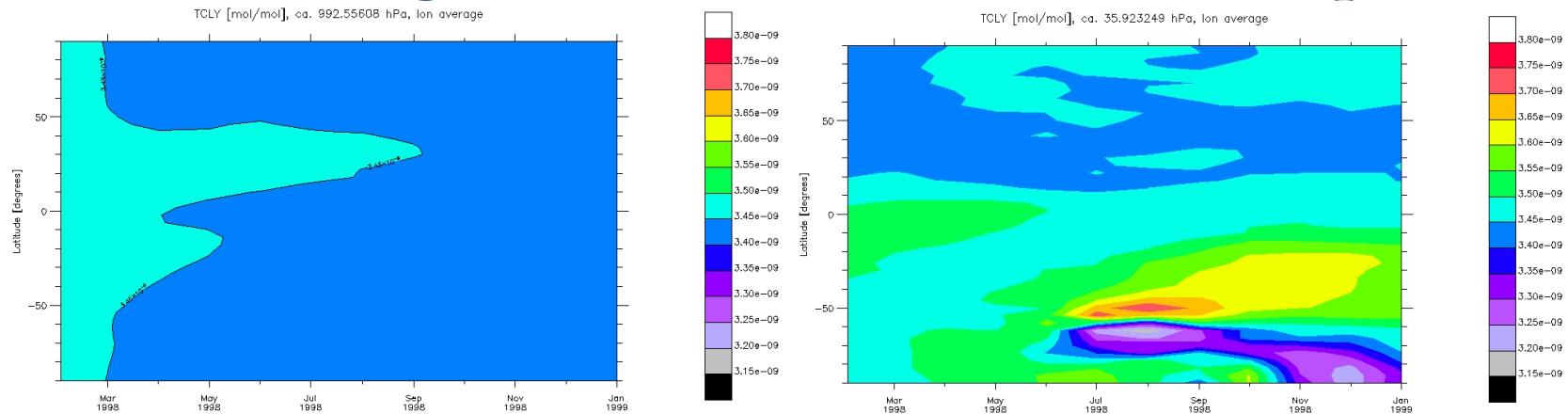
Total Chlorine

$$TCLY = T_{Cl}^{ORG} + T_{Cl}^{INORG}$$

Total chlorine TCLY should be conserved in the upper troposphere and stratosphere (despite complex chemical reactions between the different chlorine species)!

Reactants	Products	Rate
PAN + M	→ CH ₃ CO ₃ + NO ₂ + M	k(CH ₃ CO ₃ +NO ₂ +M)·1.111E28 ·exp(-14000/T)
CH ₃ CO ₃ + CH ₃ CO ₃	→ 2·CH ₃ O ₂ + 2·{CO ₂ }	2.50E-12·exp(500/T)
GLYALD + OH	→ HO ₂ + .2·GLYOXAL + .8·CH ₂ O + .8·{CO ₂ }	1.00E-11
GLYOXAL + OH	→ HO ₂ + CO + {CO ₂ }	1.10E-11
CH ₃ COOH + OH	→ CH ₃ O ₂ + {CO ₂ } + H ₂ O	7.00E-13
C ₂ H ₅ OH + OH	→ HO ₂ + CH ₃ CHO	6.90E-12·exp(-230/T)
C ₃ H ₆ + OH + M	→ PO ₂ + M	ko=8.00E-27·(300/T) ^{3.50} ; ki=3.00E-11; f=0.50

Conserving sum of “families” of species



(left) longitude-averaged surface TCLY as a function of time and latitude: Constant!
 (right) same as (left) but near tropopause: Spurious 7% deviations (near sharp gradients)!

Problem?

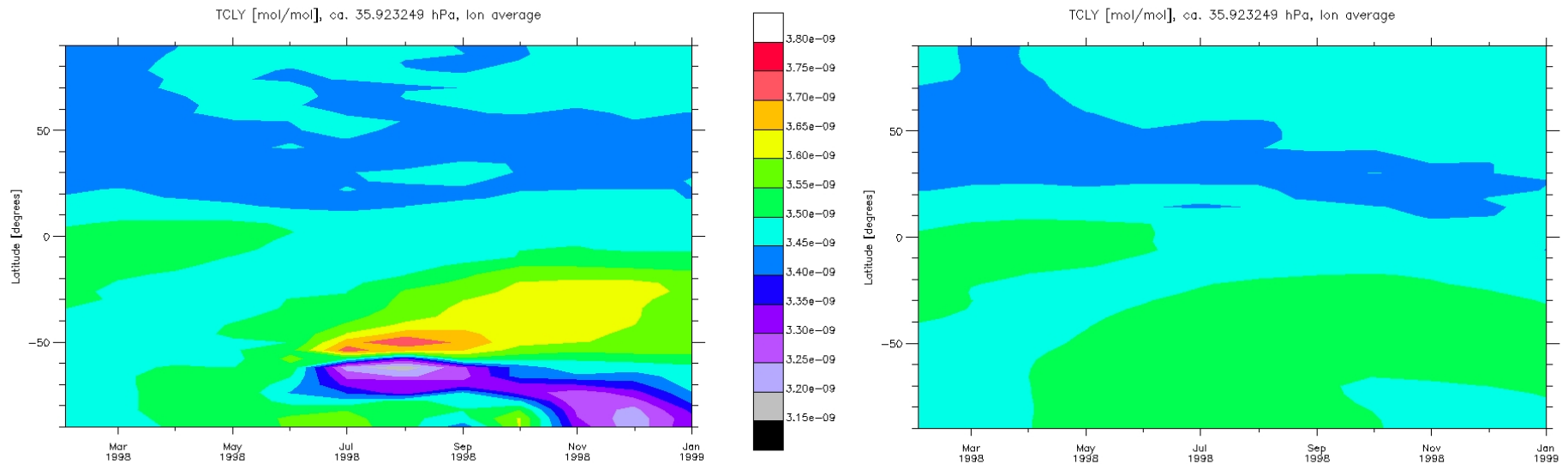
Transport scheme can not maintain the sum when transporting the species individually:

$$\sum_{i=1}^{N_x} \mathcal{T}(\chi_i) \neq \mathcal{T} \left(\sum_{i=1}^{N_x} \chi_i \right),$$

“Semi-linear” property is a necessary but not sufficient condition for conserving a sum of more than 2 tracers

where N_x is the number of species χ_i .

Conserving sum of “families” of species



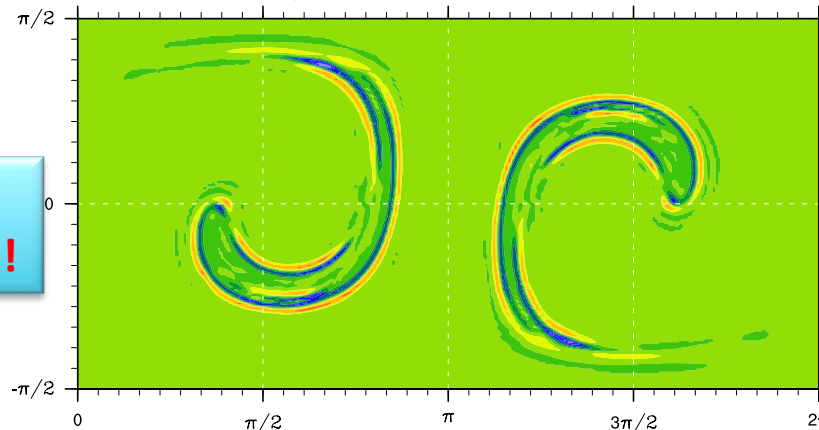
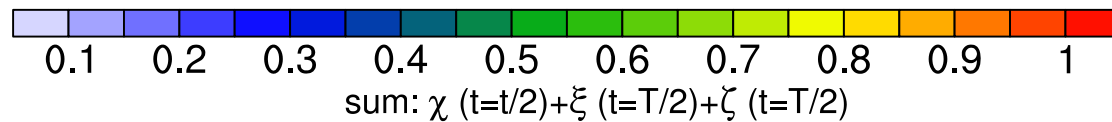
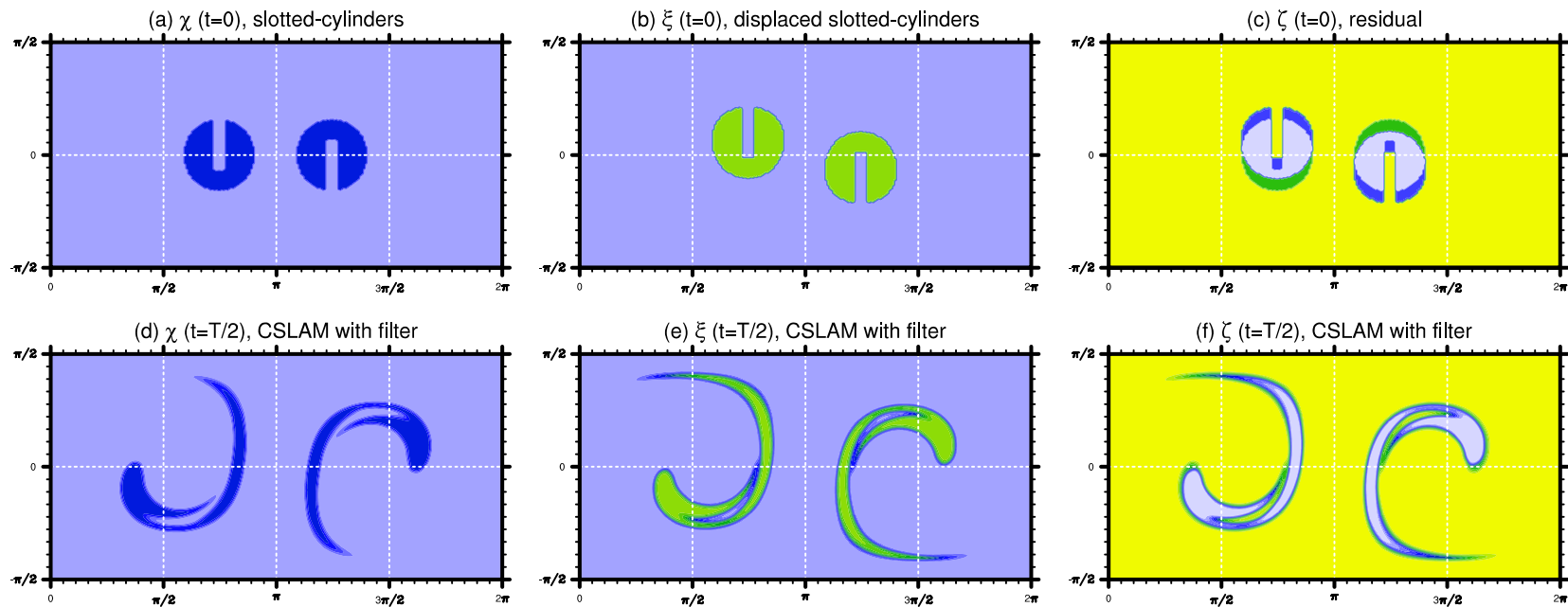
(left) same as previous slide:

- large unphysical deviations from constancy in TCLY near the edge of the polar stratospheric vortex \Rightarrow less TCLY over South pole \Rightarrow less ozone loss (error on the order of 10%).

(right) same as (left) but using a fixer:

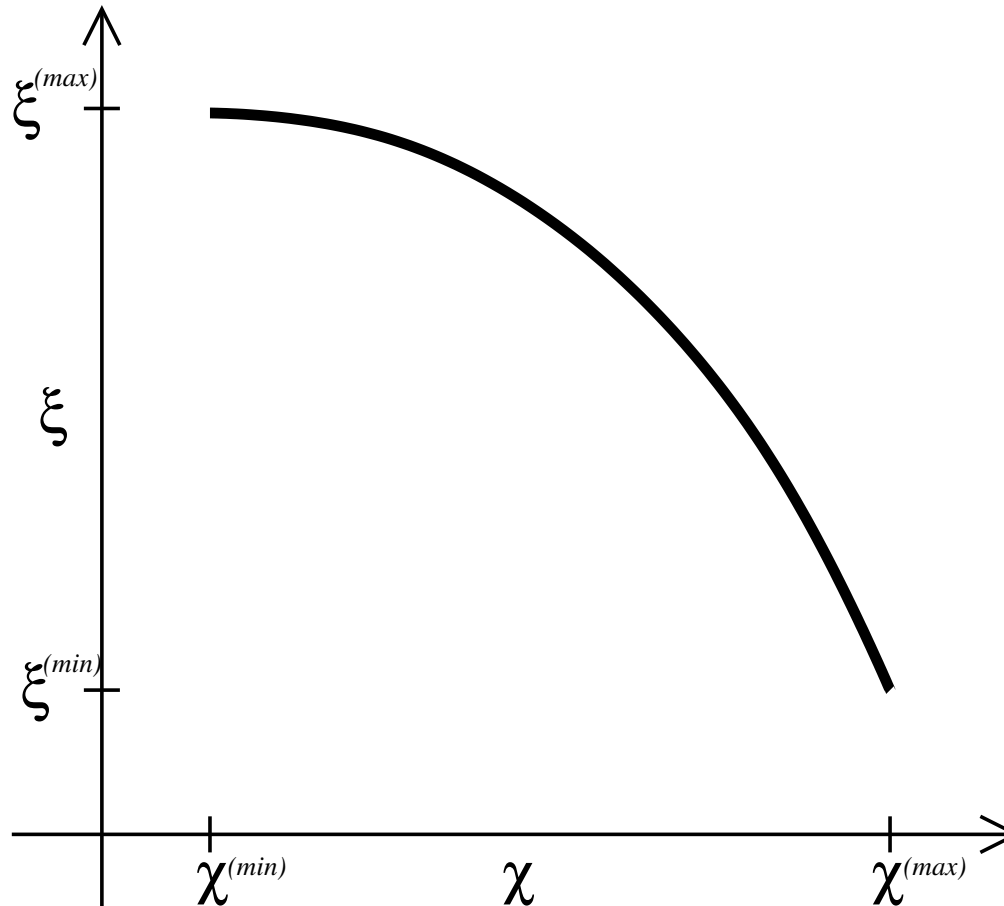
- (i) transport the individual species
- (ii) transport the total
- in each grid cell scale the individual species by the difference between (i) and (ii)

Simple idealized “family of species” test



This test does not rely on an analytical solution!

Analyzing scatter plots

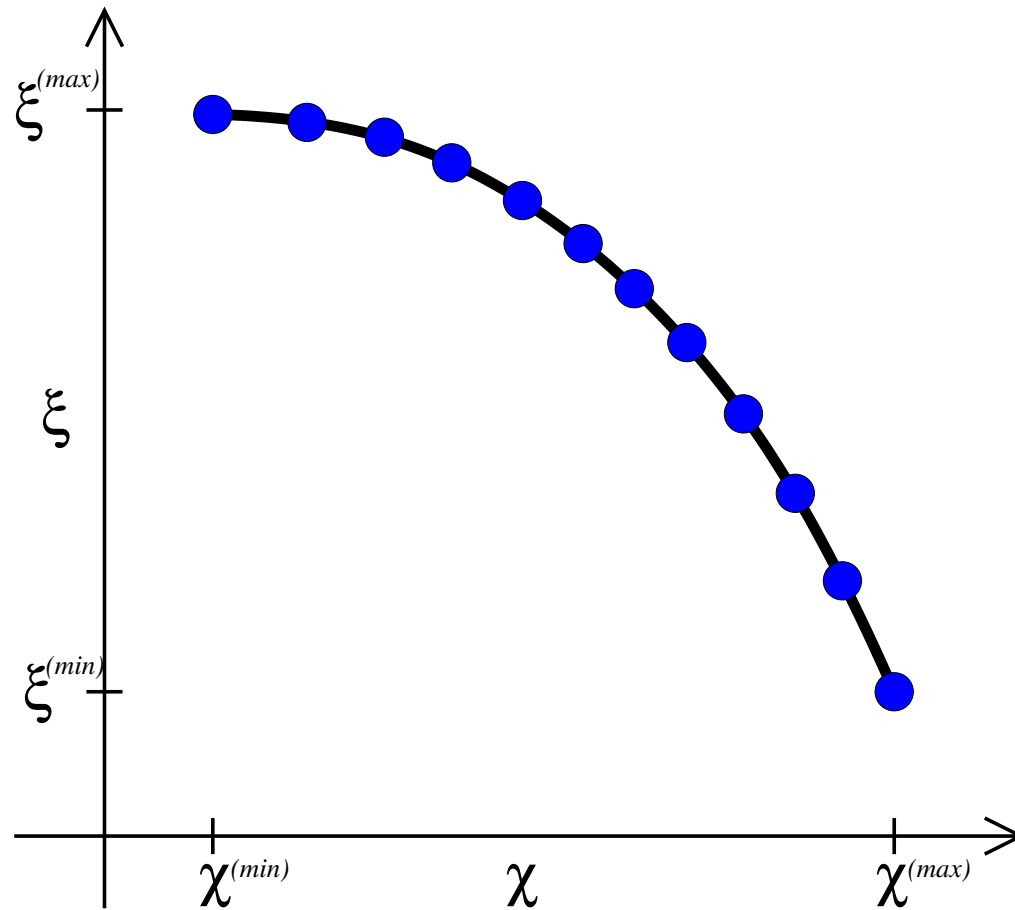


Analytical pre-existing functional relationship curve ψ

$$\xi = \psi(\chi) = a \cdot \chi^2 + b,$$

where a and b are constants so that ψ is concave or convex in $[\chi^{(min)}, \chi^{(max)}]$

Analyzing scatter plots

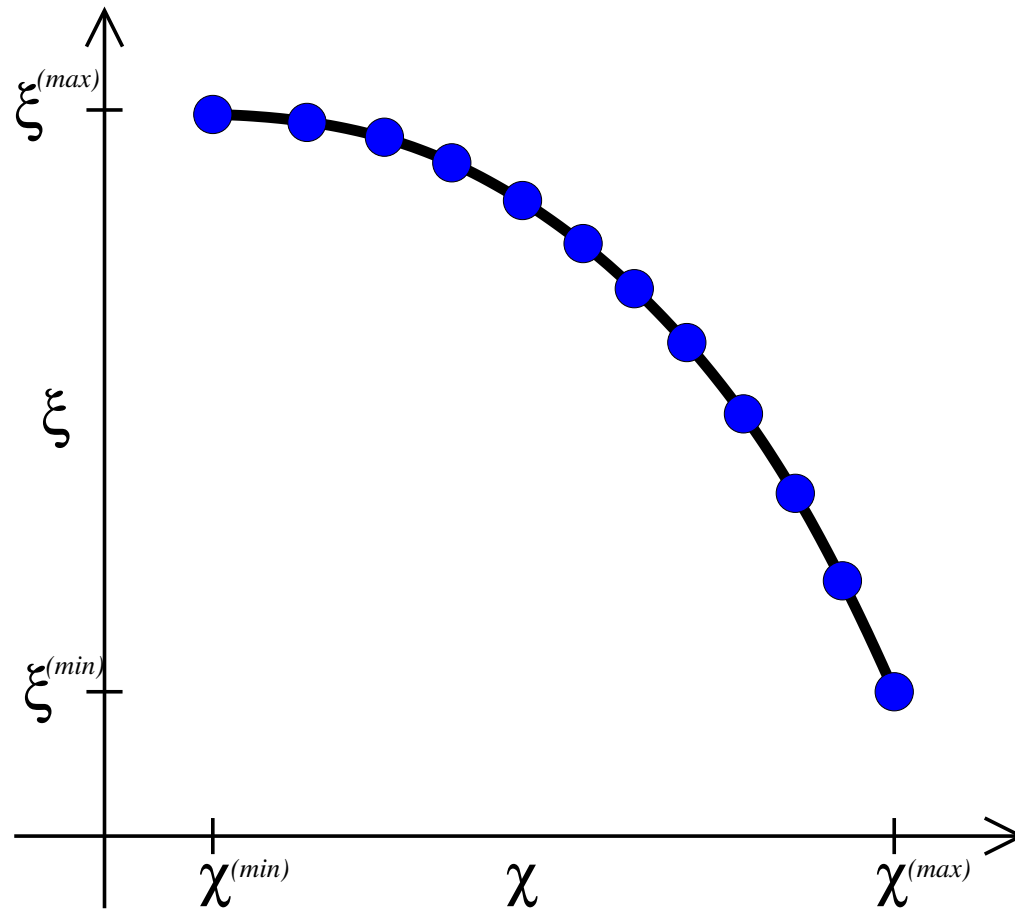


Discrete pre-existing functional relation (initial condition)

$$\xi_k = \psi(\chi_k) = a \cdot (\chi_k)^2 + b, \quad k = 1, \dots, K,$$

where a and b are constants so that ψ is concave or convex in $[\chi^{(min)}, \chi^{(max)}]$

Analyzing scatter plots

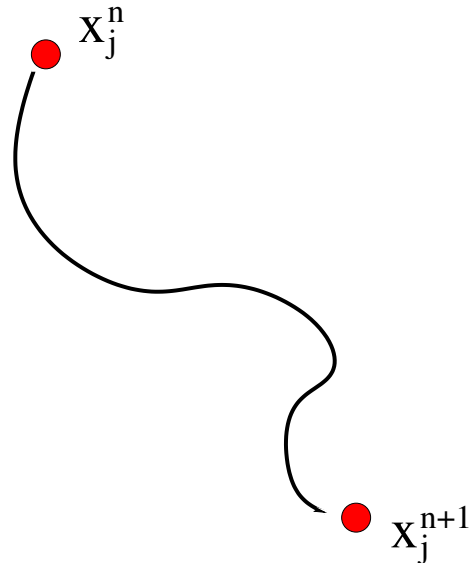


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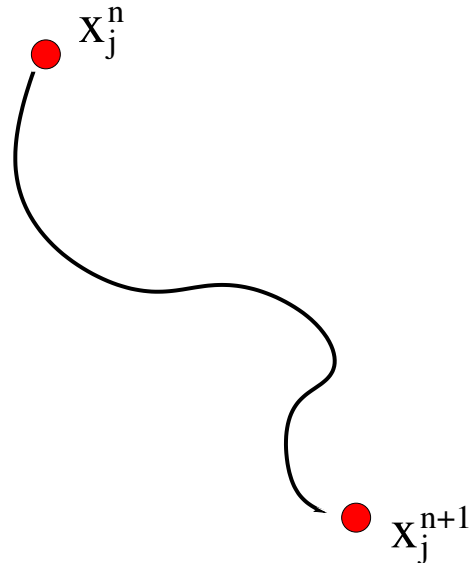


A fully Lagrangian model will maintain pre-existing functional relation

$$\chi_k^{n+1} = \chi_k^n, \quad \xi_k^{n+1} = \xi_k^n$$

following parcel trajectories (without 'contour-surgery' or other mixing mechanisms)

Analyzing scatter plots

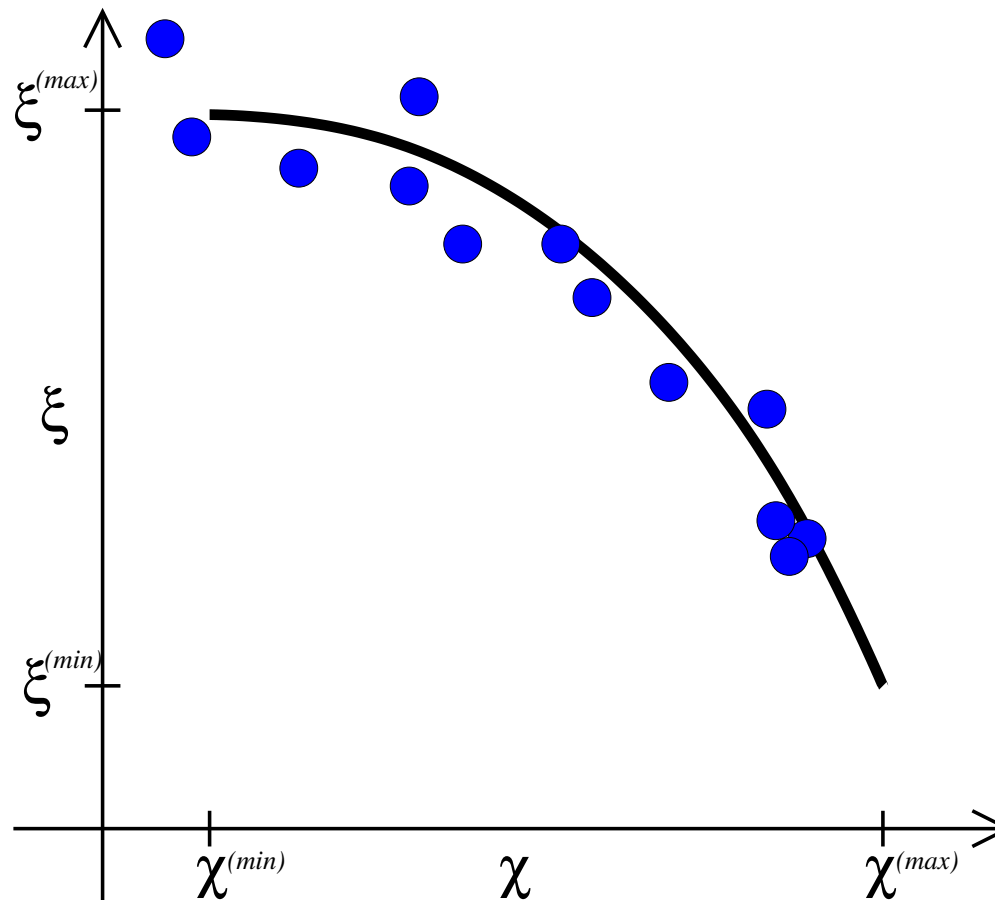


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Analyzing scatter plots

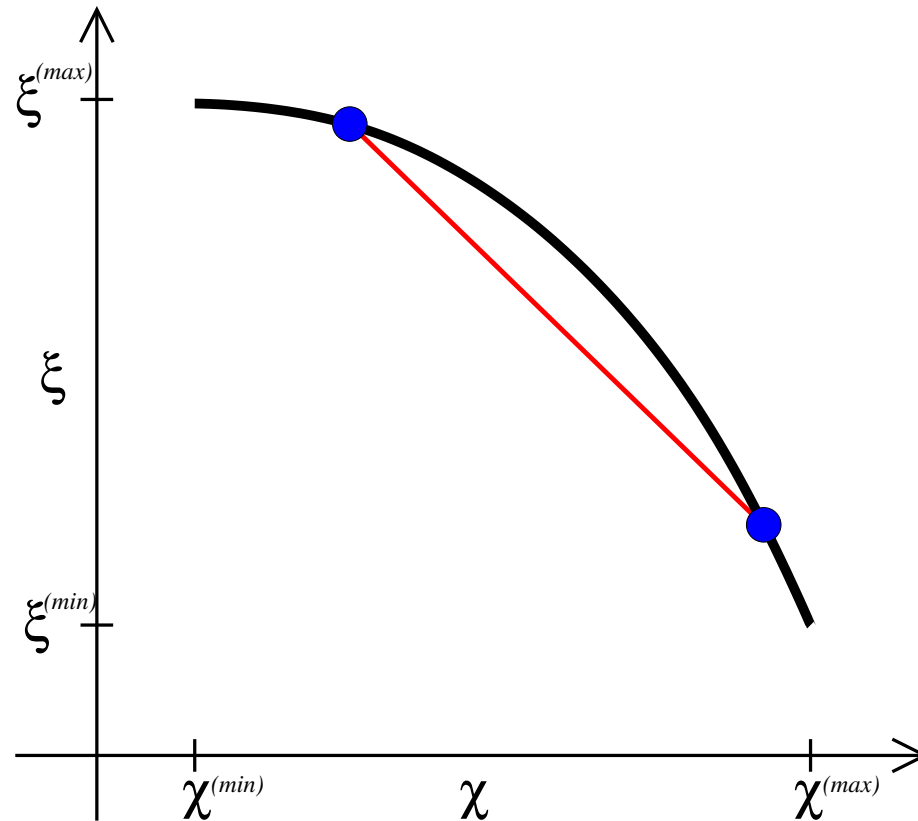


Any Eulerian/semi-Lagrangian scheme will disrupt pre-existing functional relation

$$\xi_k^{n+1} = \mathcal{T}(\xi_j^n) \neq a \cdot \mathcal{T}(\chi_j^n)^2 + b, \quad j \in \mathcal{H}$$

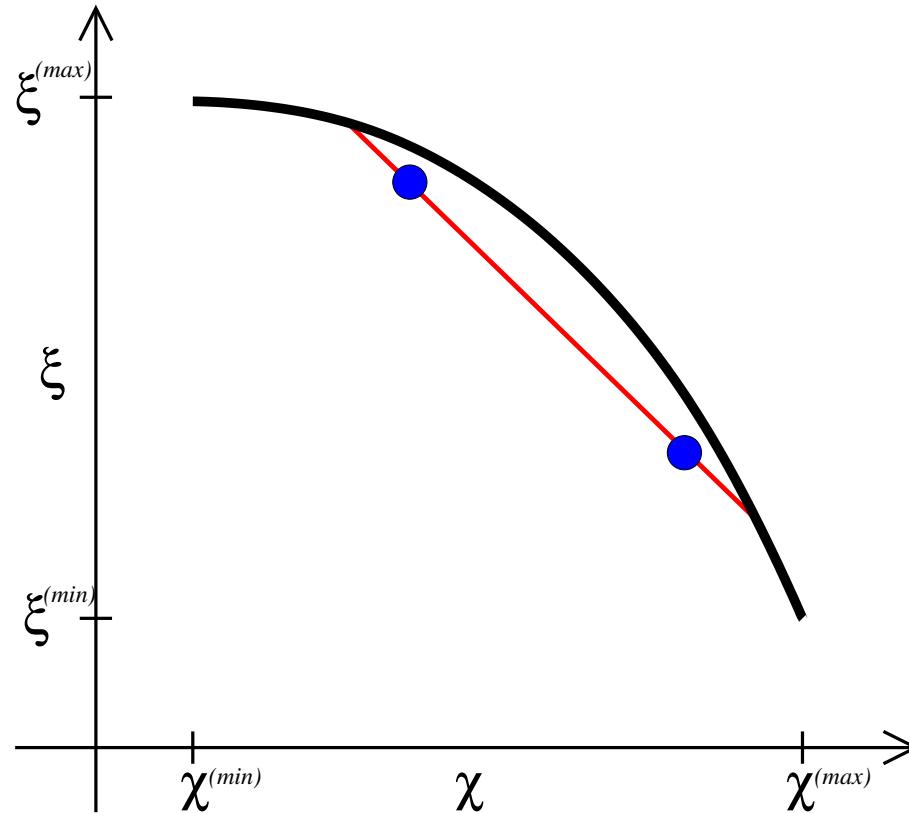
where \mathcal{T} is the transport operator and \mathcal{H} the set of indices defining the 'halo' for \mathcal{T} .

'Real' mixing, e.g., observed during polar vortex breakup (Vaugh et al., 1997)



'Real mixing' (when occurring) will tend to replace the functional relation by a scatter by linearly interpolating along mixing lines between pairs of points

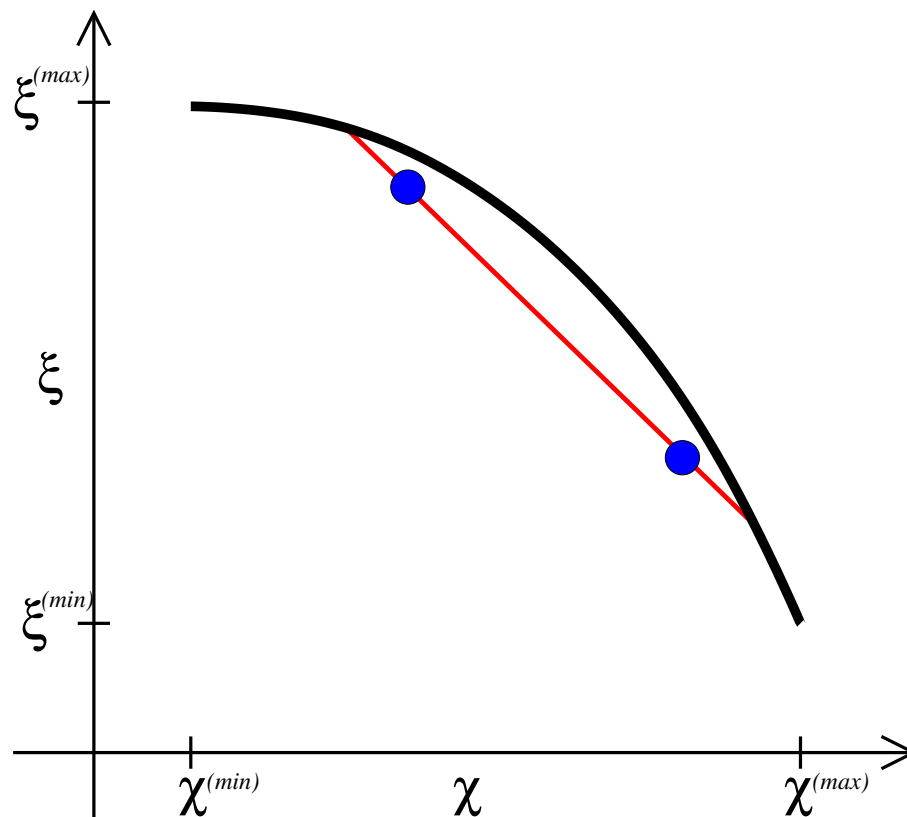
'Real' mixing, e.g., observed during polar vortex breakup



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→ Ideally numerical mixing should = 'real mixing'!

However, it may be shown mathematically that schemes that exclusively introduce 'real mixing' are 1st-order schemes (Thuburn and McIntyre, 1997).

Classification of numerical mixing on scatter plots



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Classification of numerical mixing on scatter plots

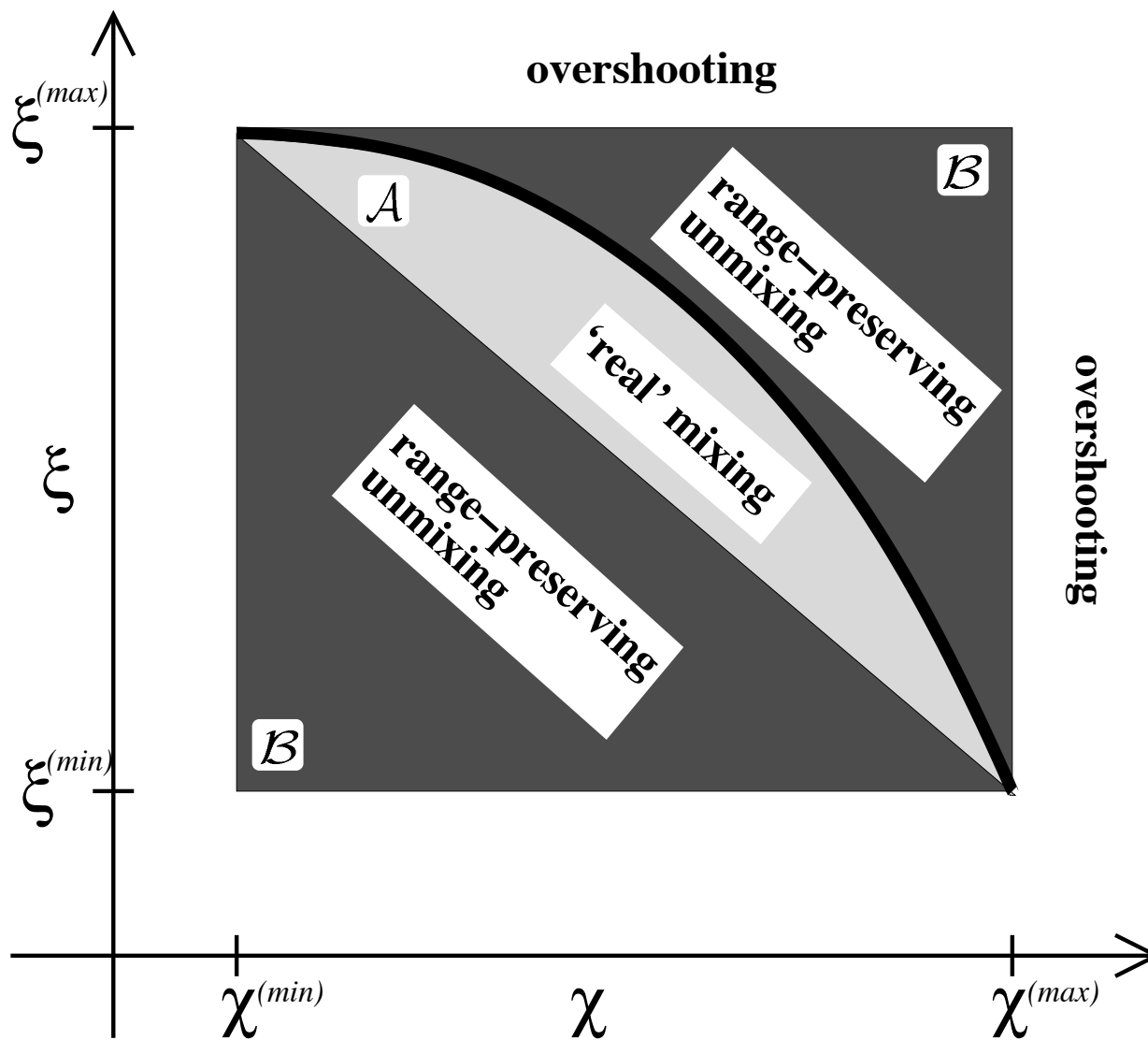
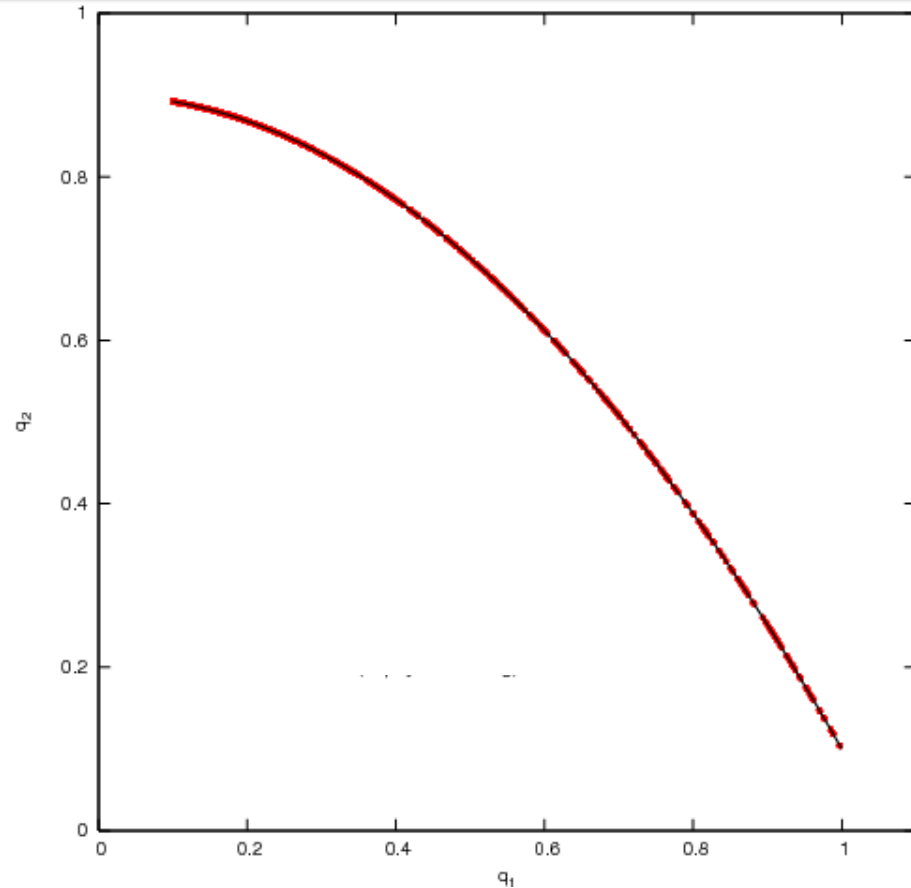
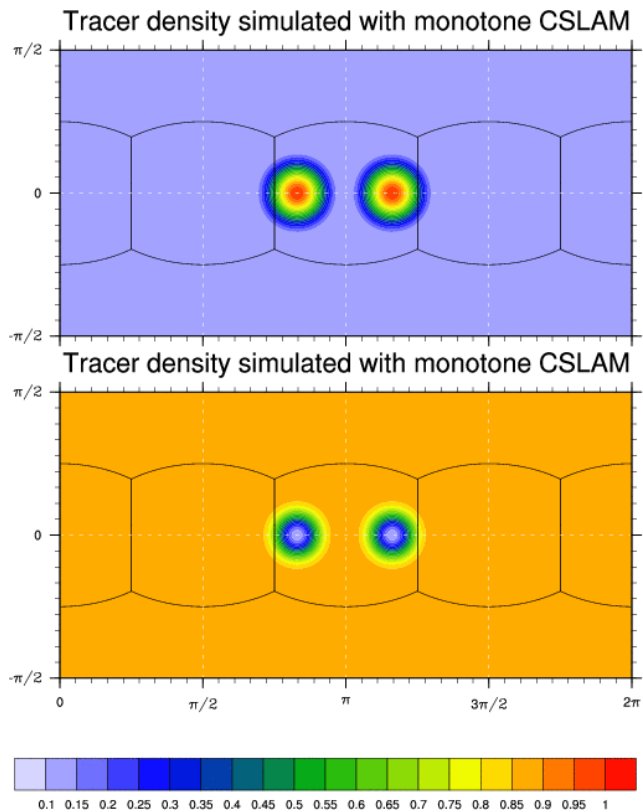


Figure from (Lauritzen and Thuburn, 2012)

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

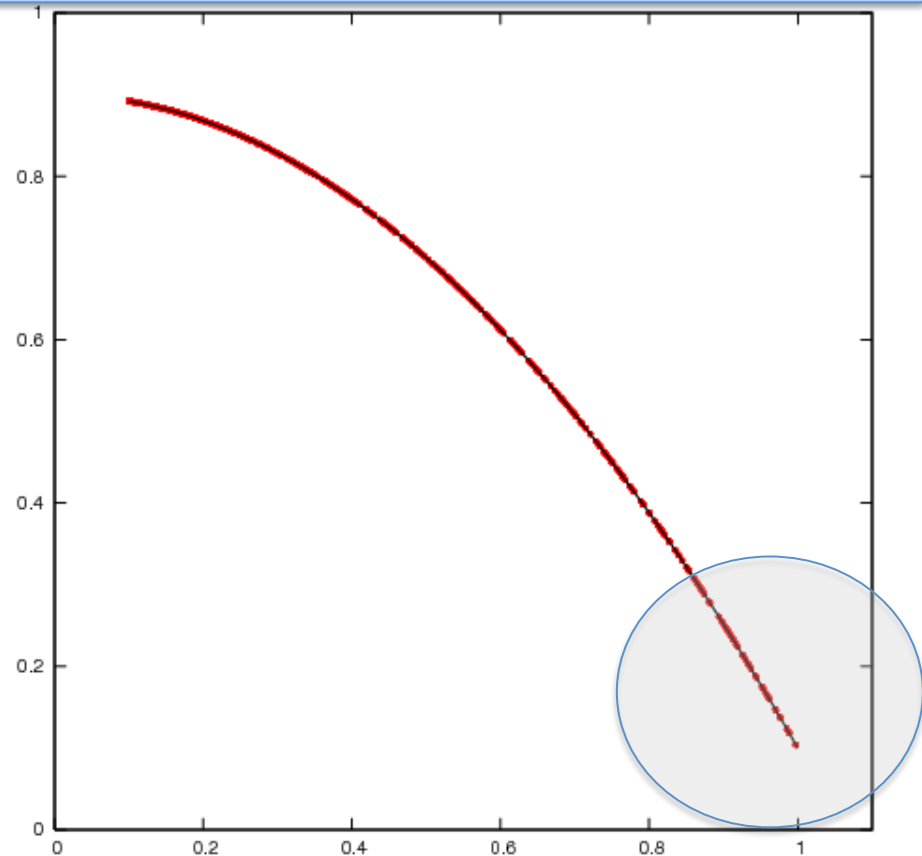
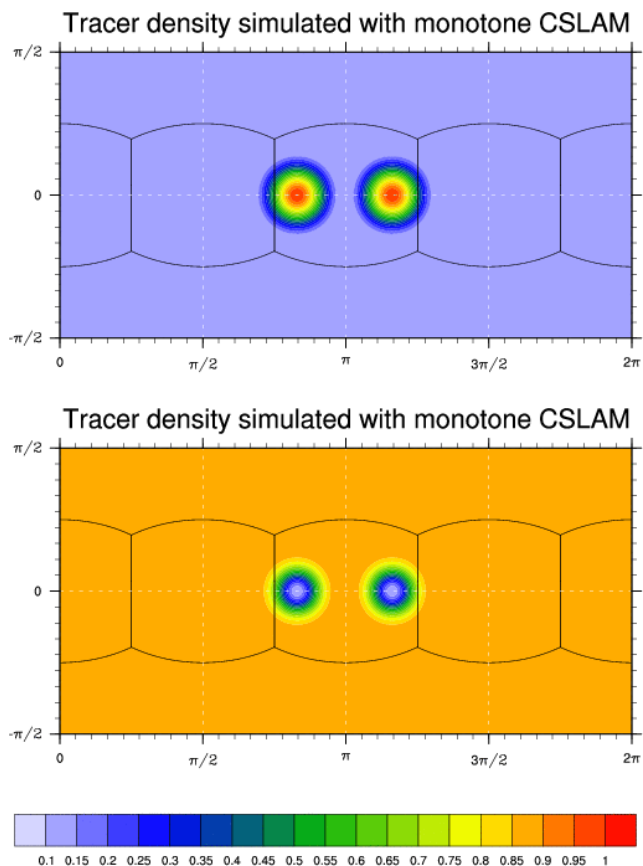
First-order scheme: only 'real mixing'



Nair and Lauritzen (2010) flow field

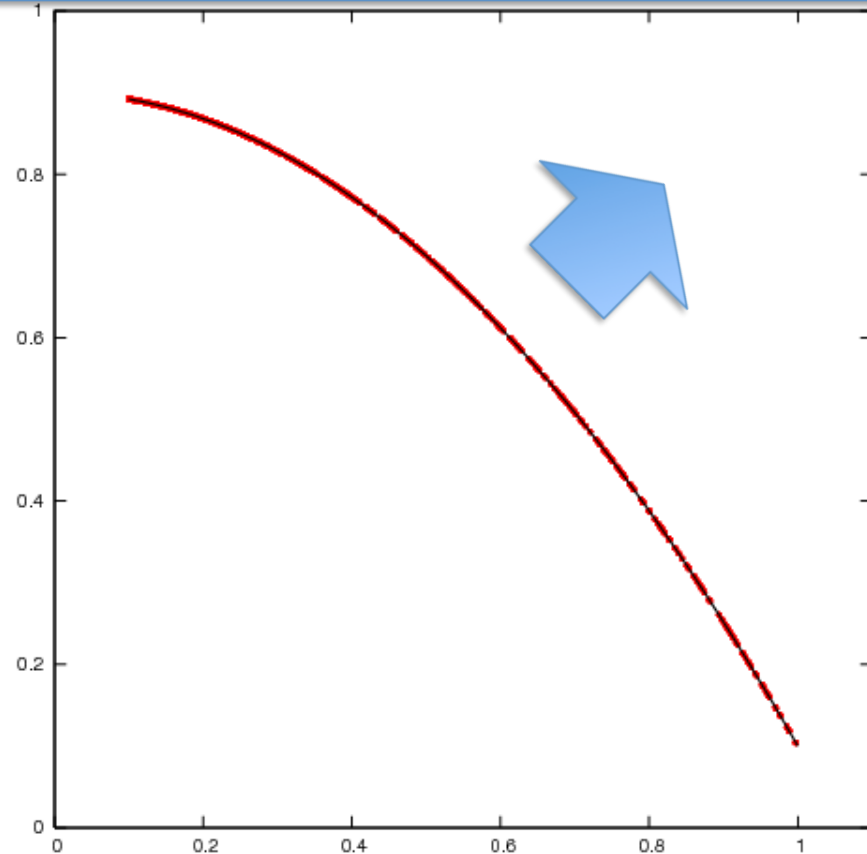
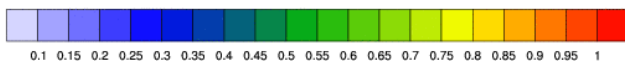
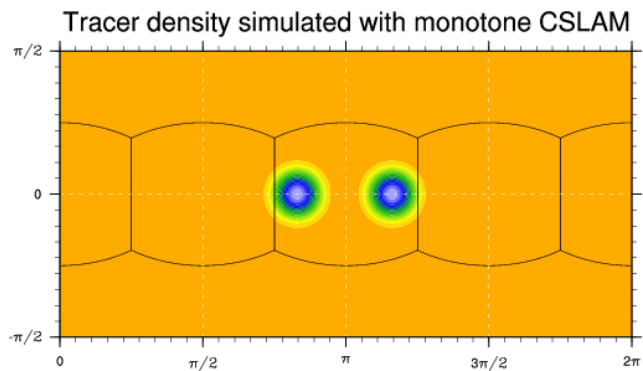
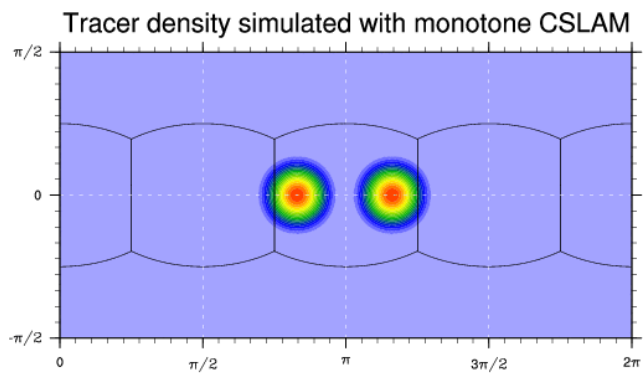
Preserving pre-existing functional relation between tracers under challenging flow conditions

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



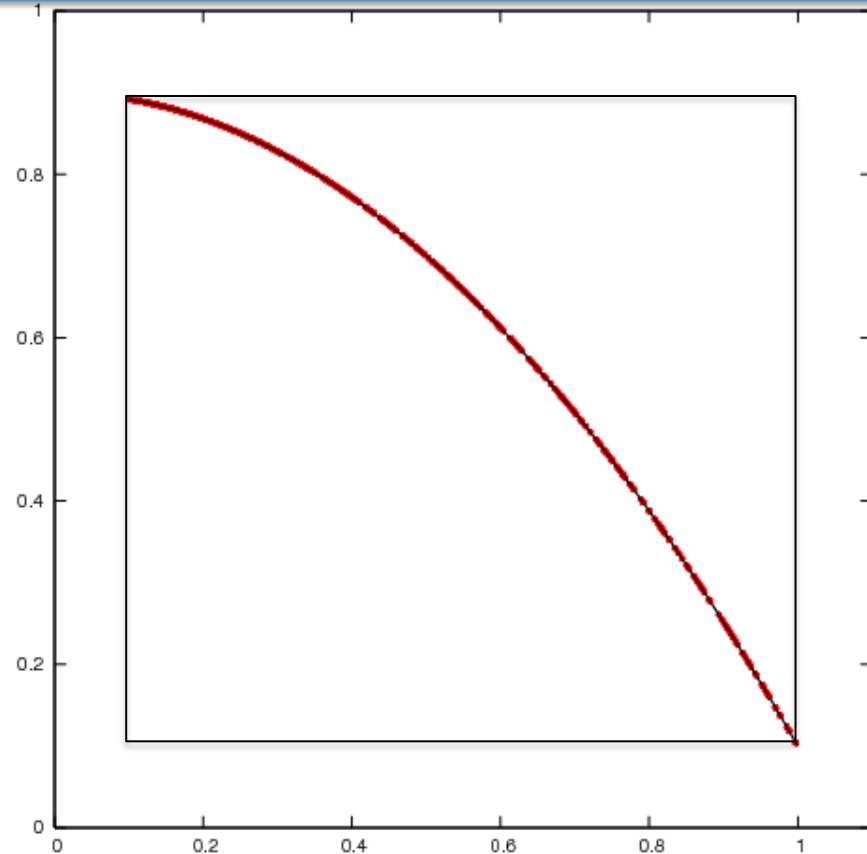
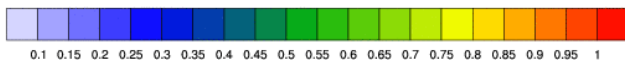
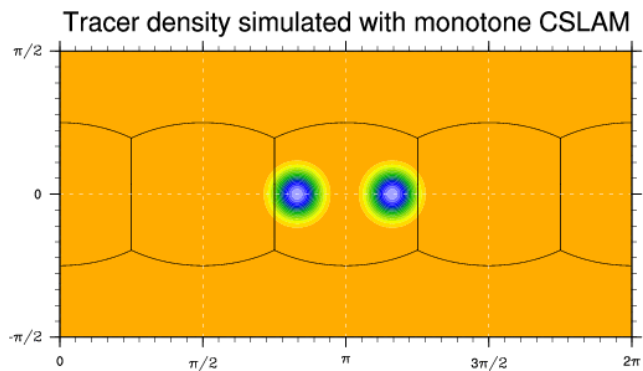
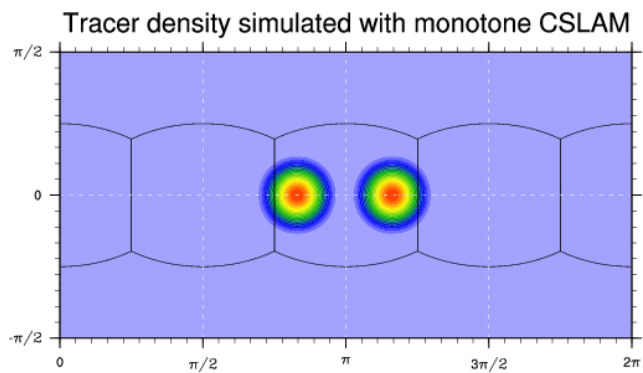
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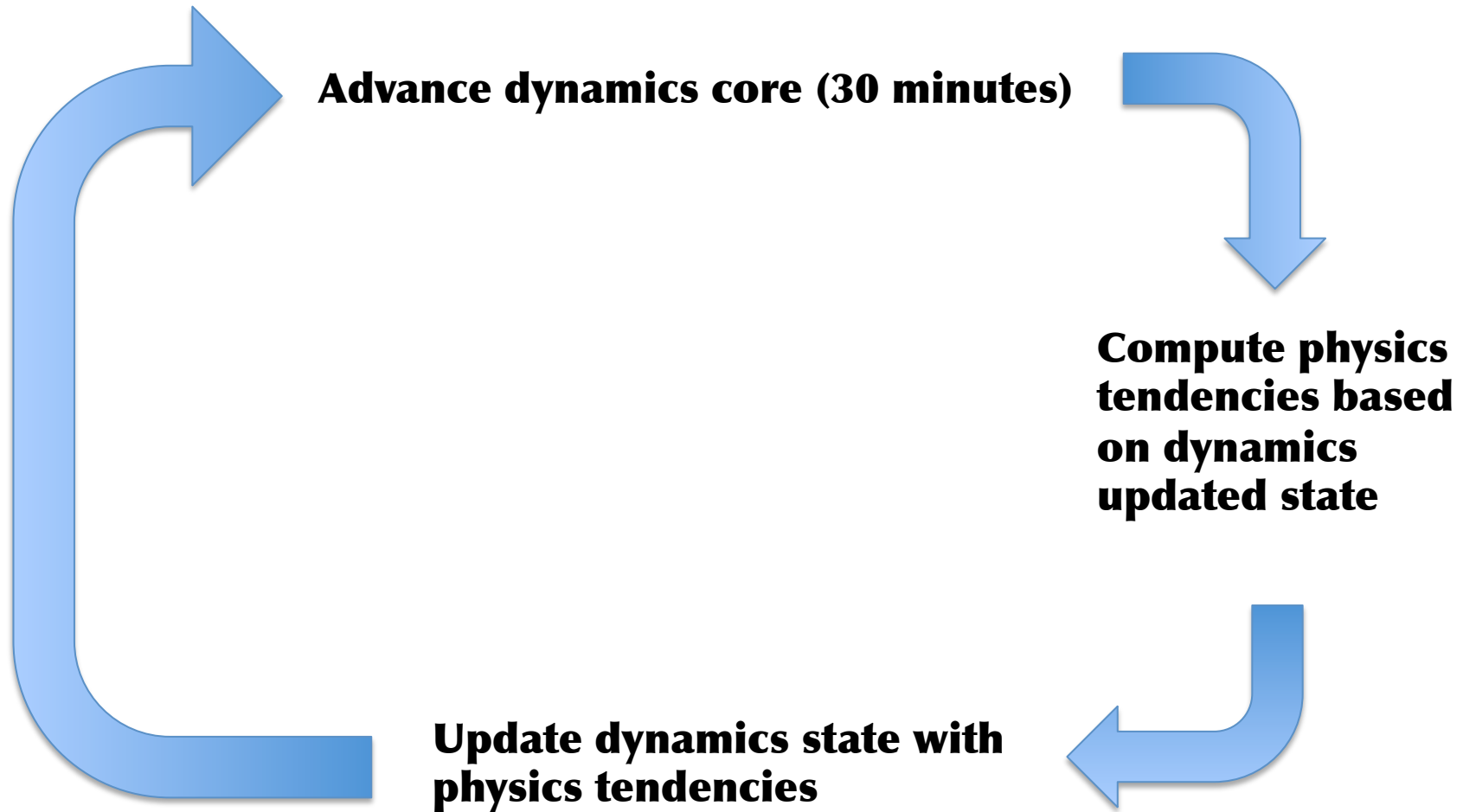


Preserving pre-existing functional relation between tracers under challenging flow conditions

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



Physics dynamics coupling methods



Physics dynamics coupling methods

Advance dynamics core (30 minutes)

For long physics time-steps and less diffusive dynamical cores this can create spurious noise!

Noise can be detected by computing

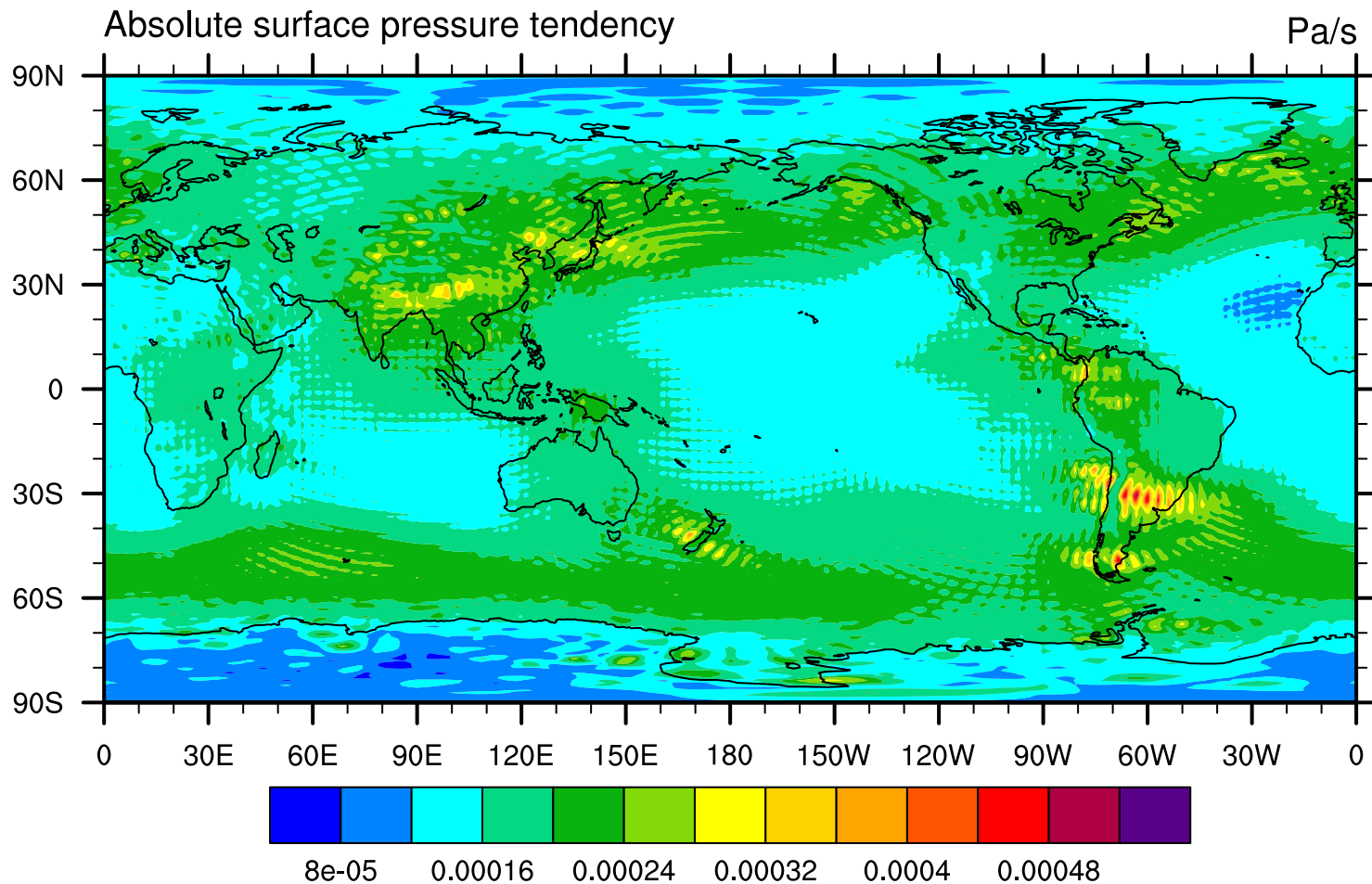
$$\frac{d}{dt} |p_s|$$

Compute physics tendencies based on dynamics updated state

Update dynamics state with physics tendencies

Physics dynamics coupling methods

10 year average of $\frac{d}{dt}|p_s|$ from AMIP run



Physics dynamics coupling methods

**Advance dynamics core (30 minutes):
add physics tendency “chunks”
during the dynamics time-stepping
- every 15 minutes in this example
(I refer to it as “**dribbling**”)**

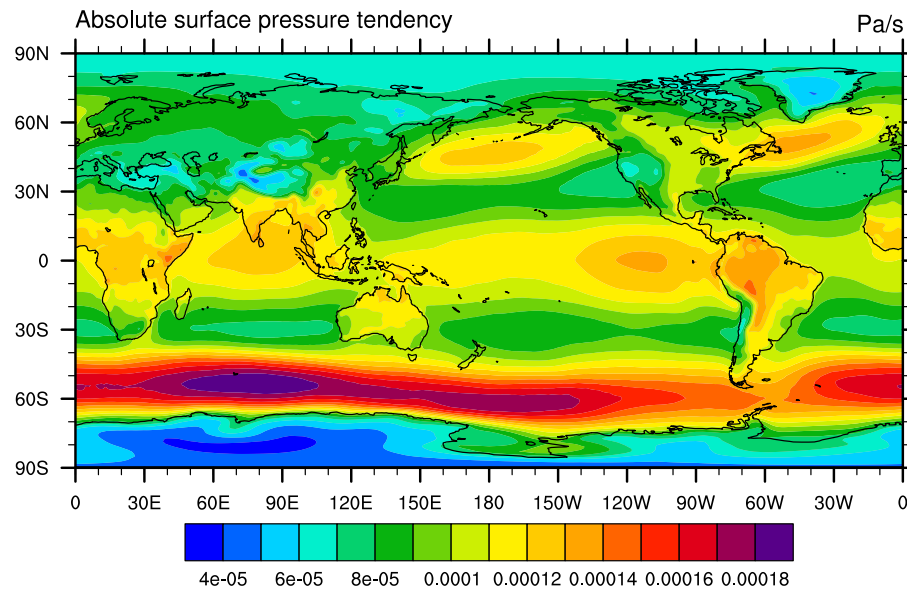
**Compute physics
tendencies based
on dynamics
updated state**

**Split physics tendencies into
a number of “chunks”**

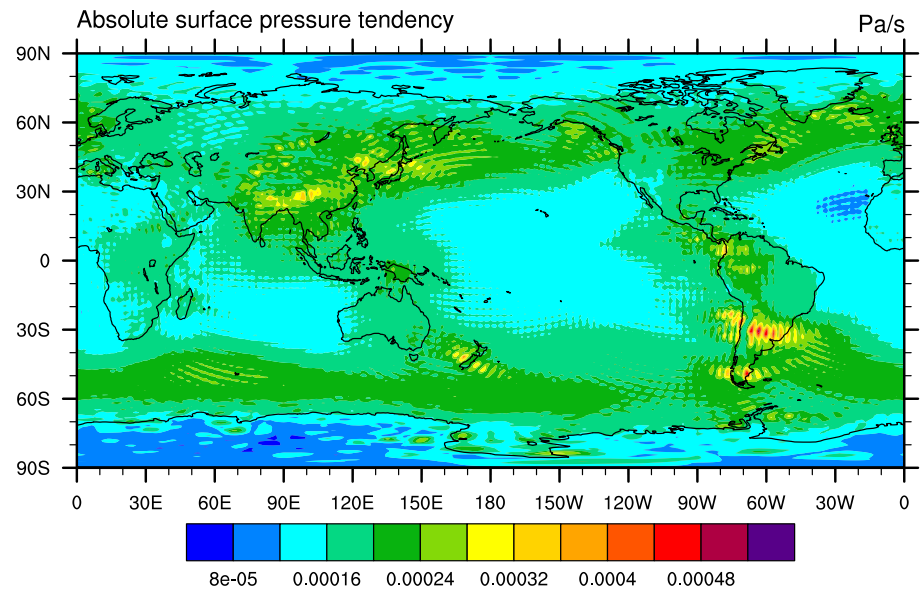
Physics dynamics coupling methods

10 year average of $\frac{d}{dt}|p_s|$ from AMIP run

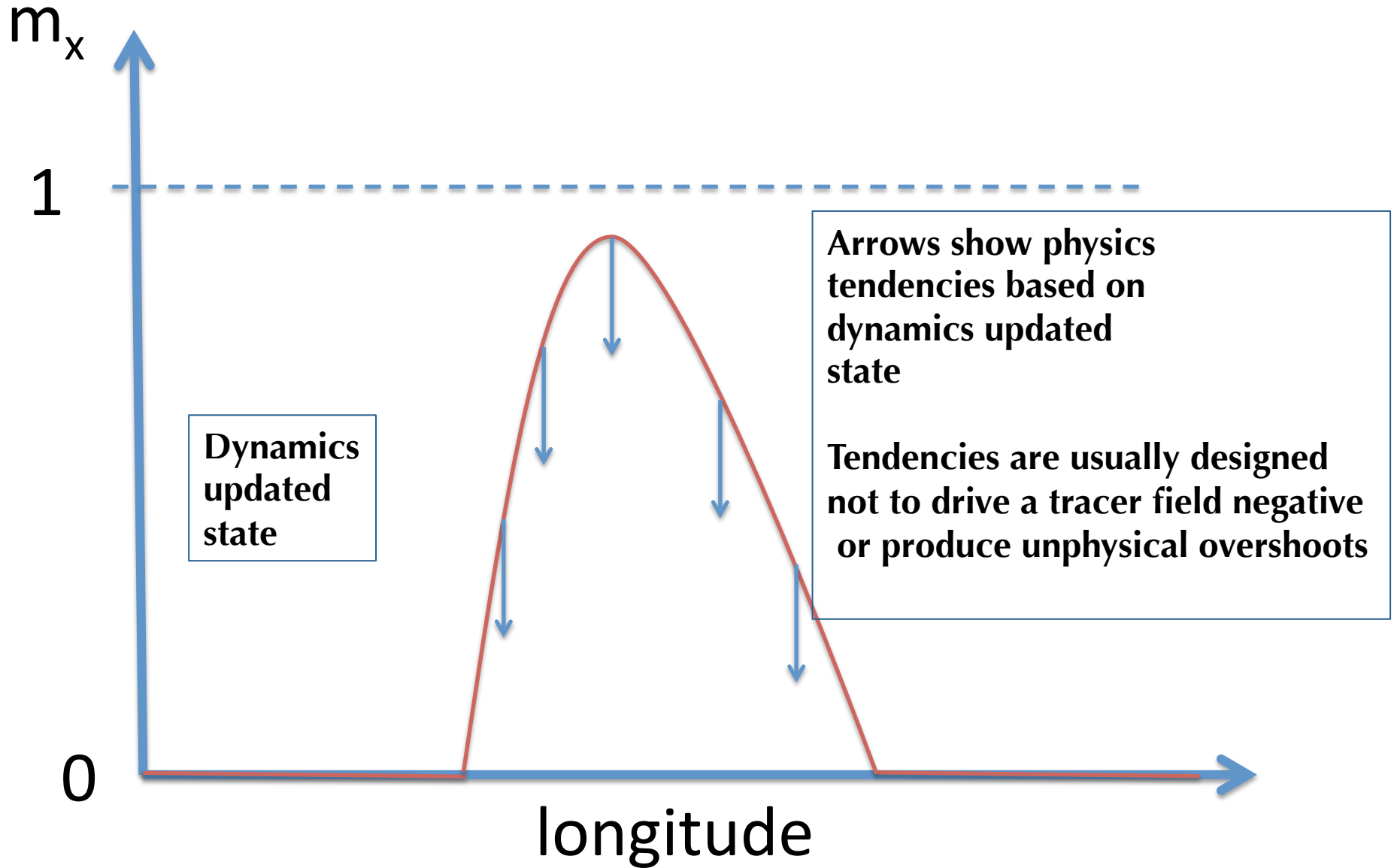
“Dribbling” physics tendencies



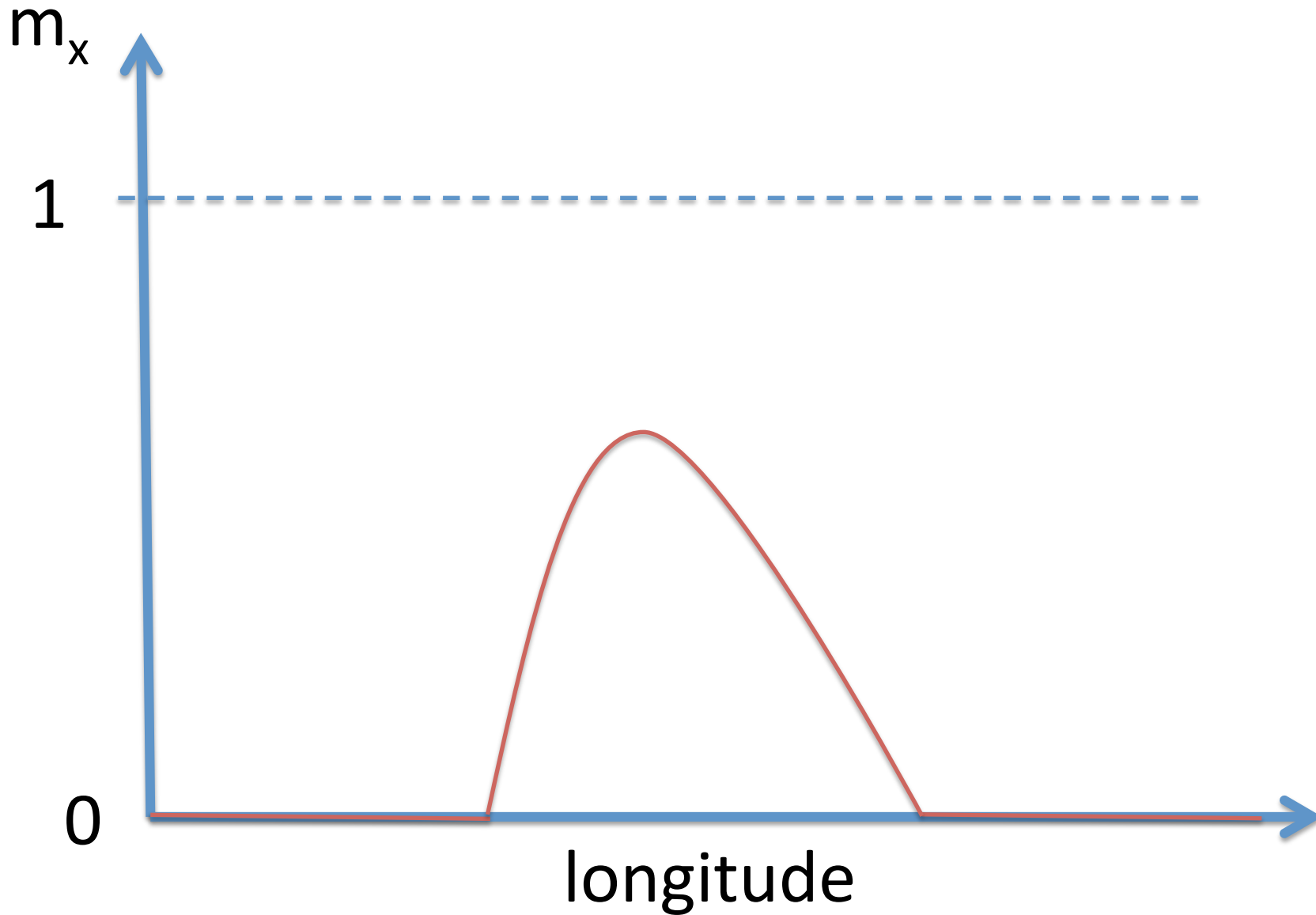
State updated every 30 minutes



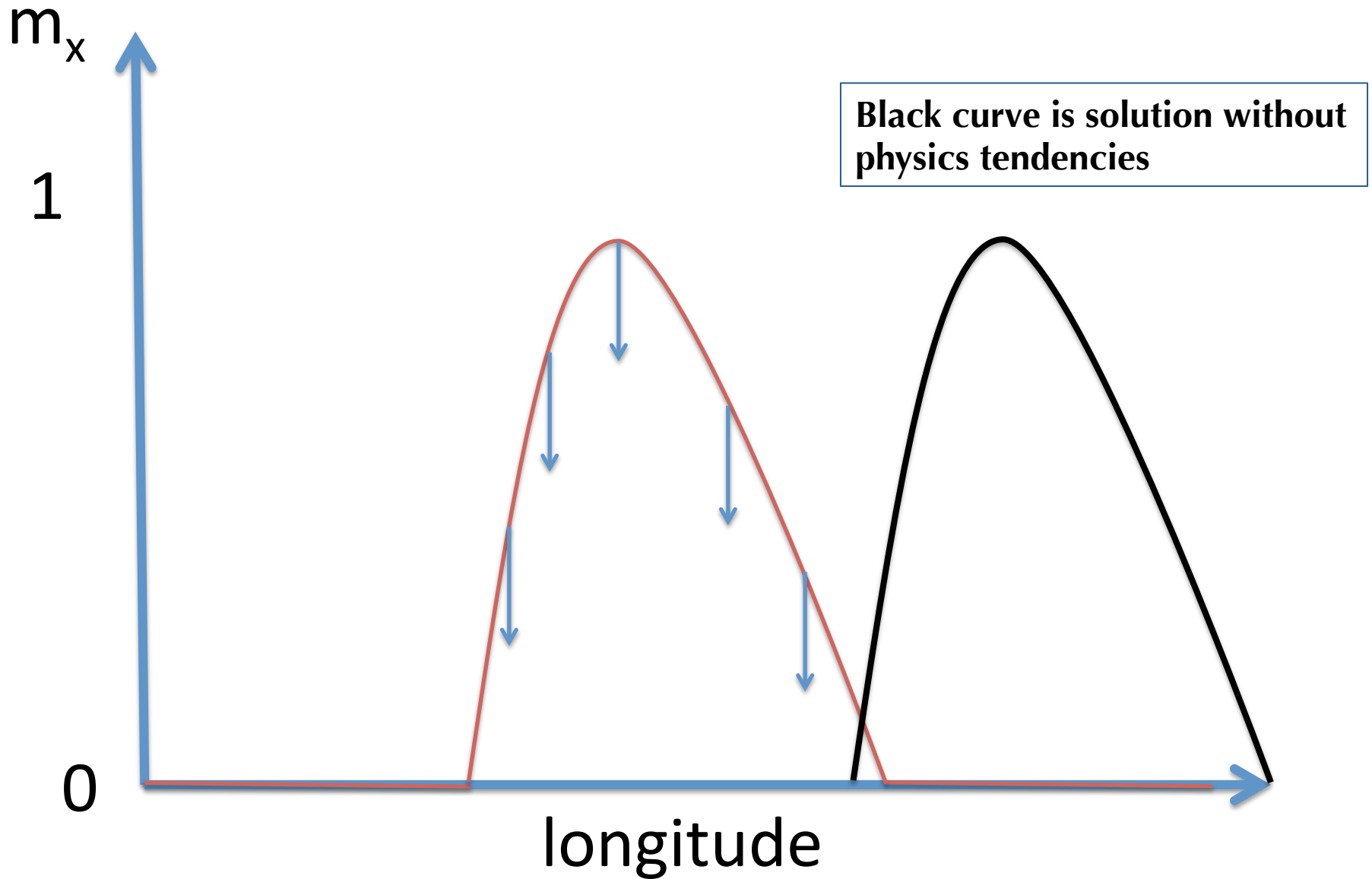
Physics-dynamics coupling: state update



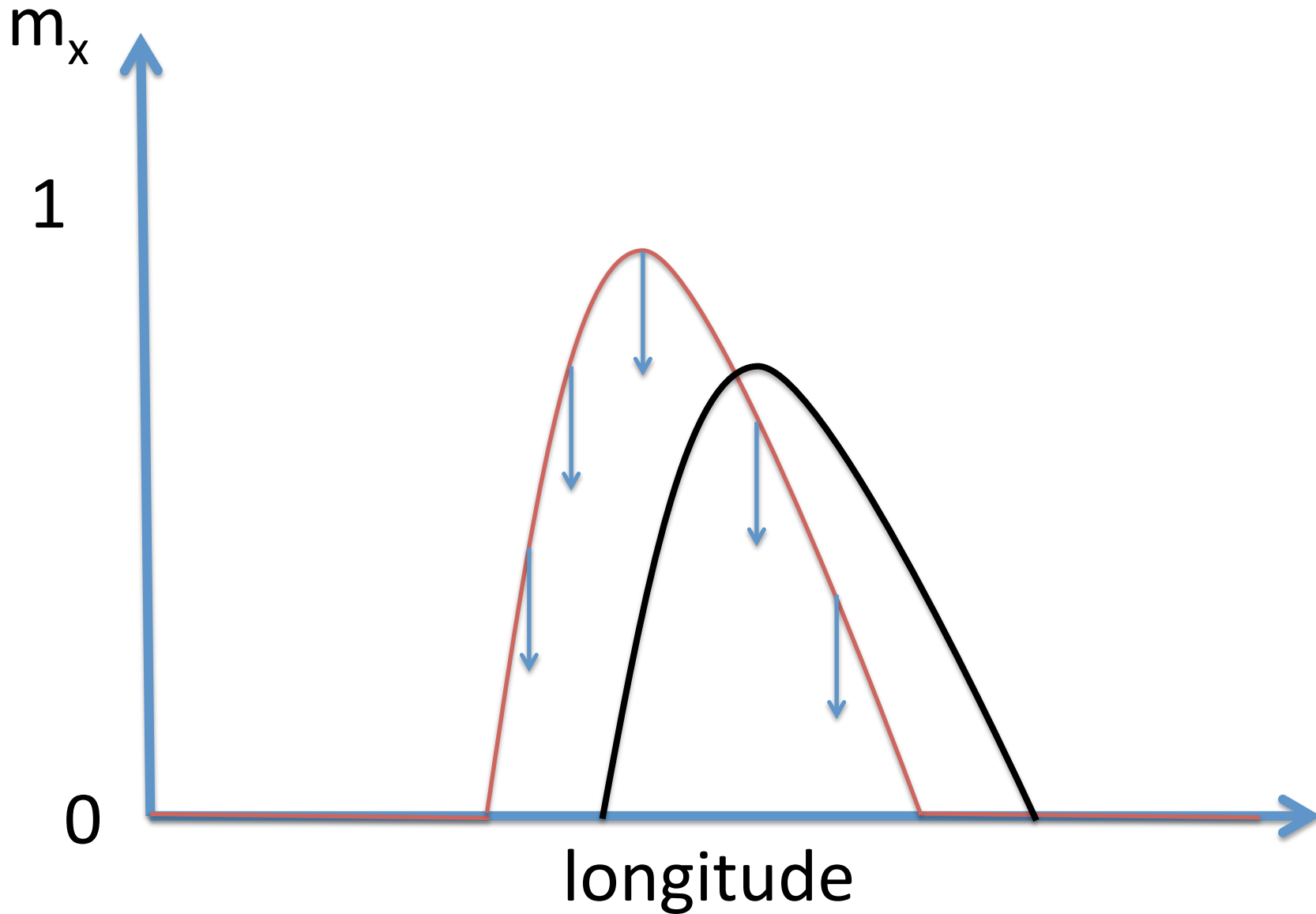
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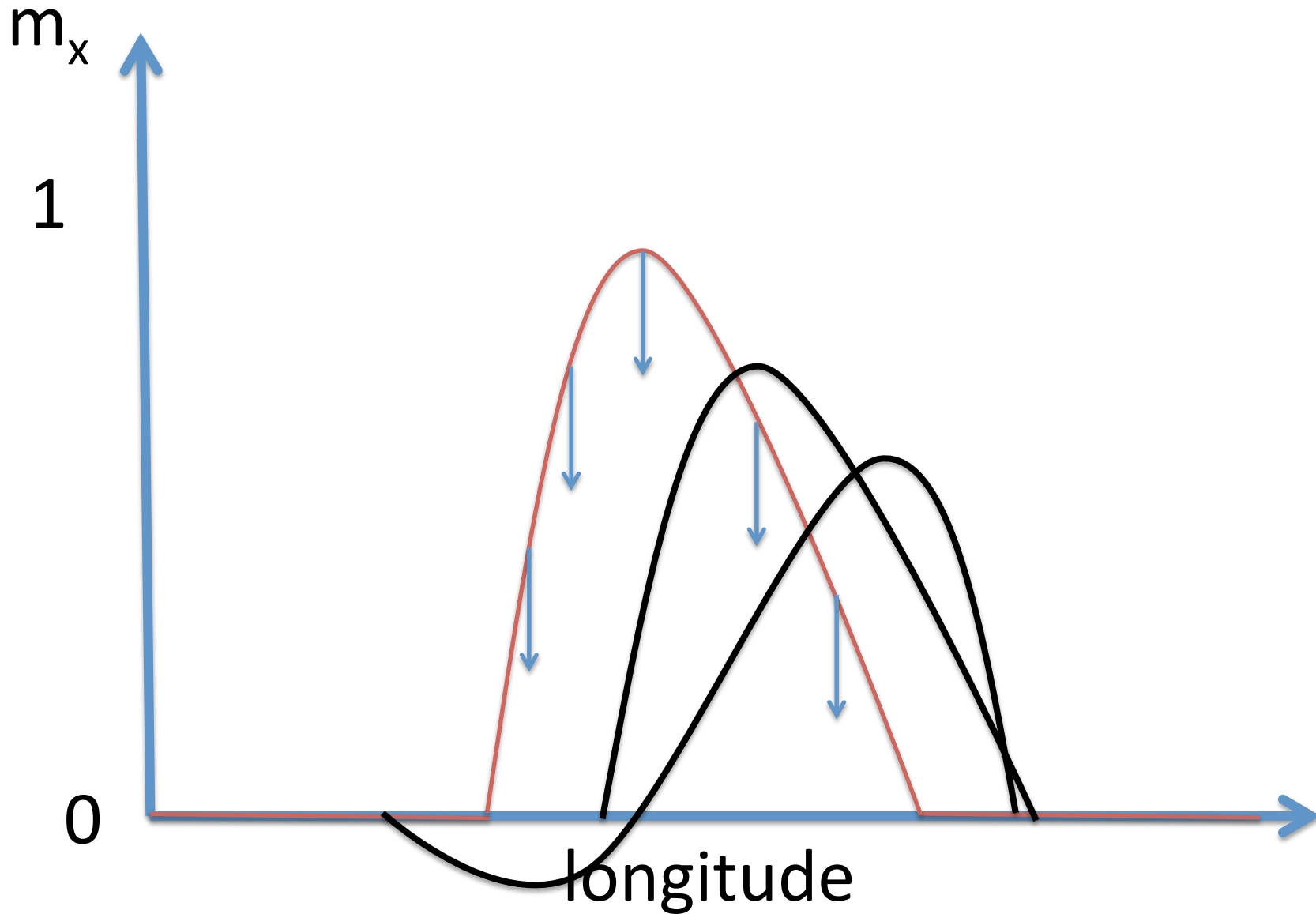
Physics-dynamics coupling: “dribbling” tendencies



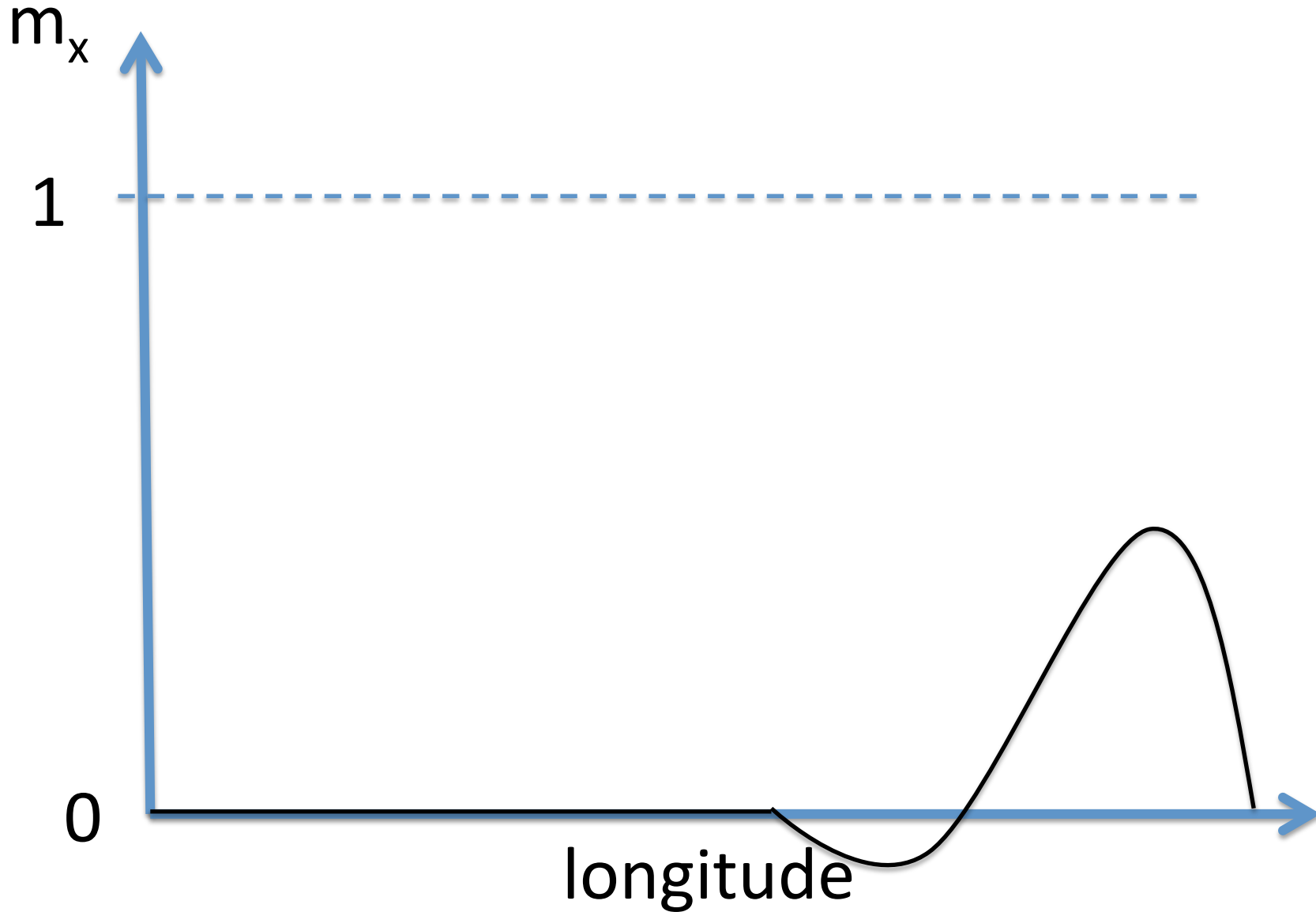
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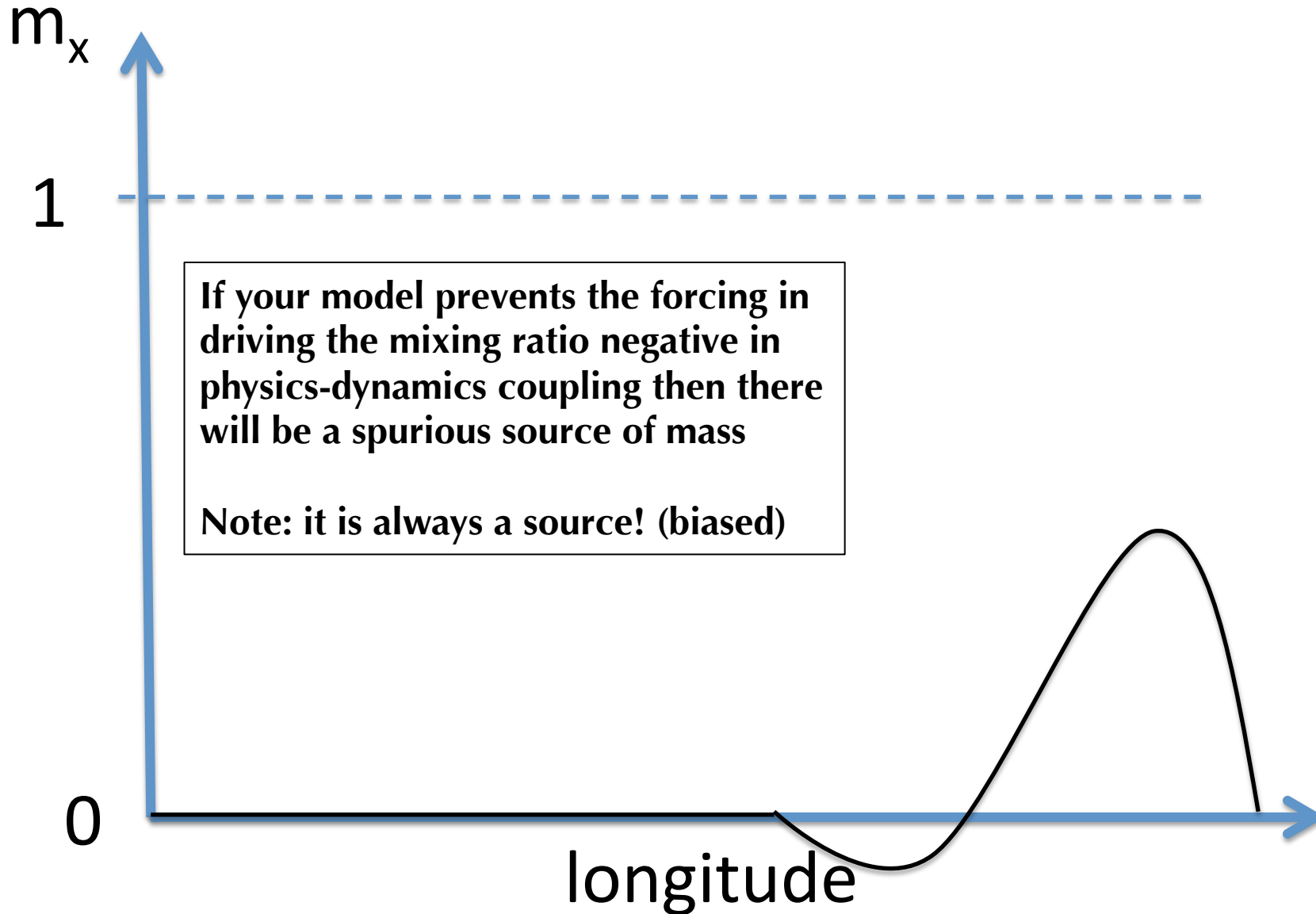
Physics-dynamics coupling: “dribbling” tendencies



Physics-dynamics coupling: “dribbling” tendencies



Physics-dynamics coupling: “dribbling” tendencies





More information: <http://www.cgd.ucar.edu/cms/pel>

Email: pel@ucar.edu