



# Desirable properties of transport schemes

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# 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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JOHN B. DRAKE

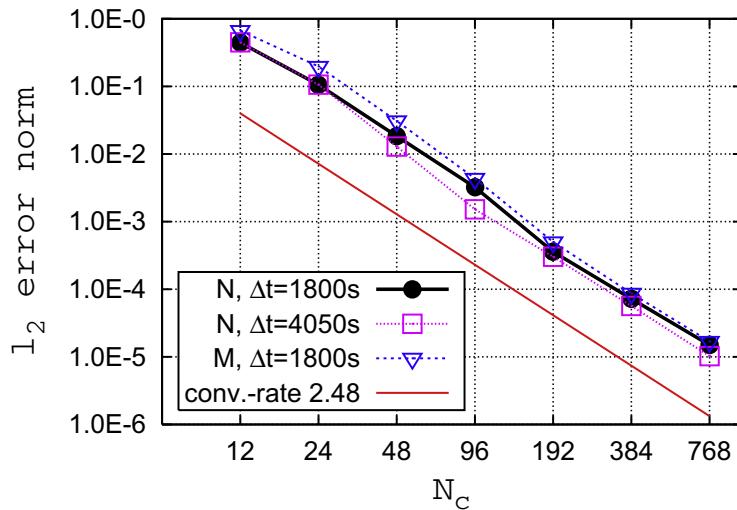
*Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*

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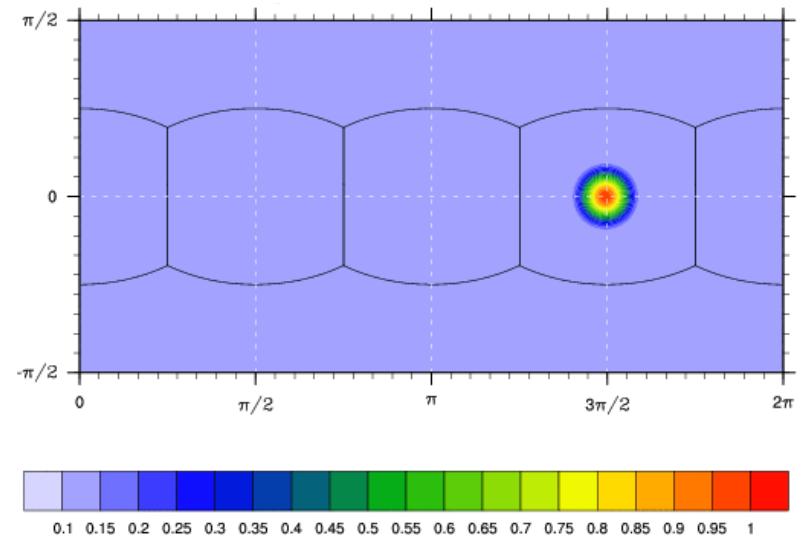
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### Test 1: Solid-body advection



Received June 17, 1991



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

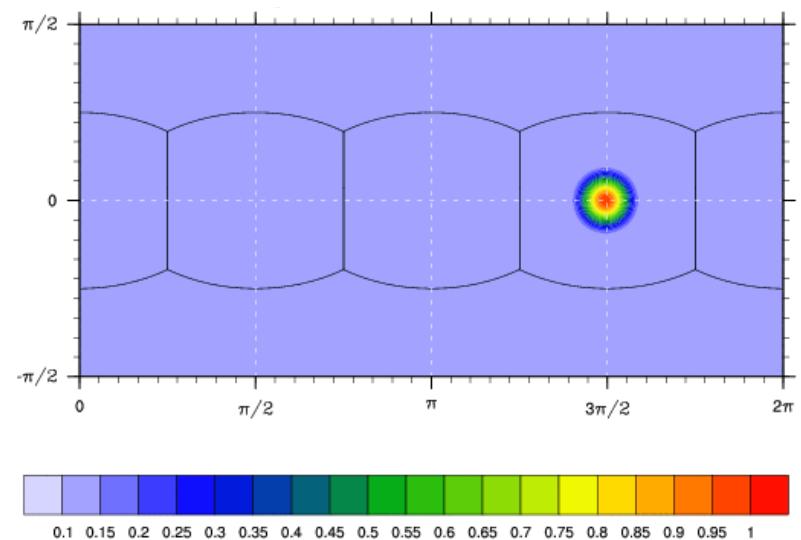
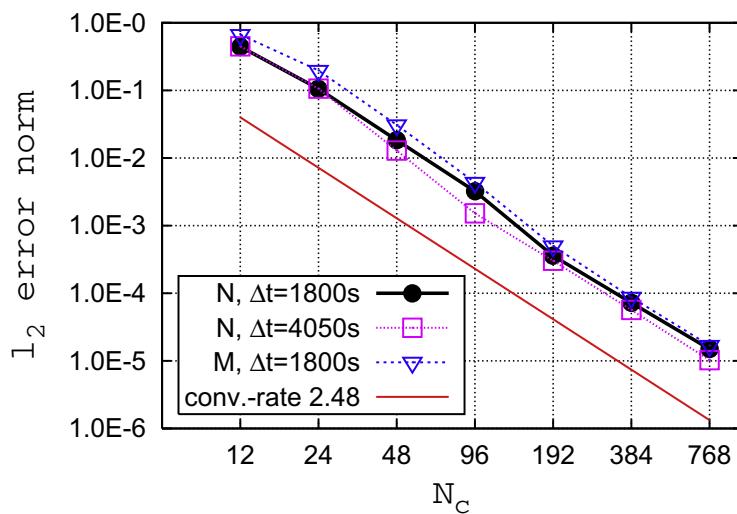


## **Test 1: Solid-body advection**

# 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):

$$\begin{aligned}\ell_2 &= \left[ \frac{I[(\phi - \phi_T)^2]}{I[(\phi_T)^2]} \right]^{1/2}, \\ \ell_\infty &= \frac{\max_{\forall \lambda, \theta} |\phi - \phi_T|}{\max_{\forall \lambda, \theta} |\phi_T|}, \\ \phi_{\max} &= \frac{\max_{\forall \lambda, \theta} (\phi) - \max_{\forall \lambda, \theta} (\phi_T)}{\Delta \phi_0}, \\ \phi_{\min} &= \frac{\min_{\forall \lambda, \theta} (\phi) - \min_{\forall \lambda, \theta} (\phi_T)}{\Delta \phi_0},\end{aligned}$$

where  $\phi_T$  and  $\phi_0$  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, ...)

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

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

Integrate (1) over entire atmosphere  $\Omega_{tot}$

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

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

# 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

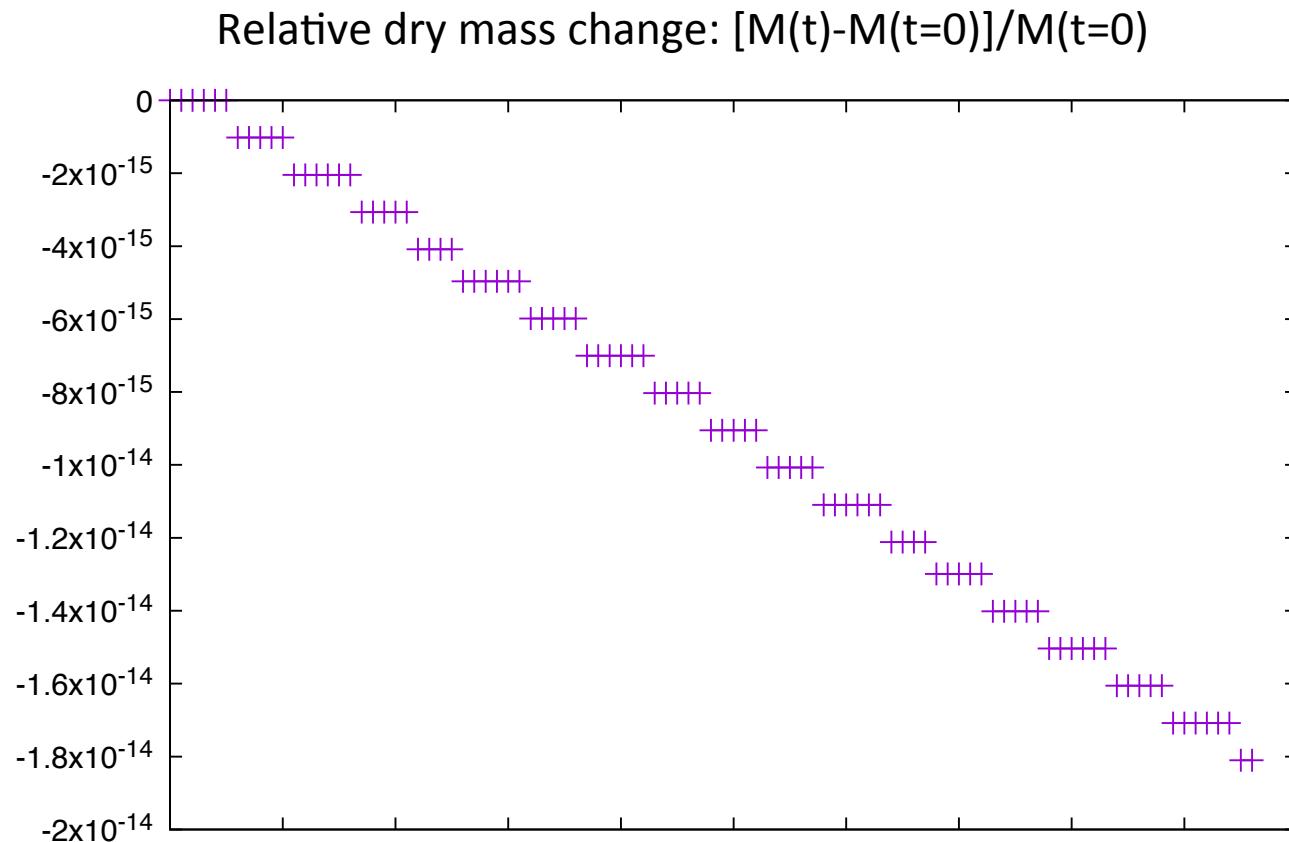
**Why is that a problem?**

Integrate (1) over entire atmosphere  $\Omega_{tot}$

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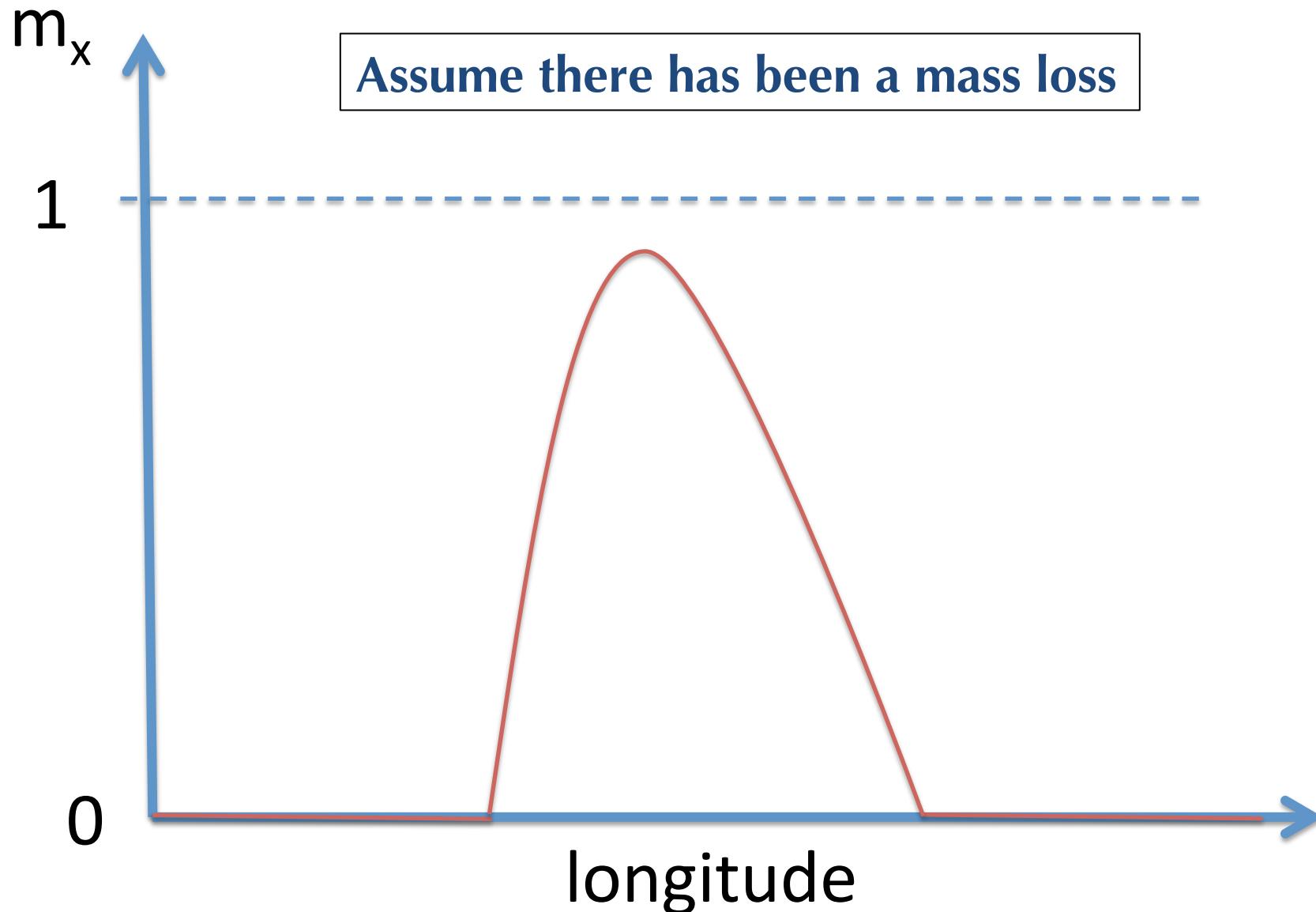
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# Accumulation of error

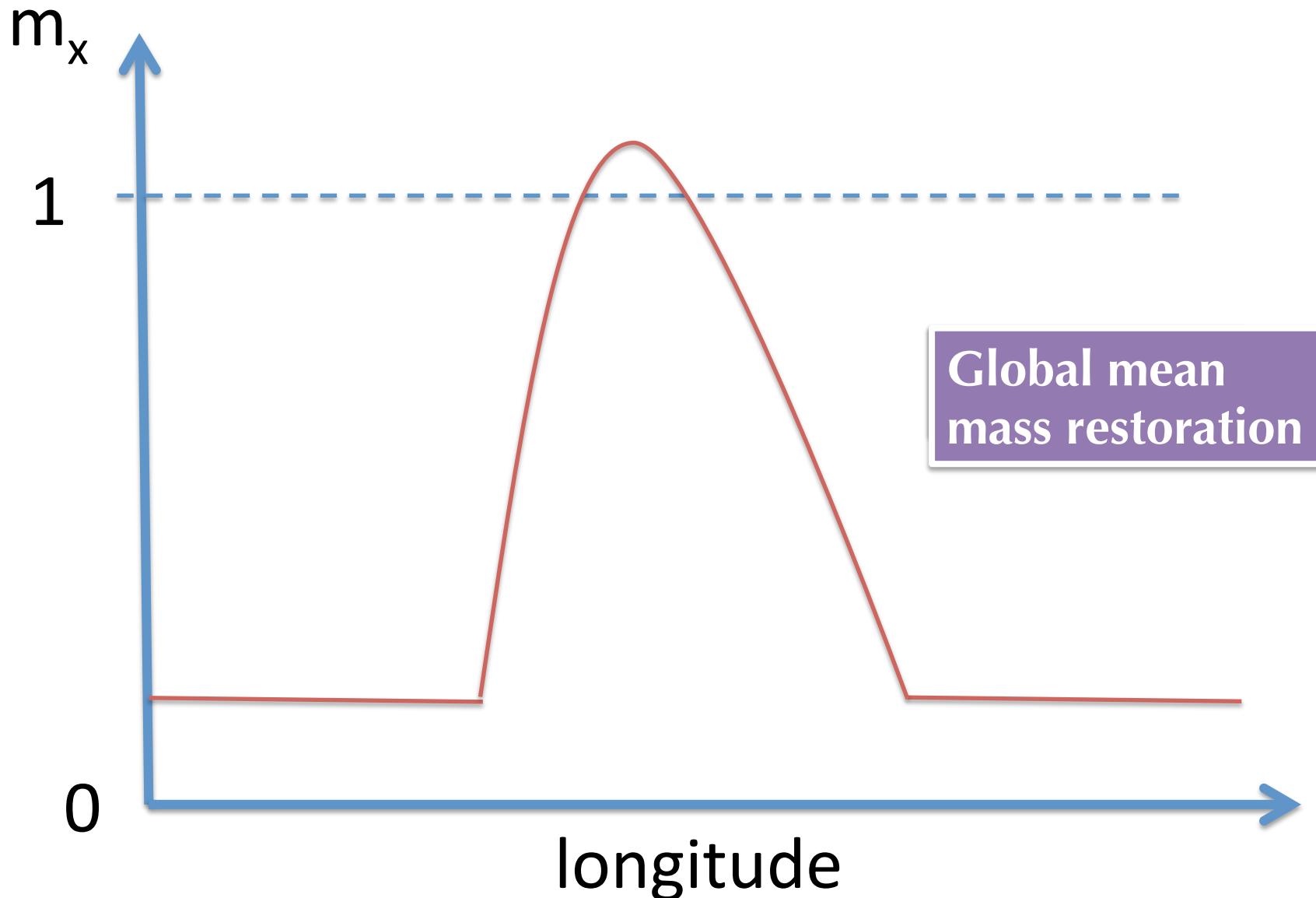


1000 year simulation  $\approx O(10^7)$  30 minute time-steps

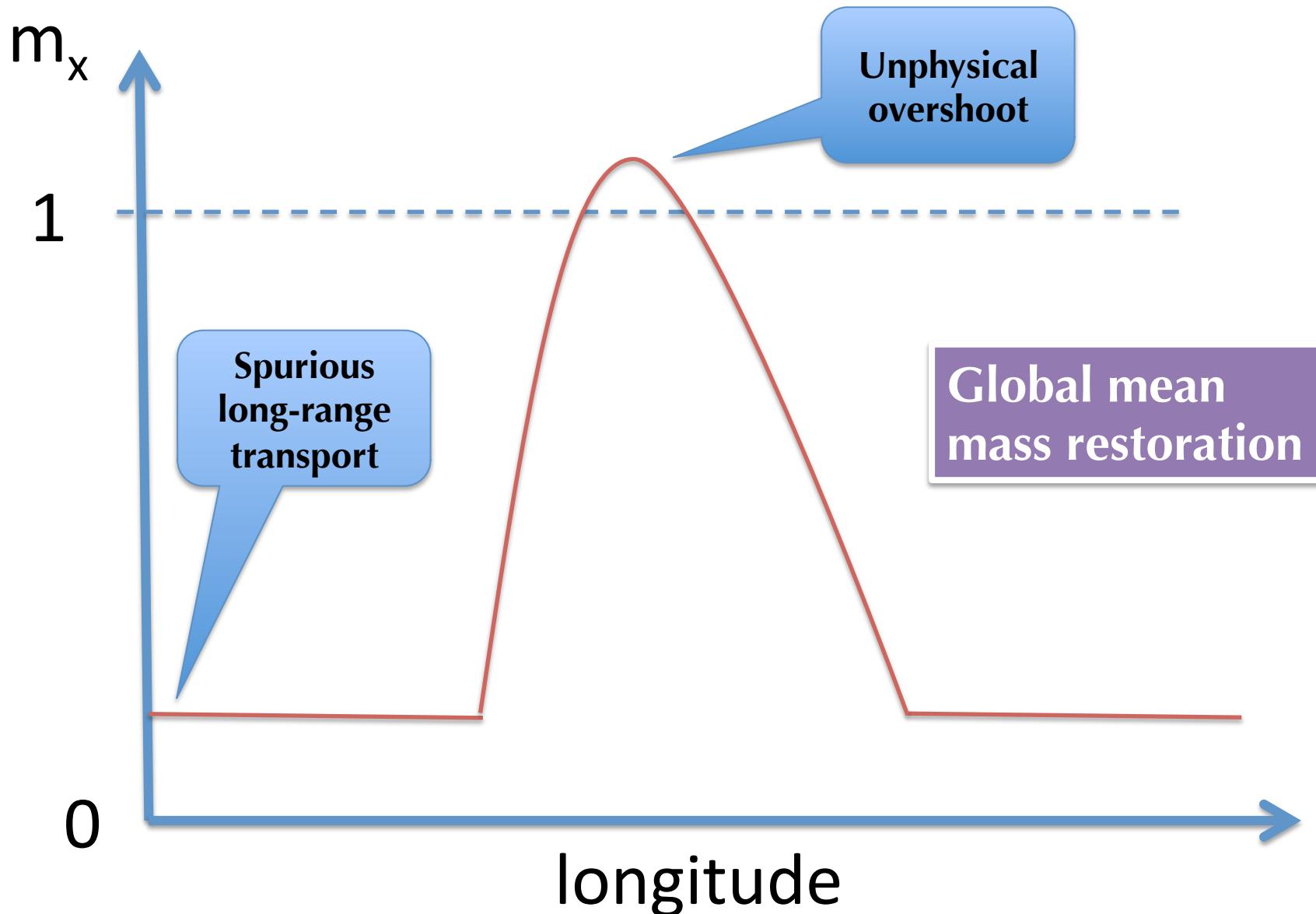
# Ad hoc mass fixers are inherently problematic



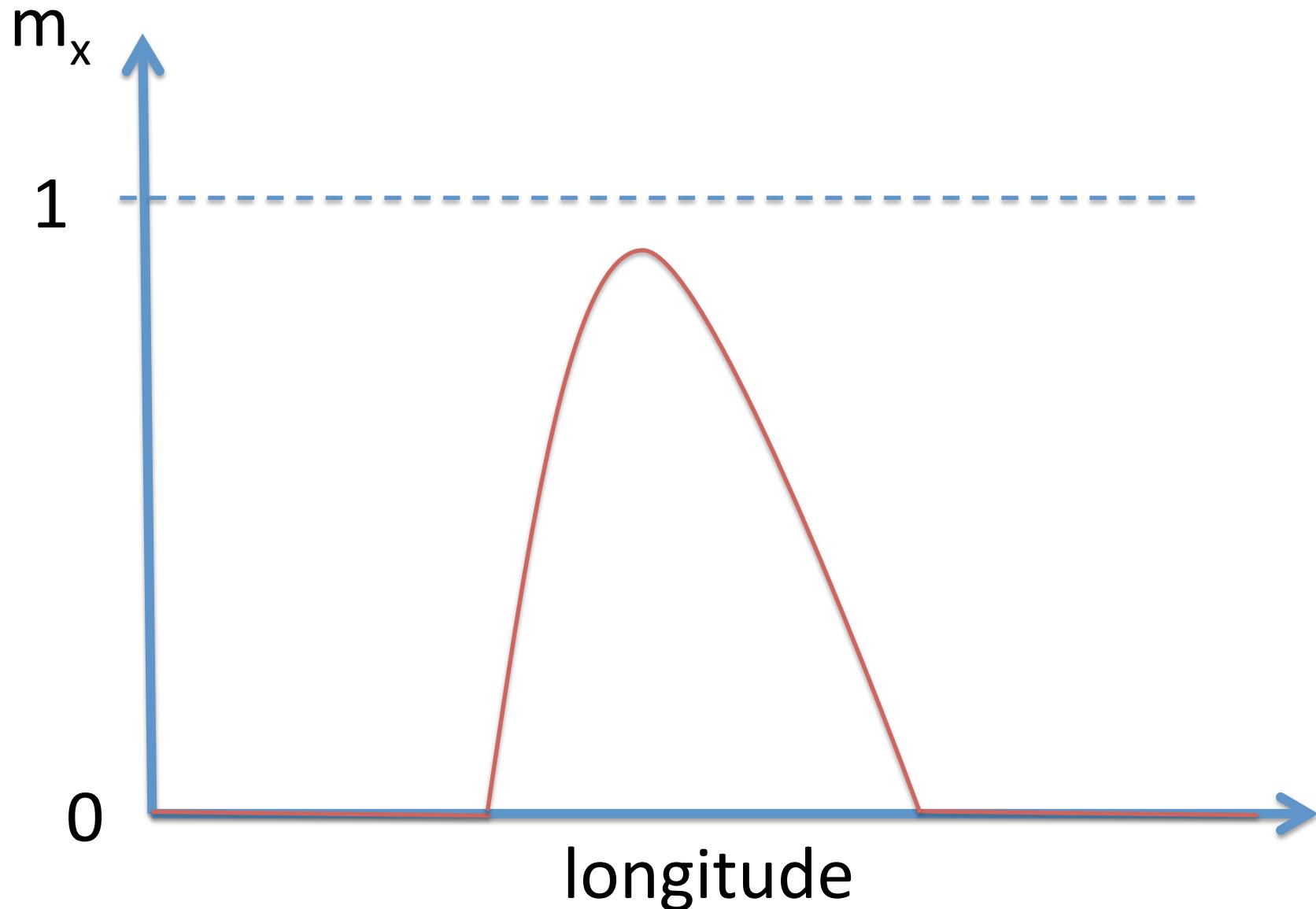
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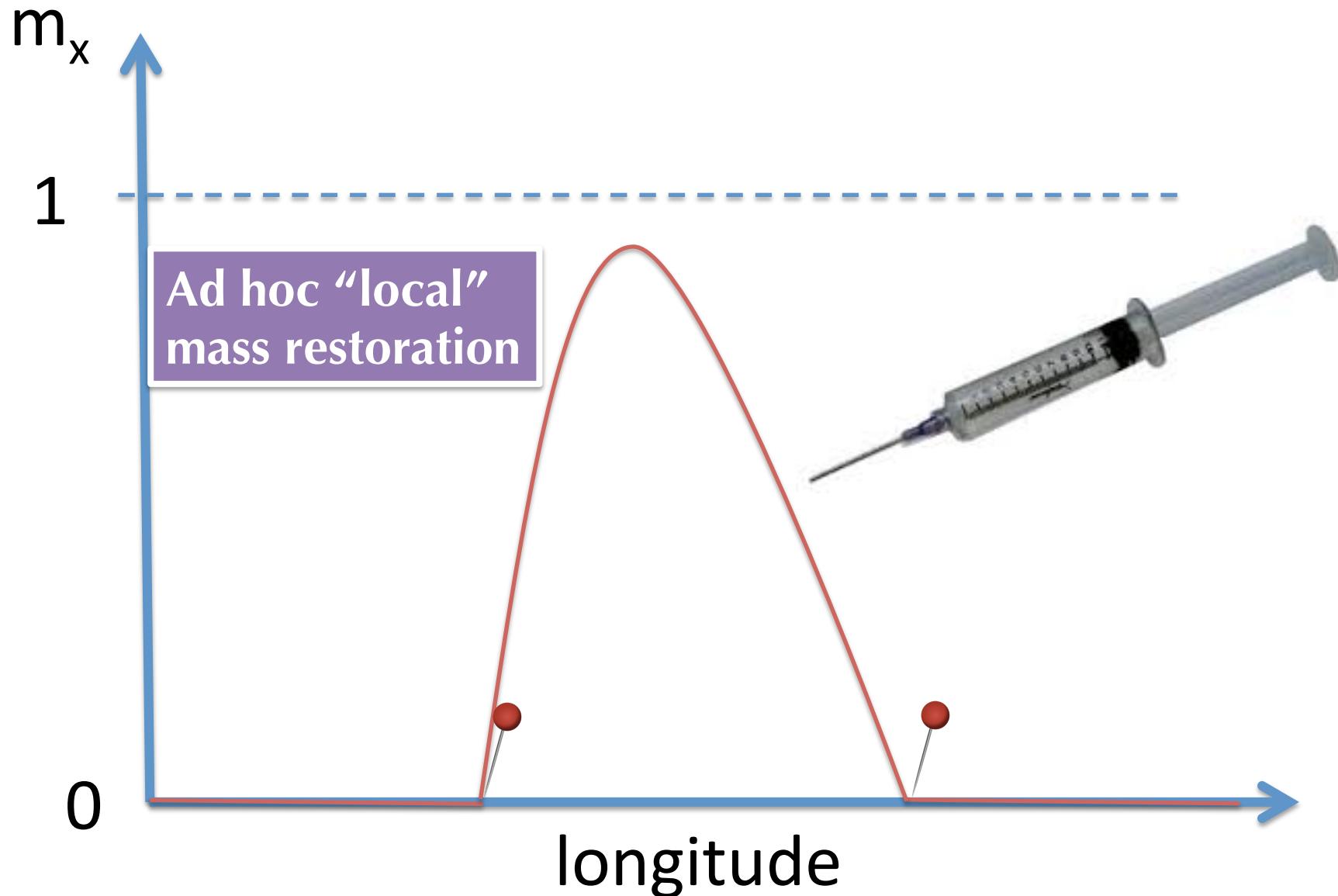
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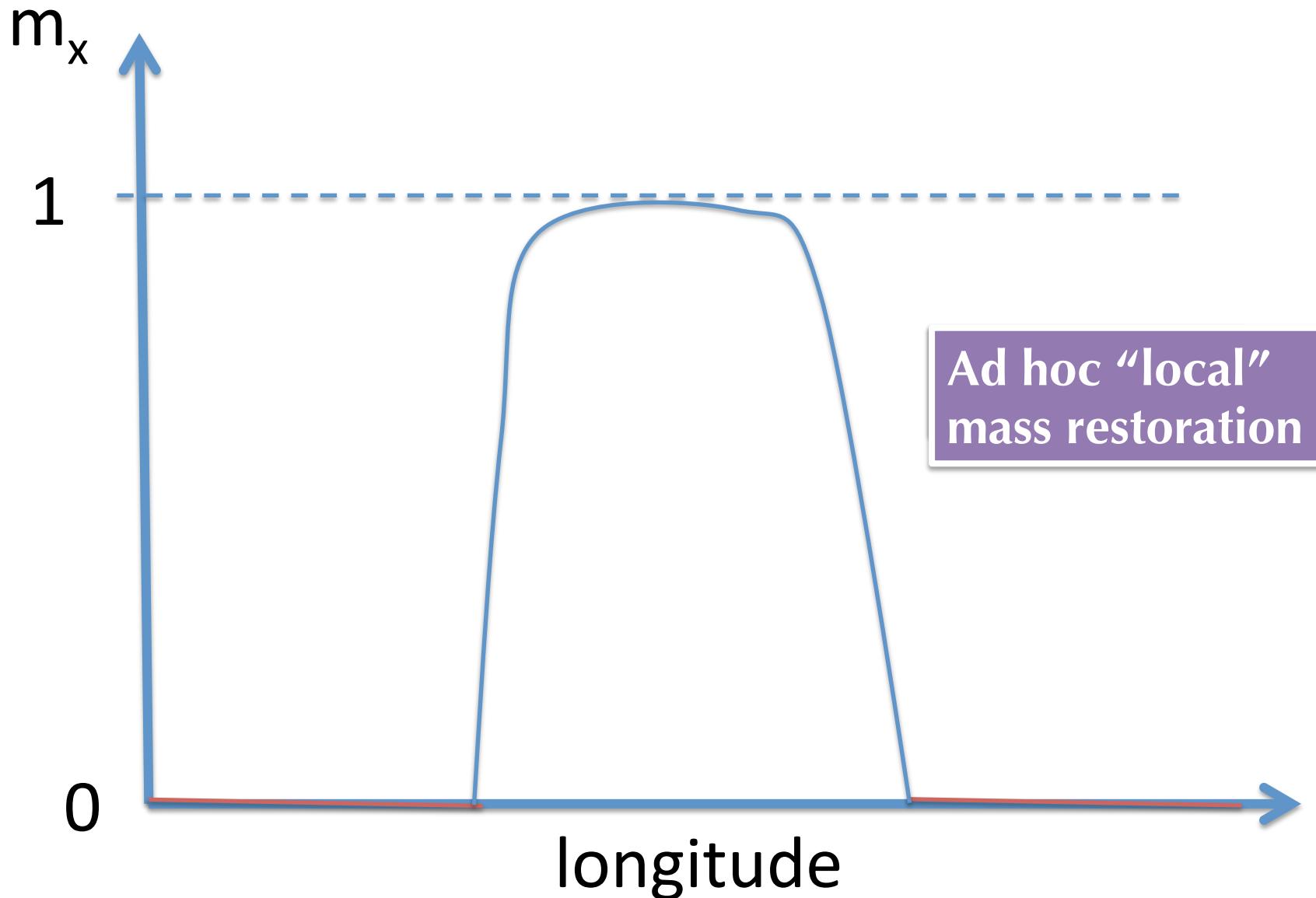
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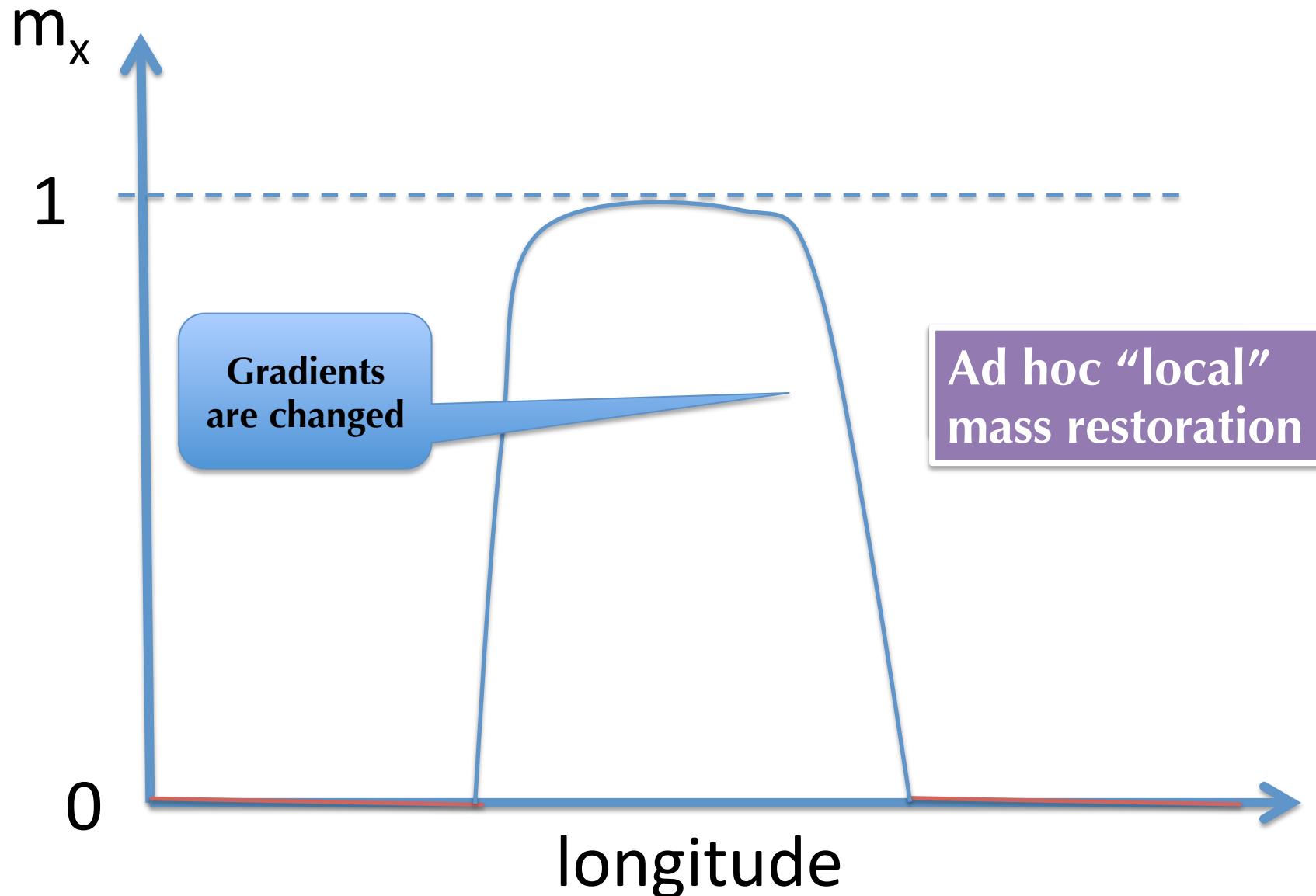
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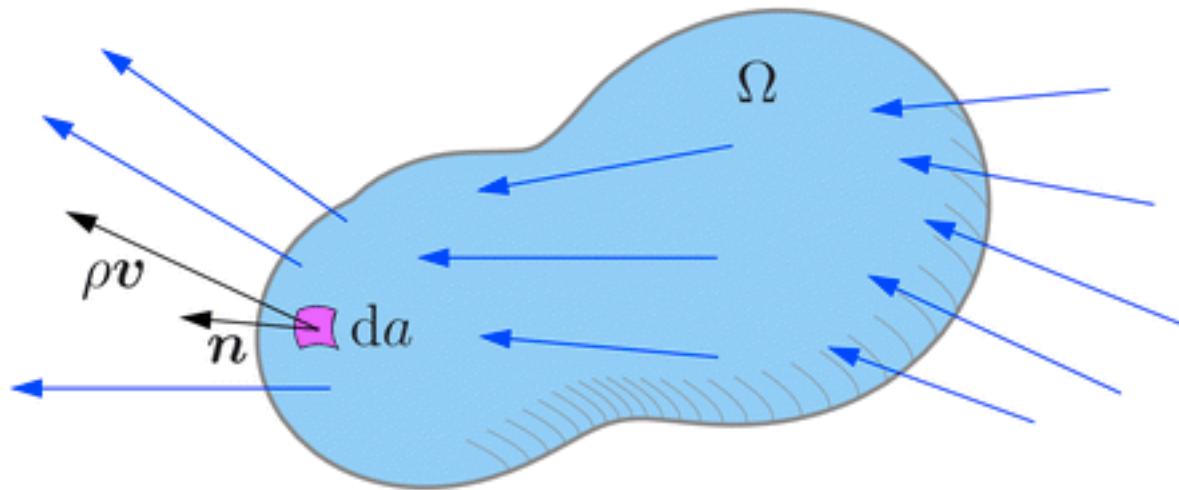
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# Ad hoc mass fixers are inherently problematic



# Inherent local mass-conservation is desirable



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

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

## 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

$$\frac{D m_X}{D t} = S^{m_X},$$

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

## Conservation of $m_x$ along parcel trajectories

Consider the continuity equation for dry air and  $X$

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \vec{v}) = 0$$
$$\frac{\partial}{\partial t} (m_x \rho_d) + \nabla \cdot (m_x \rho_d \vec{v}) = 0$$

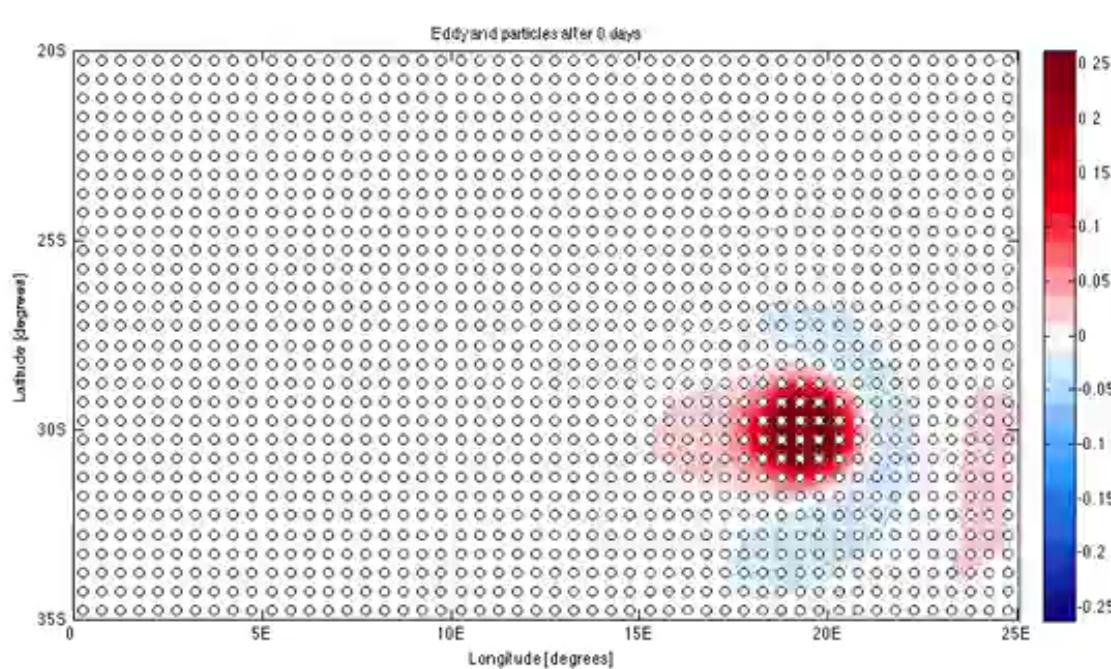
respectively. Applying the chain rule to the second equation and substituting (2) implies

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

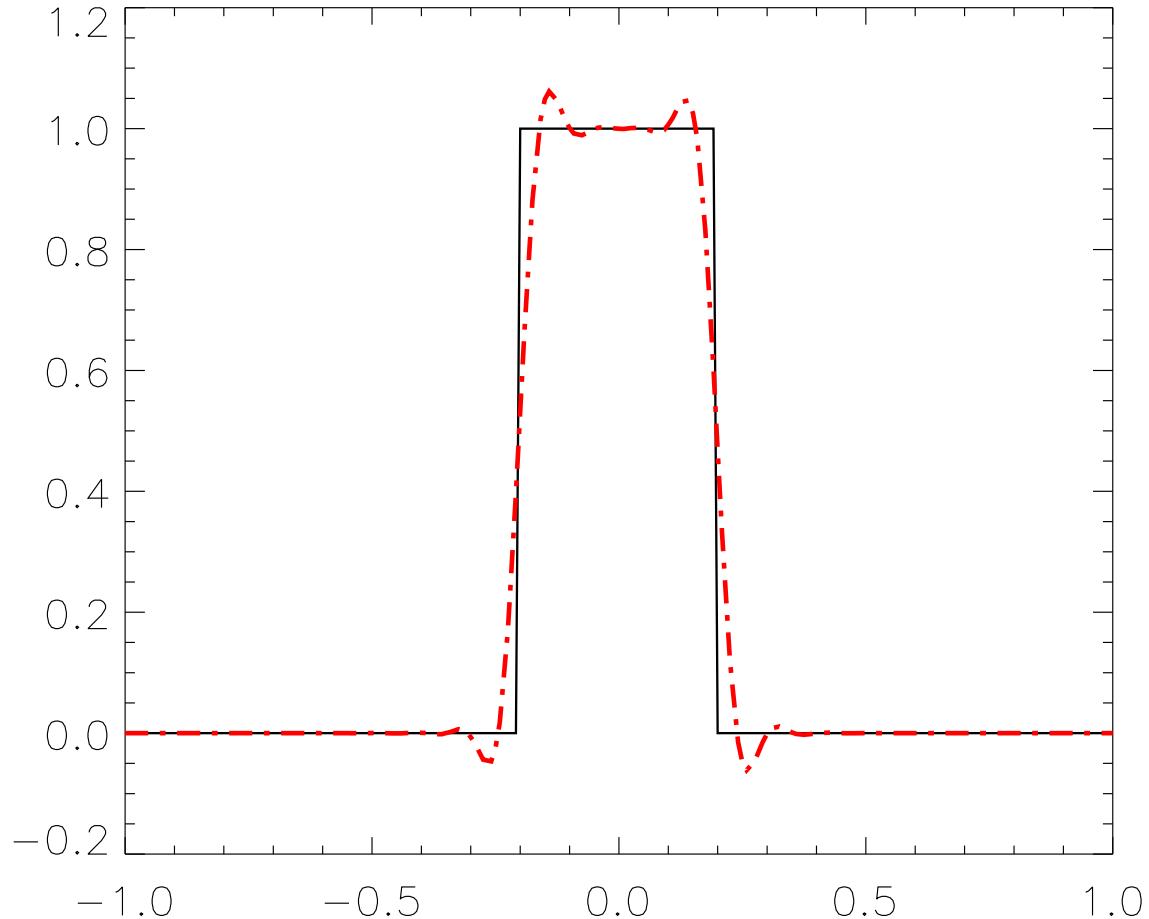
# **Conservation of $m_x$ along parcel trajectories (if no sources/sinks of $m_x$ )**



- 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’!**

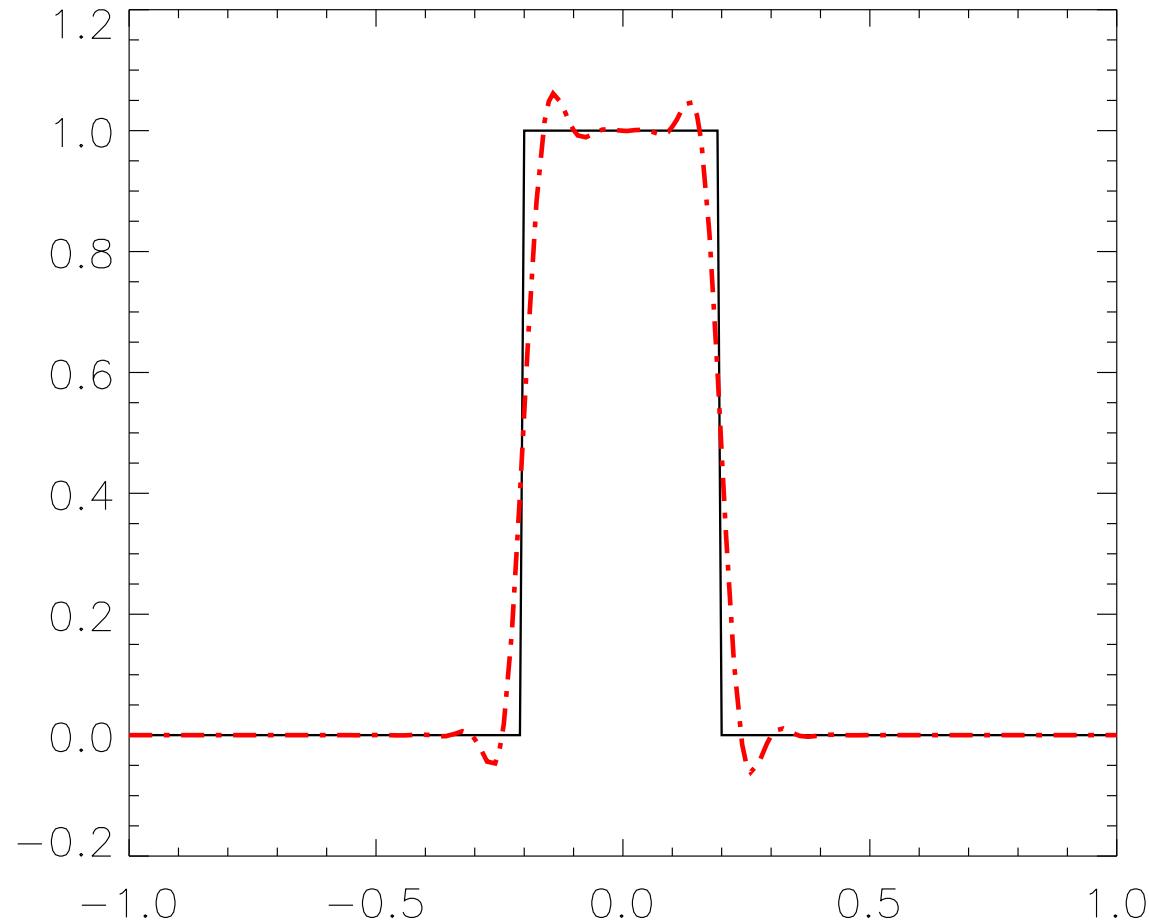
When modelers refer to “non-oscillatory”, “shape-preserving”, “physical realizable” or “monotone” they usually refer to the **monotonicity property** as defined by Harten (1983):

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

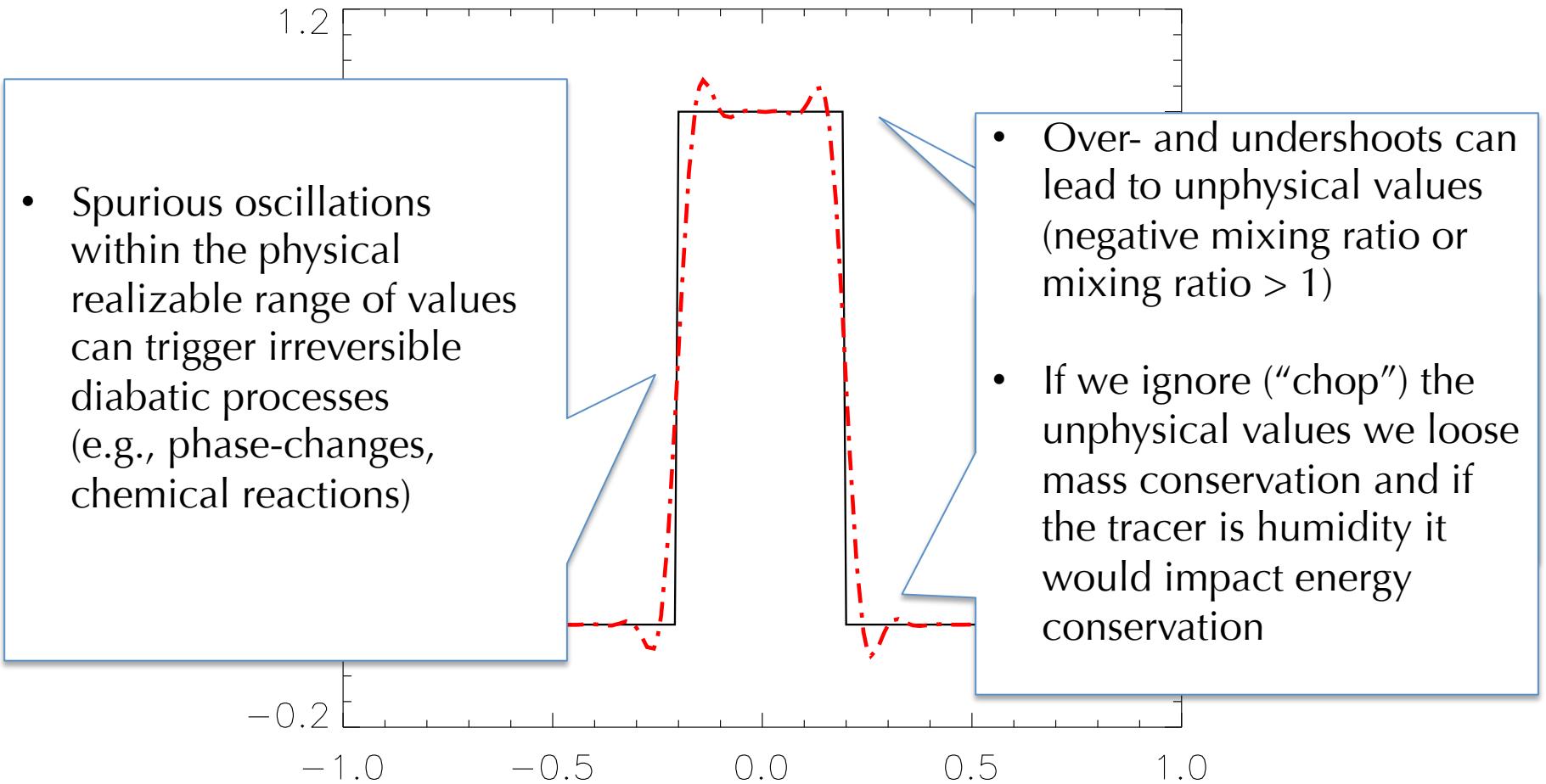
**=> the monotonicity property applies to mixing ratio  $m_x$  and not tracer mass!**

# 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  $\rho_d$  over a Lagrangian volume  $\Omega_L$  then

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

# Lagrangian volumes are rapidly distorting

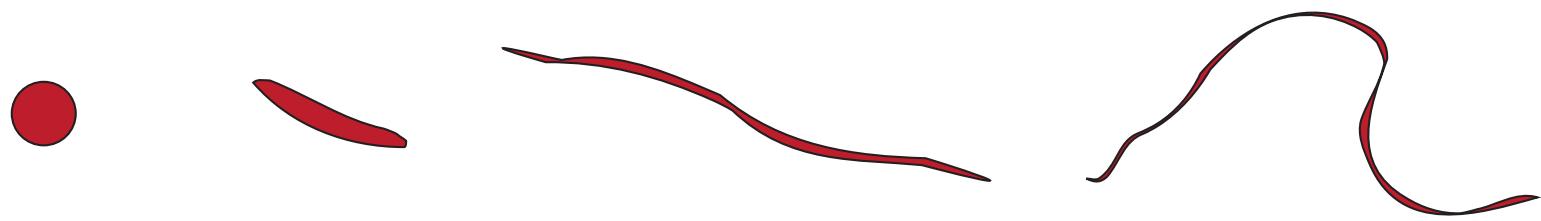
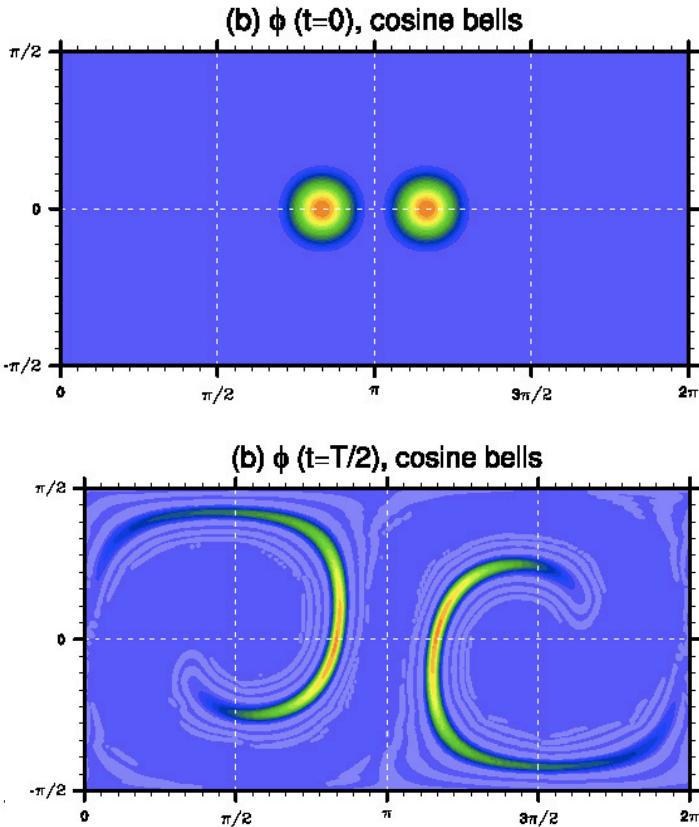


Fig. 2: In the highly nonlinear flows that characterize fluid motion in the atmosphere and ocean, Lagrangian control volumes are rapidly distorted due the presence of strong shear, rotation and dilation. The rapid distortion of Lagrangian control volumes makes the formulation of numerical models within 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  $\tau$  is the threshold value. For a non-divergent flow field and a passive and inert tracer  $\phi$ , 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  $\Delta A_k$  is the spherical area for which  $\phi_k$  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  $\Delta A_k$  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

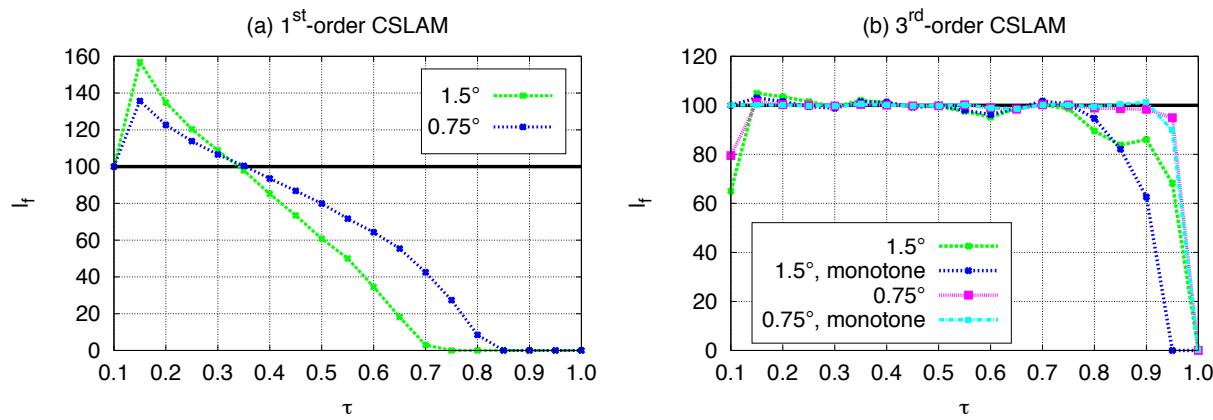
$$\ell_f(\tau, t) = \begin{cases} 100.0 \times \frac{A(\tau, t)}{A(\tau, t=0)} & \text{if } A(\tau, t=0) \neq 0, \\ 0.0, & \text{otherwise.} \end{cases} \quad (30)$$

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  $\tau$ . 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  $\tau$  for different configurations of the CSLAM scheme with Courant number 5.5. (a)  $1^{\text{st}}$ -order version of CSLAM at  $\Delta\lambda = 1.5^\circ$  and  $\Delta\lambda = 0.75^\circ$ , and (b)  $3^{\text{rd}}$ -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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respectively.

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

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## Examples of tracer mass and air mass consistency violation

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

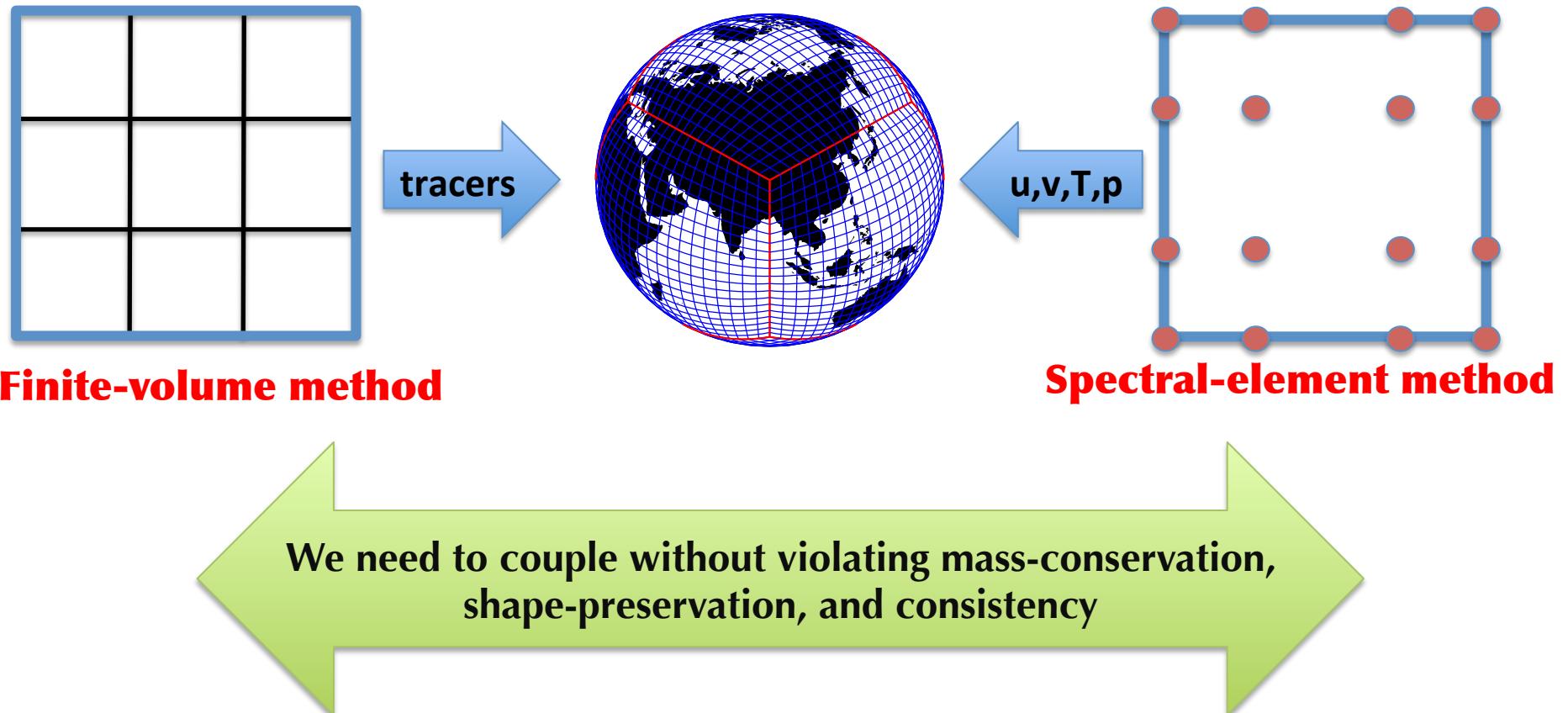
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$$\frac{\partial}{\partial t} (m_x \rho_d) + \nabla \cdot (m_X \rho_d \mathbf{v}) = 0, \quad (5)$$

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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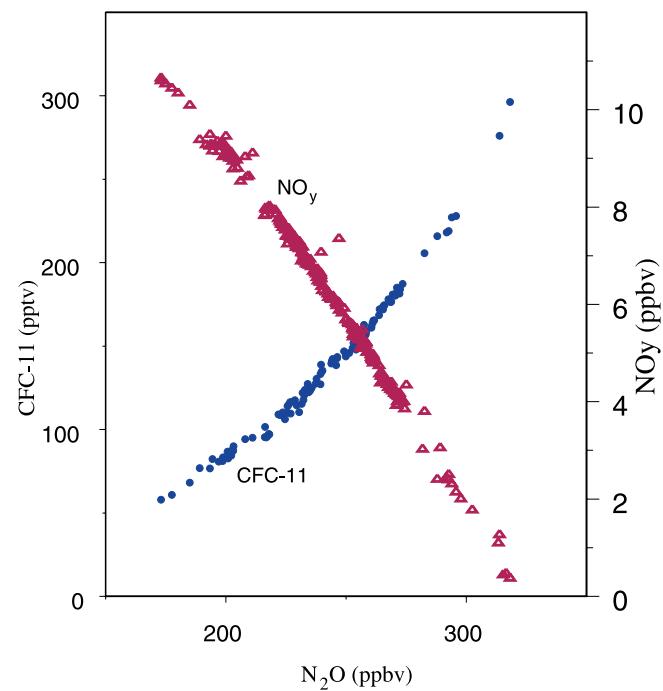
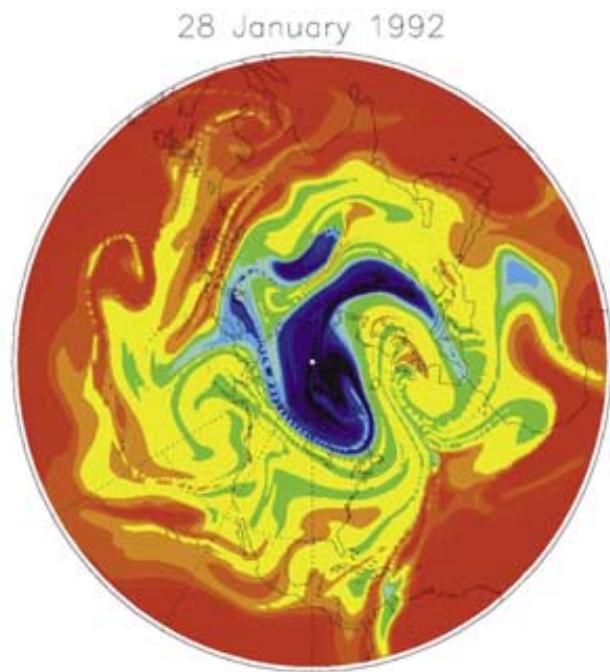
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# Correlations between long-lived species in the stratosphere

*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

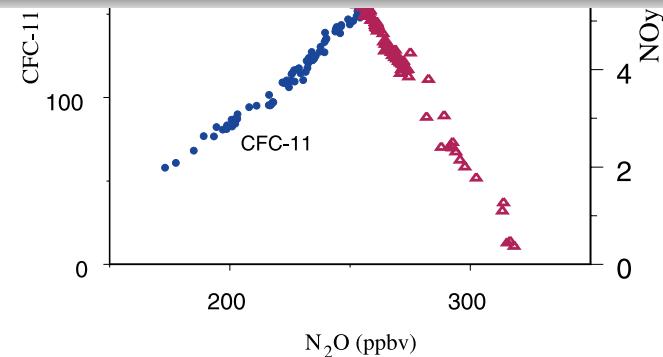
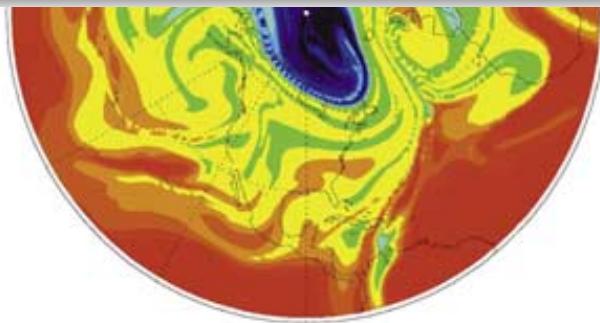
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Similarly:

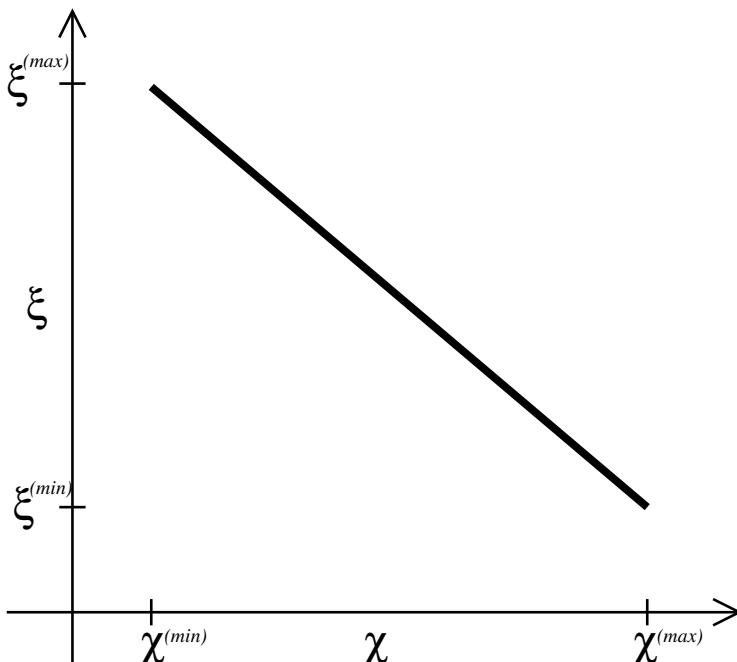
- The total of chemical species within some chemical family may be preserved following an air parcel although the individual species have a complicated relation to each other and may be transformed into each other through chemical reactions (e.g., total chlorine)
- Aerosol-cloud interactions (Ovtchinnikov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

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



Figures from Plumb (2007).

# Analyzing scatter plots

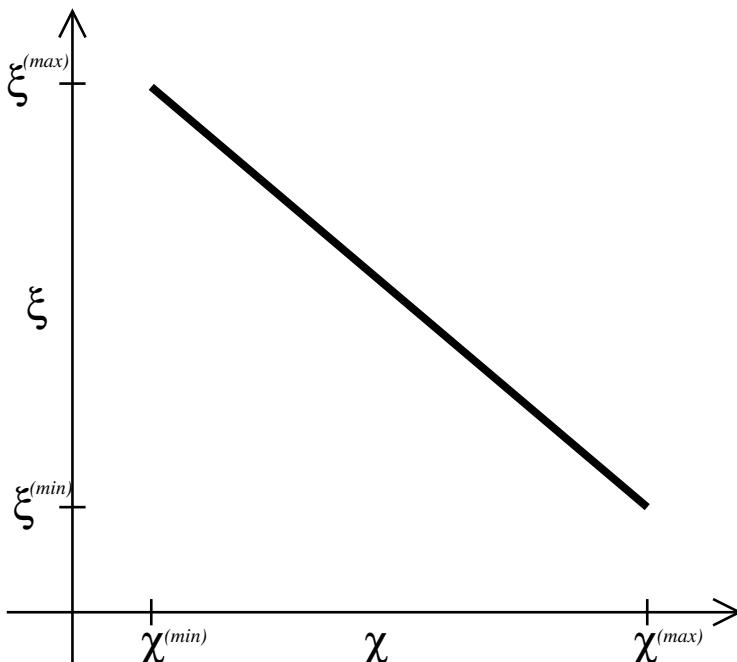


Analytical pre-existing functional relationship curve  $\psi$  (linear)

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

where  $a$  and  $b$  are constants, and  $\chi$  and  $\xi$  are the mixing ratios of the two tracers

# Analyzing scatter plots

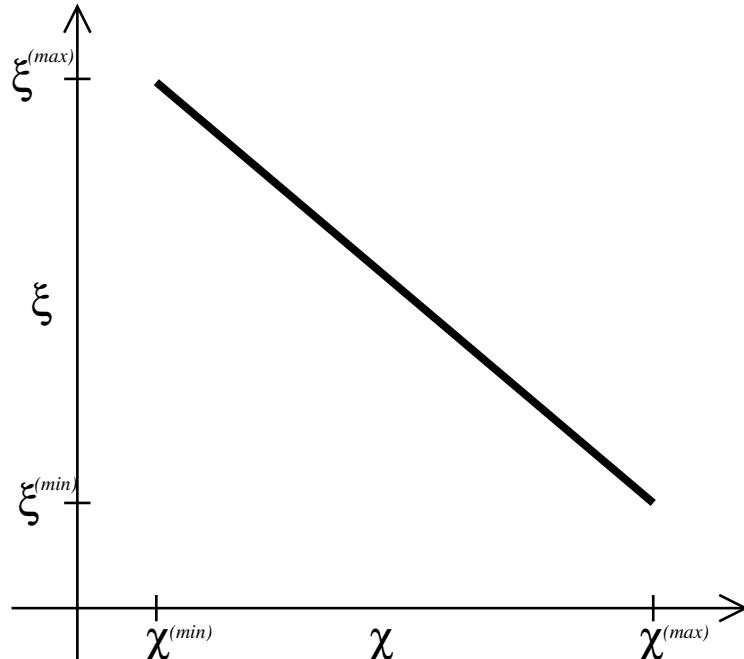


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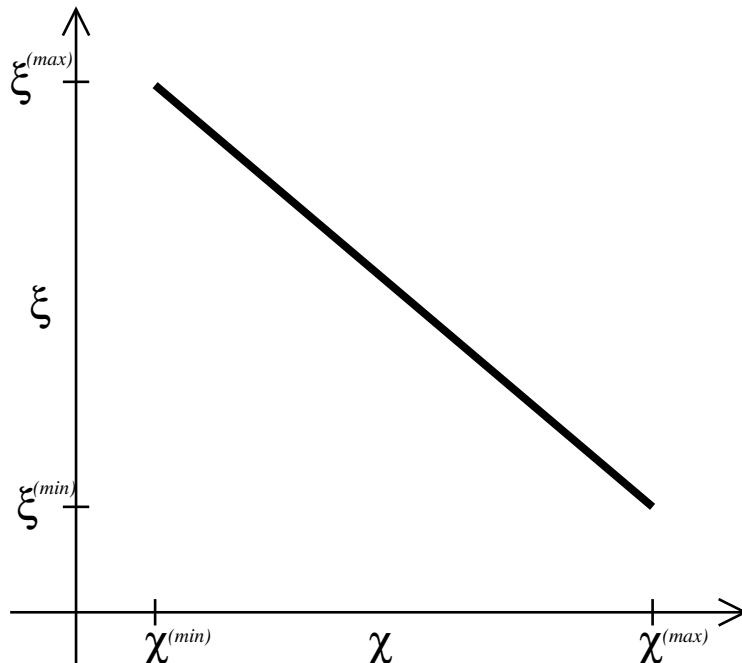
Analytical pre-existing functional relationship curve  $\psi$  (linear)

$\chi$  and  $\xi$  are transported separately by the transport scheme

$$\begin{aligned}\chi_k^{n+1} &= \mathcal{T}(\chi_j^n), \quad j \in \mathcal{H}, \\ \xi_k^{n+1} &= \mathcal{T}(\xi_j^n), \quad j \in \mathcal{H},\end{aligned}$$

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

# Analyzing scatter plots



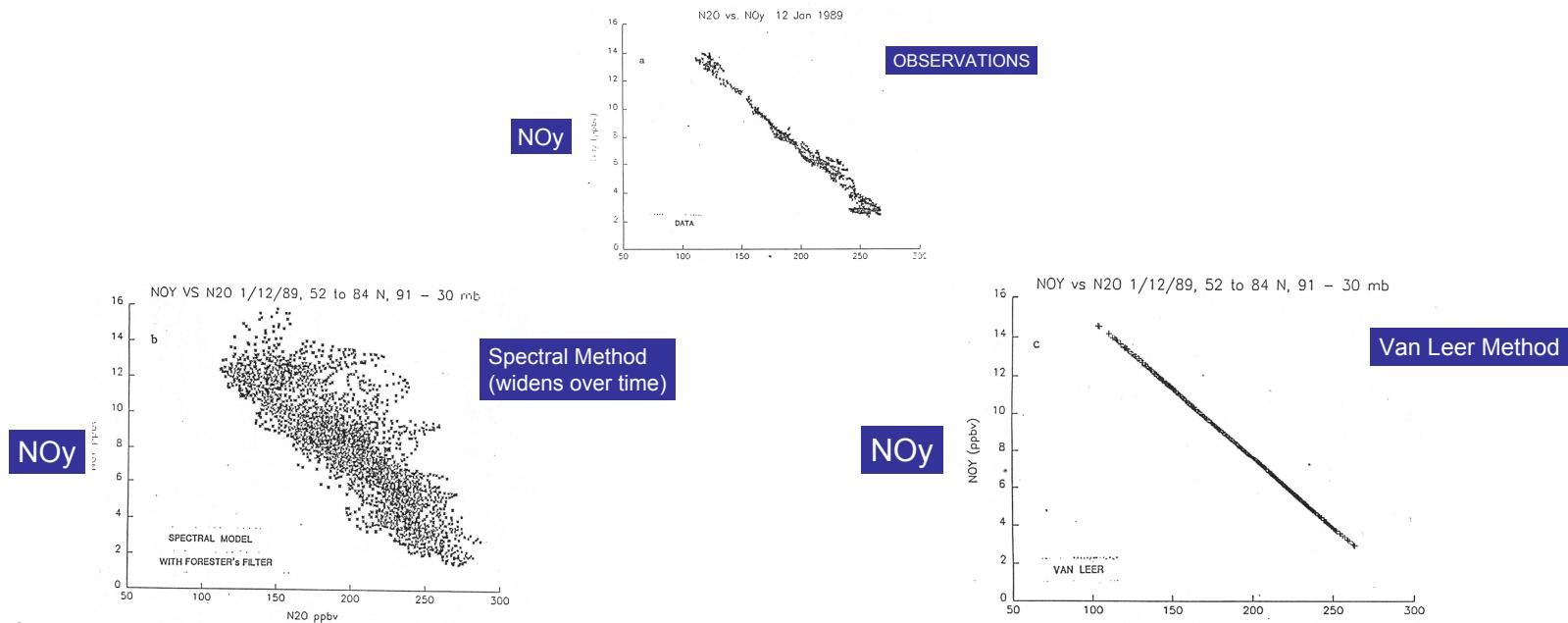
Analytical pre-existing functional relationship curve  $\psi$  (linear)

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  $\psi$  (linear)

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

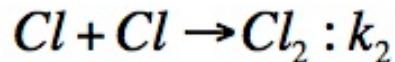
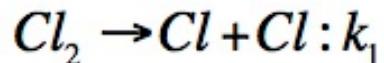
# The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

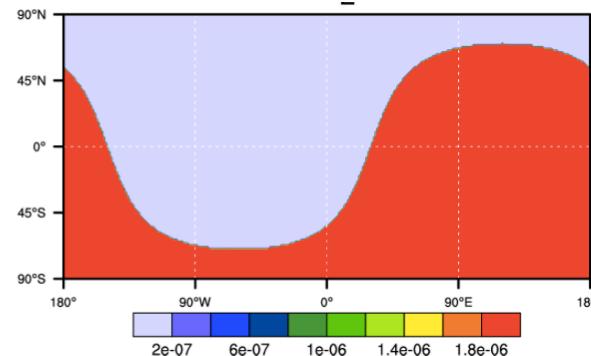
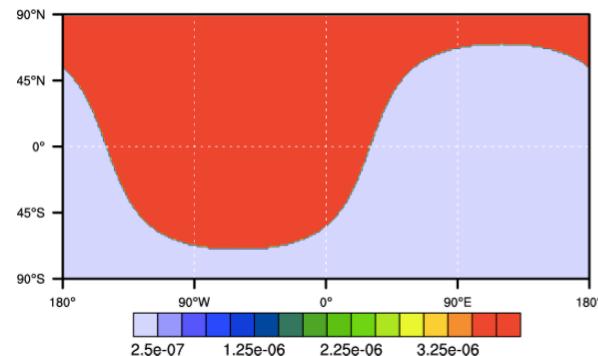
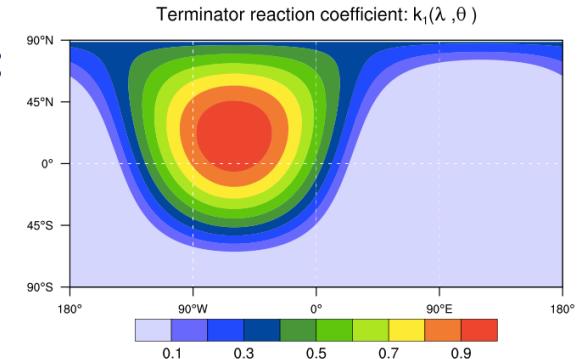
See: <http://www.cgd.ucar.edu/cms/pel/terminator.html>



- Consider 2 reactive chemical species, Cl and  $\text{Cl}_2$ :



- 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)

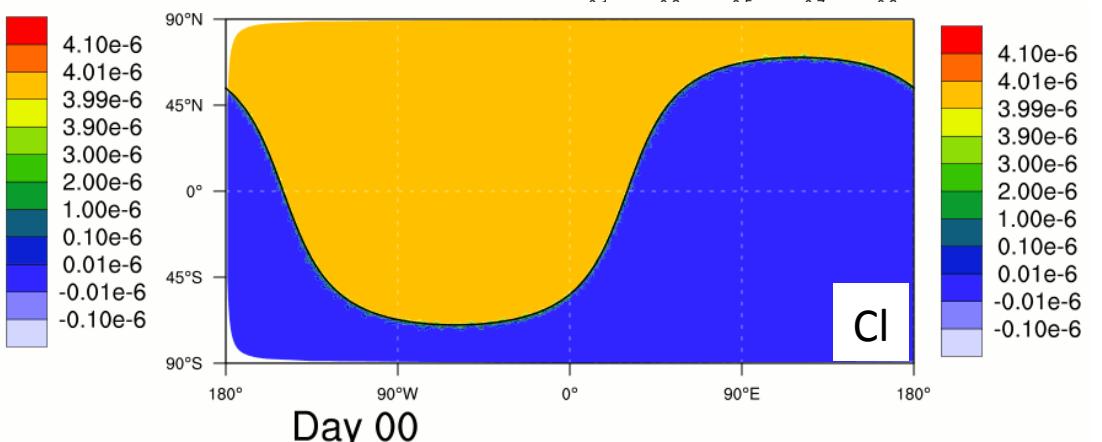
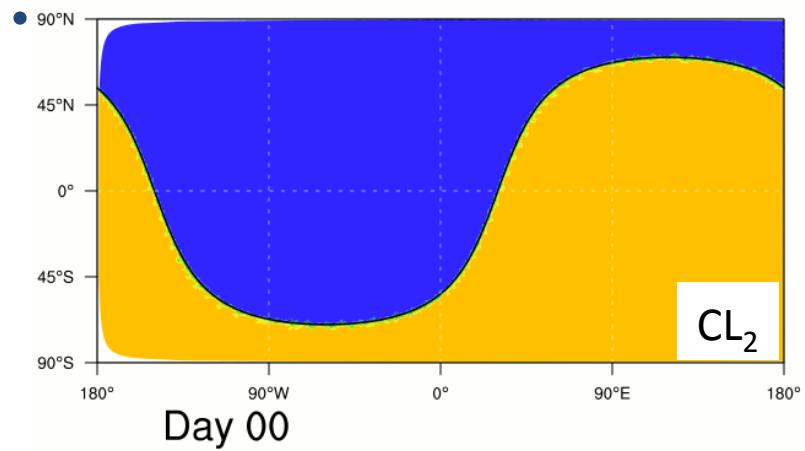
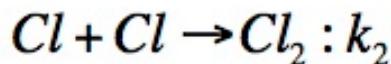
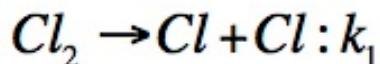
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See: <http://www.cgd.ucar.edu/cms/pel/terminator.html>



- Consider 2 reactive chemical species, Cl and  $\text{Cl}_2$ :

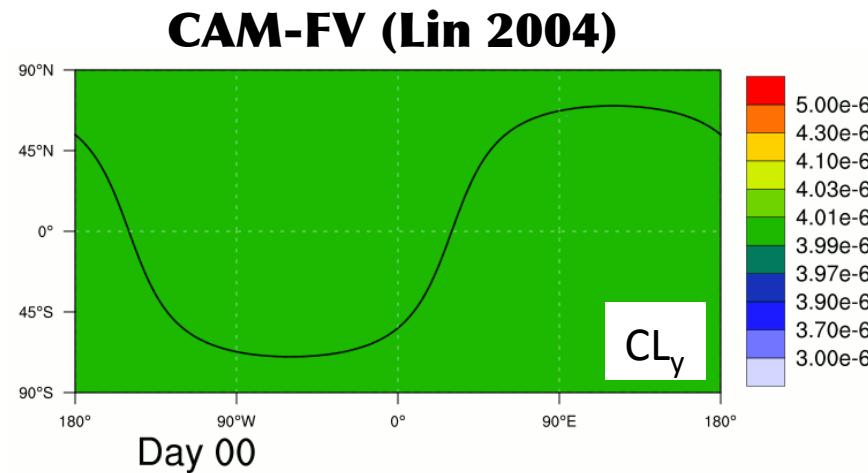
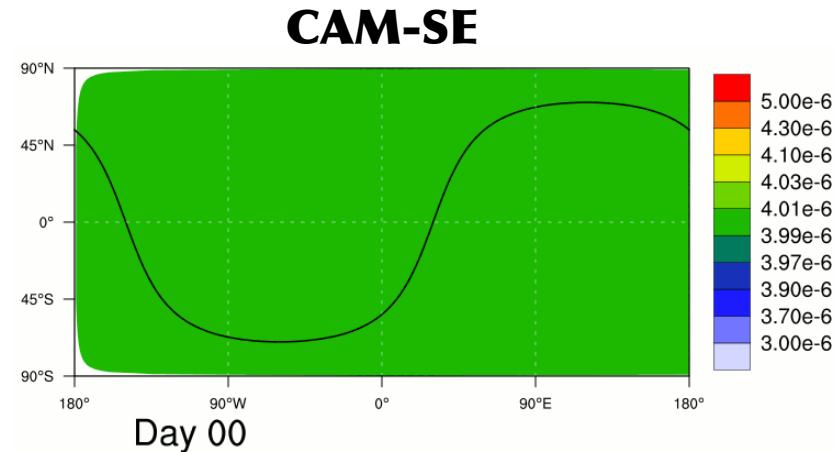


- In any flow-field  $\text{Cl}_y = \text{Cl} + 2 * \text{Cl}_2$  should be constant at all times (linear correlation preservation).

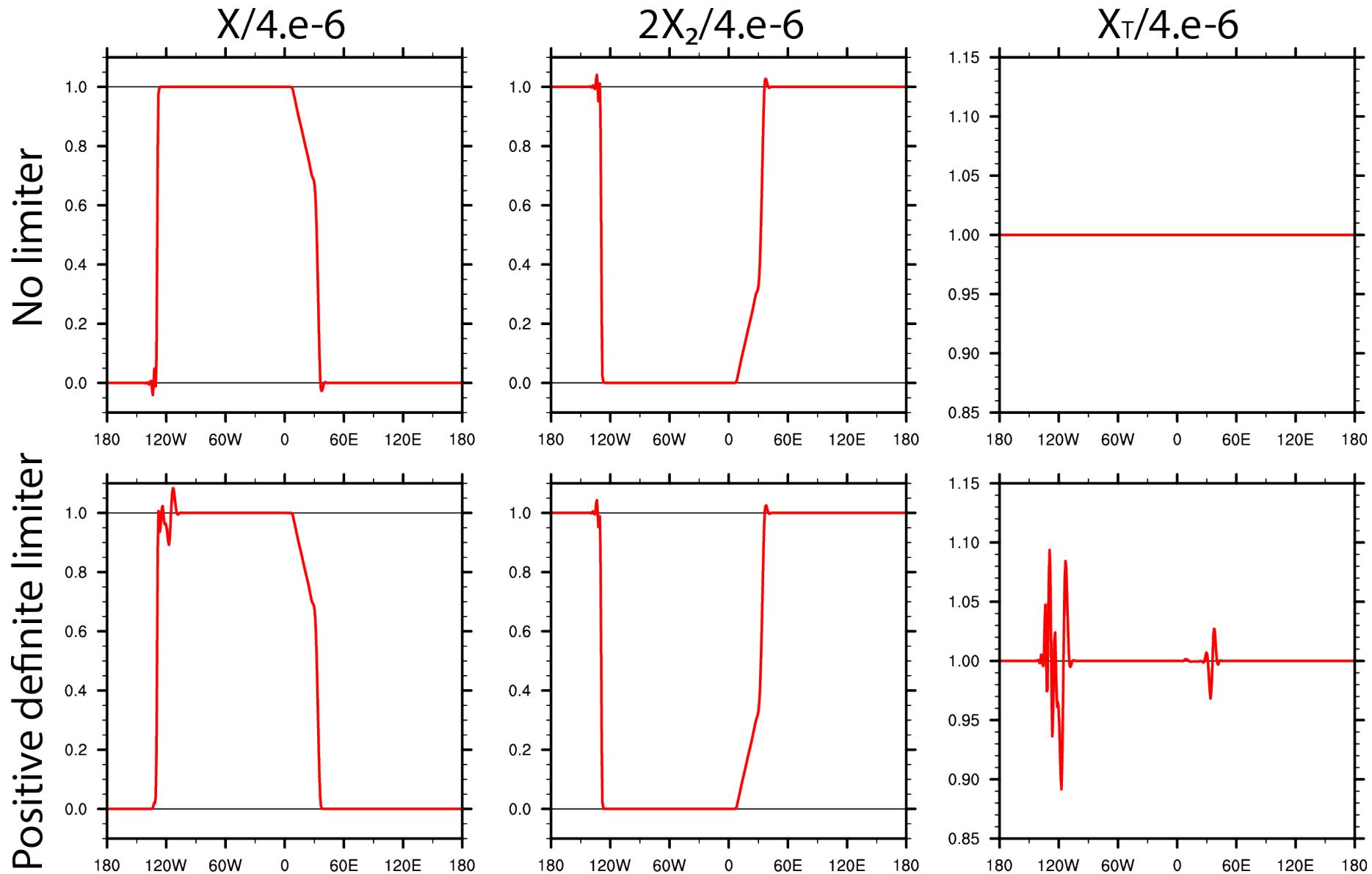
# The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

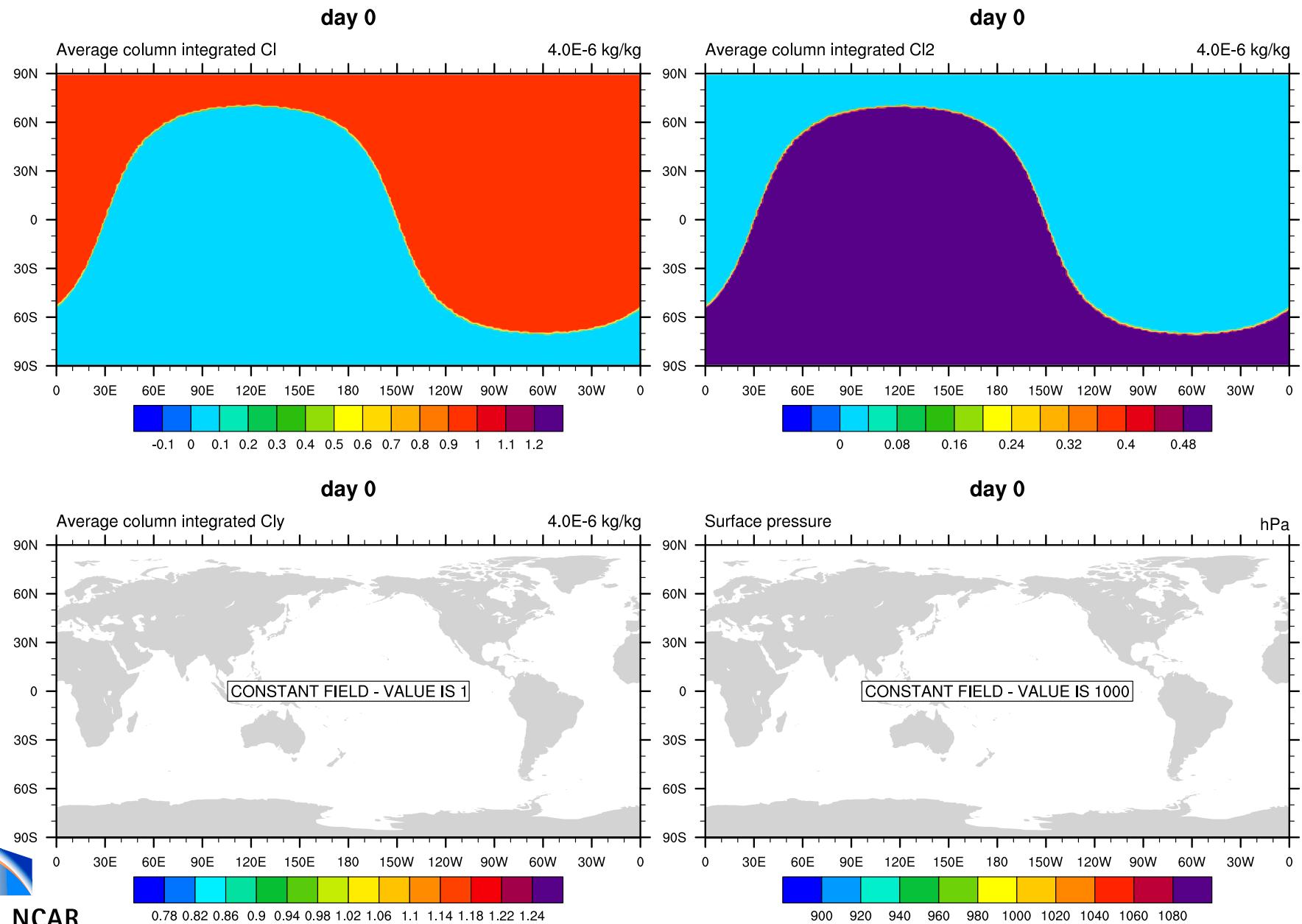
See: <http://www.cgd.ucar.edu/cms/pel/terminator.html>



- In any flow-field  $Cl_y = Cl + 2 * Cl_2$  should be constant at all times (correlation preservation).

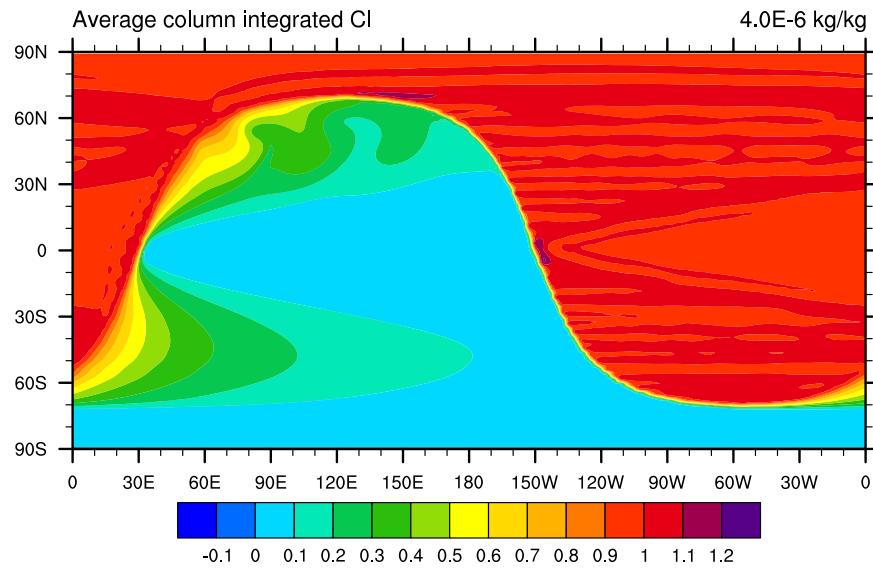


# 3D version: Initial condition

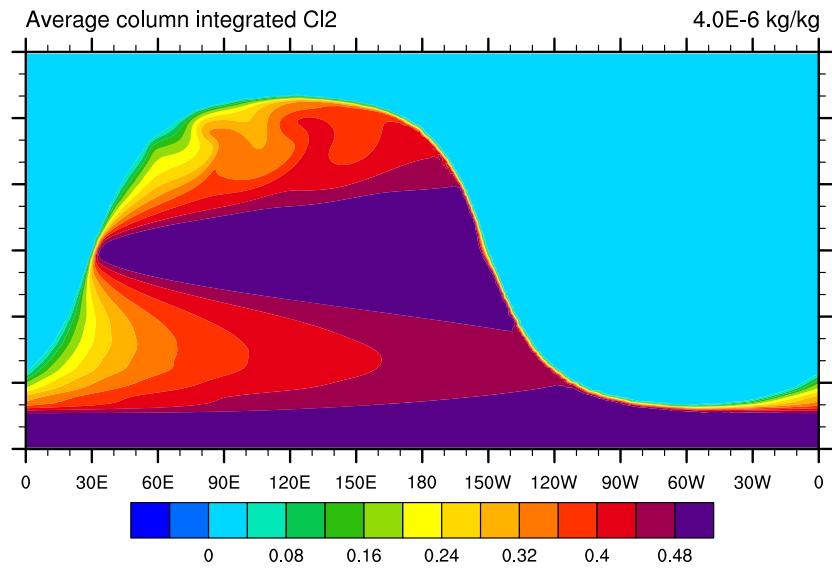


# CAM-SE

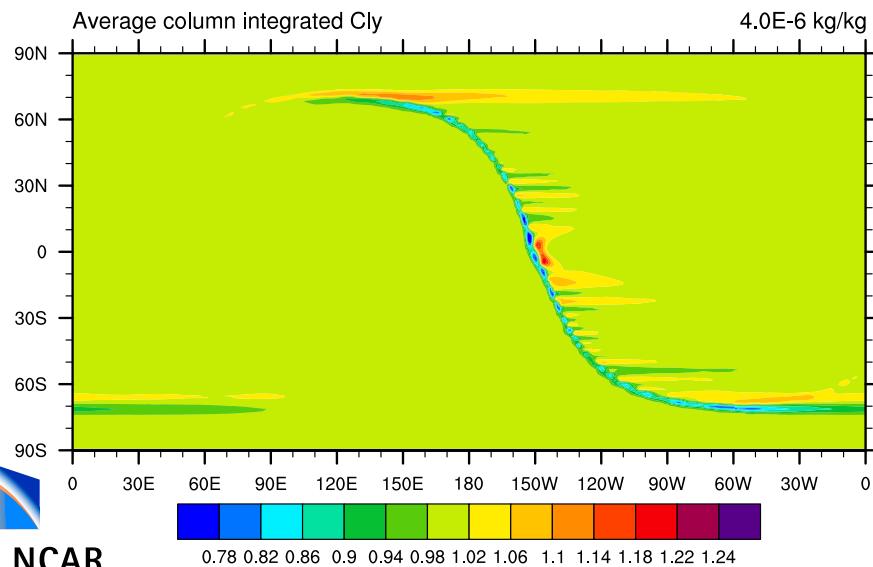
day 9



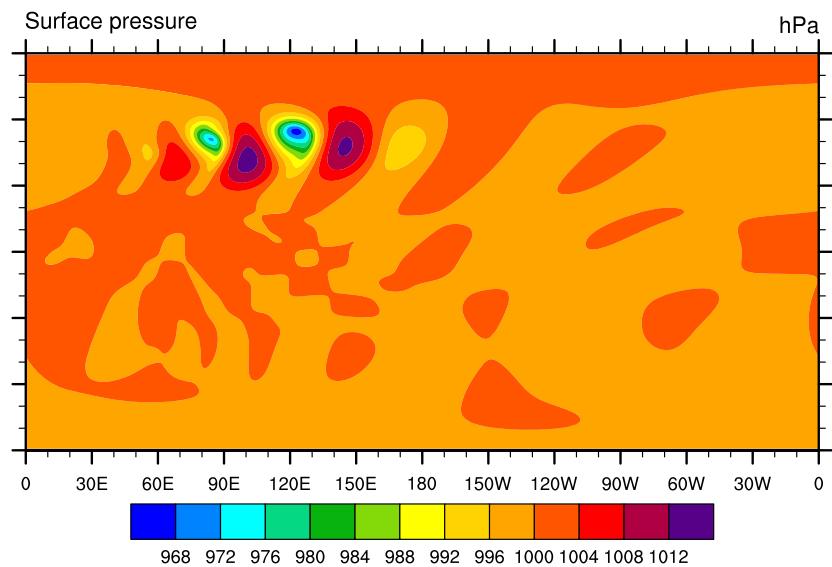
day 9



day 9

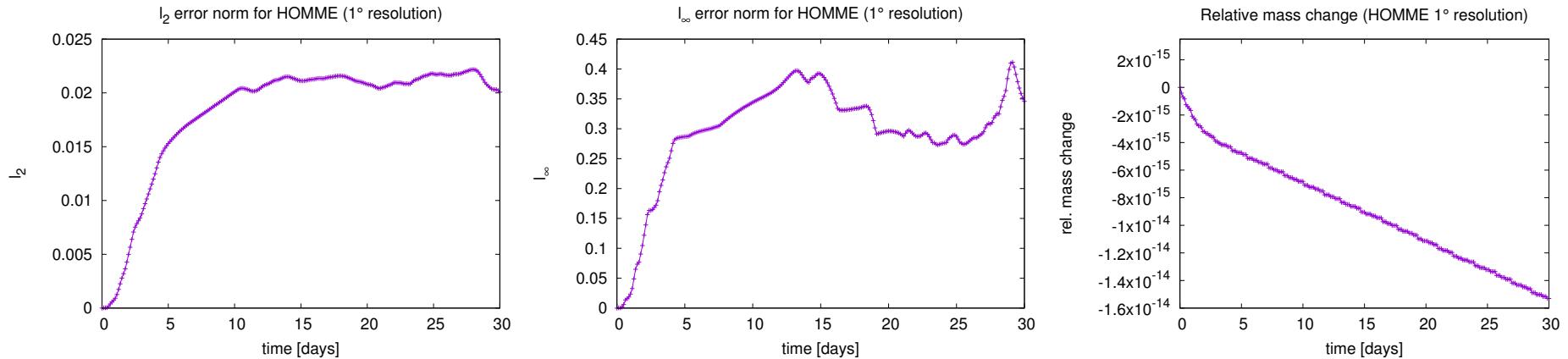


day 9

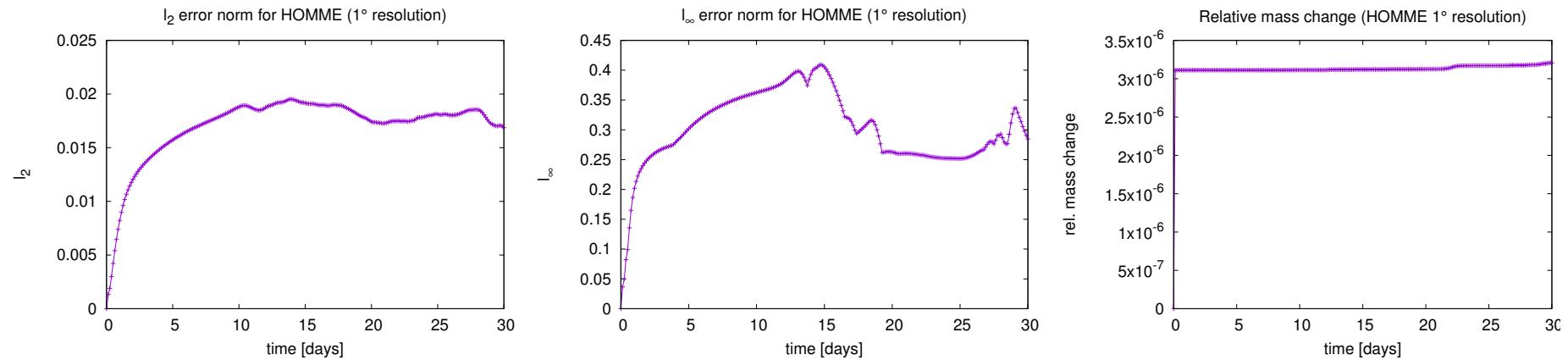


NCAR

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



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



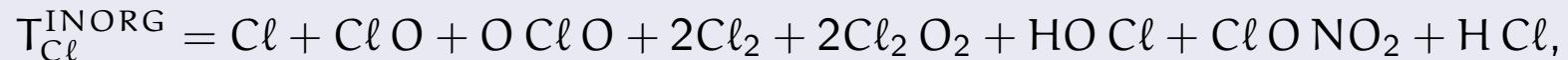
# Conserving sum of “families” of species

Chlorine (in CAM-chemistry)

Total Organic Chlorine (set at the surface)



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



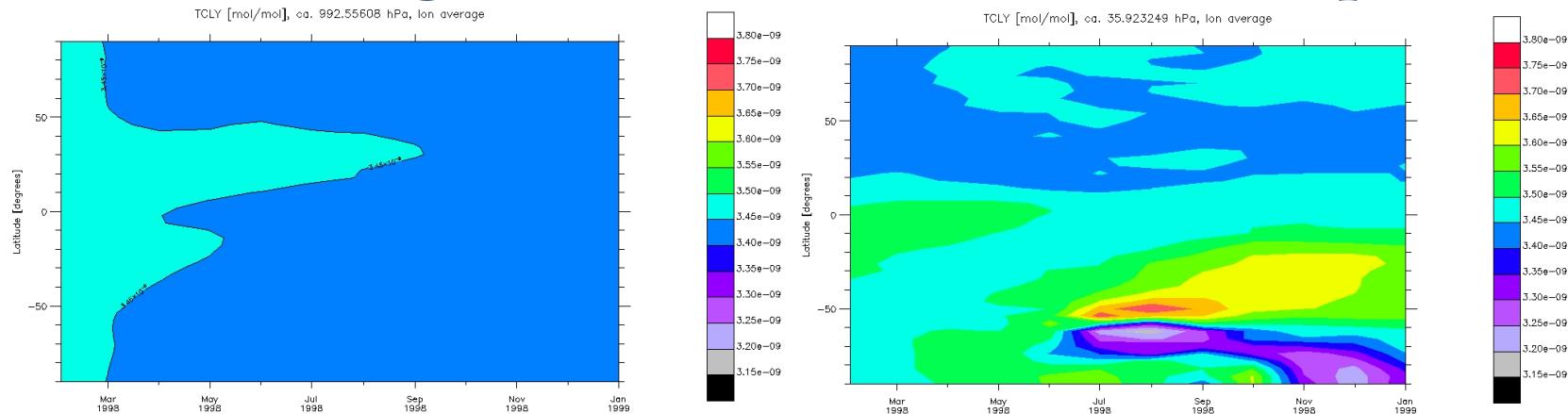
Total Chlorine

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

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	$\rightarrow$ CH <sub>3</sub> CO <sub>3</sub> + NO <sub>2</sub> + M	$k(CH_3CO_3+NO_2+M)\cdot 1.111E28 \cdot \exp(-14\,000/T)$
CH <sub>3</sub> CO <sub>3</sub> + CH <sub>3</sub> CO <sub>3</sub>	$\rightarrow$ 2·CH <sub>3</sub> O <sub>2</sub> + 2·{CO <sub>2</sub> }	2.50E-12·exp(500/T)
GLYALD + OH	$\rightarrow$ HO <sub>2</sub> + .2·GLYOXAL + .8·CH <sub>2</sub> O + .8·{CO <sub>2</sub> }	1.00E-11
GLYOXAL + OH	$\rightarrow$ HO <sub>2</sub> + CO + {CO <sub>2</sub> }	1.10E-11
CH <sub>3</sub> COOH + OH	$\rightarrow$ CH <sub>3</sub> O <sub>2</sub> + {CO <sub>2</sub> } + H <sub>2</sub> O	7.00E-13
C <sub>2</sub> H <sub>5</sub> OH + OH	$\rightarrow$ HO <sub>2</sub> + CH <sub>3</sub> CHO	6.90E-12·exp(-230/T)
C <sub>3</sub> H <sub>6</sub> + OH + M	$\rightarrow$ PO <sub>2</sub> + M	$ko=8.00E-27 \cdot (300/T)^{3.50}; ki=3.00E-11; f=0.50$

# 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?

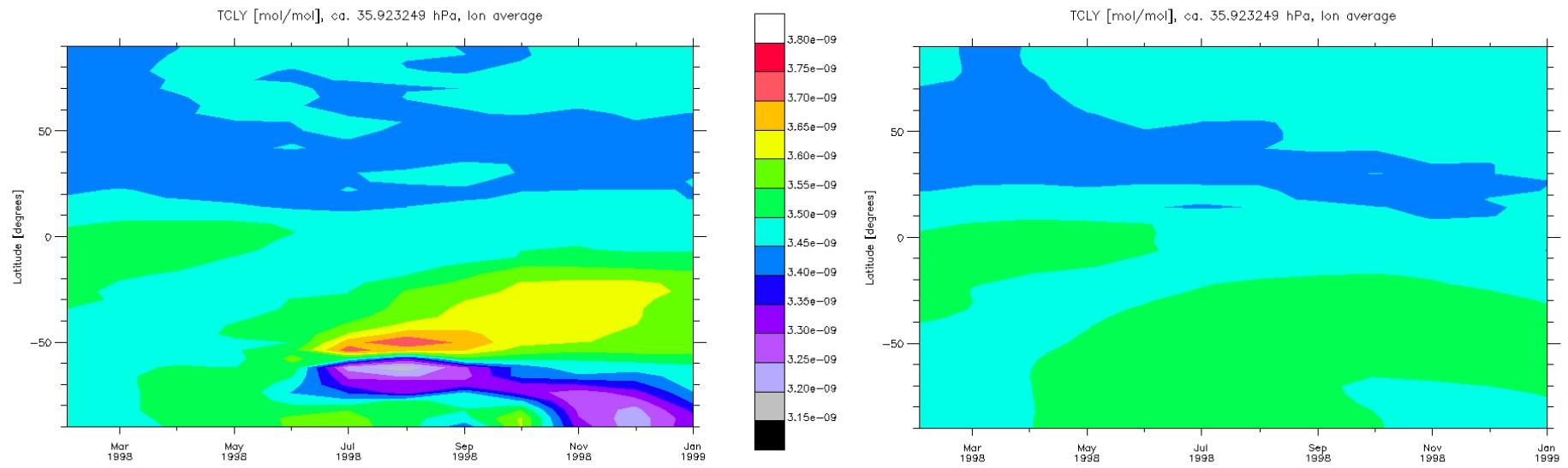
Transport scheme can not maintain the sum when transporting the species individually:

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

where  $N_x$  is the number of species  $\chi_i$ .

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

# Conserving sum of “families” of species



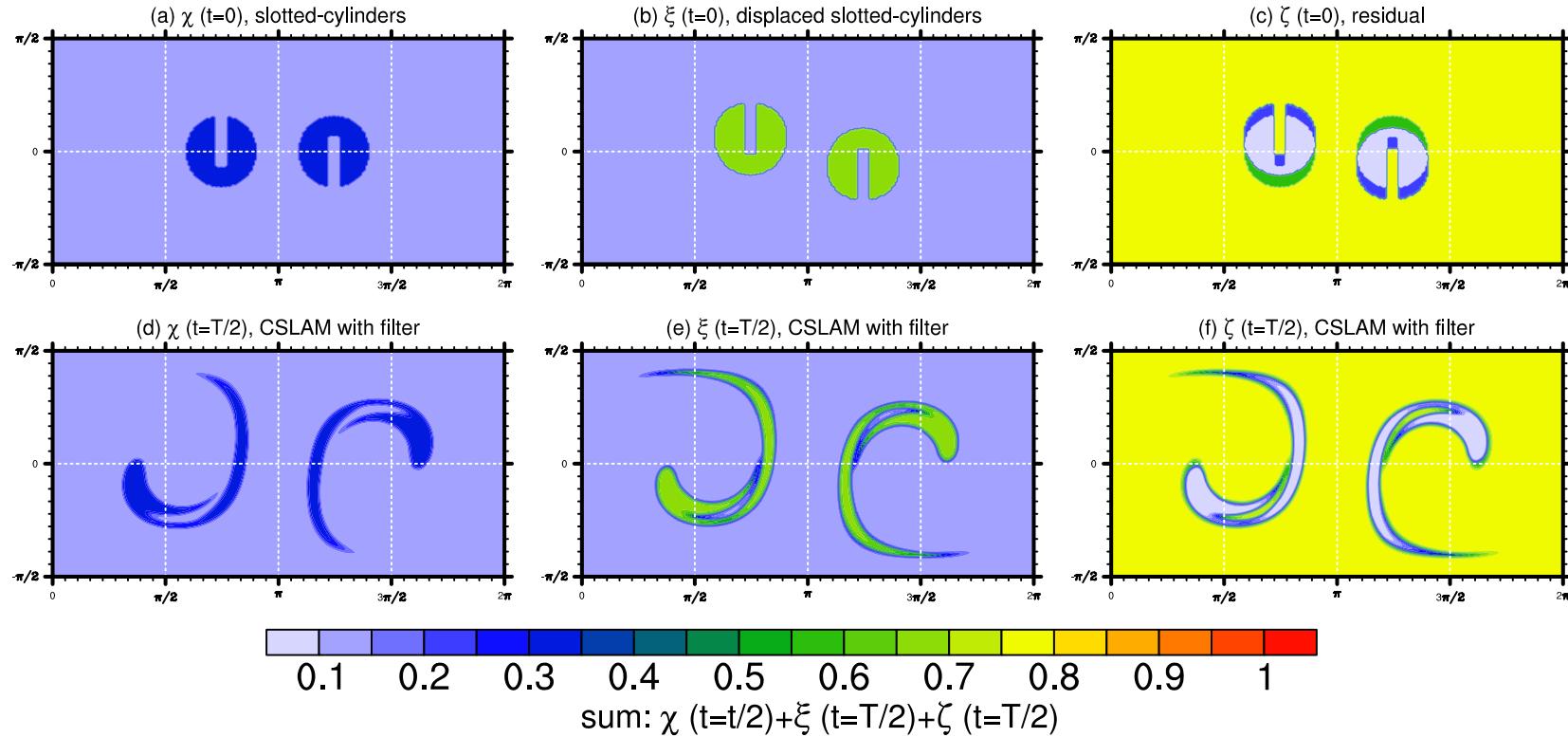
(left) same as previous slide:

- 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%).

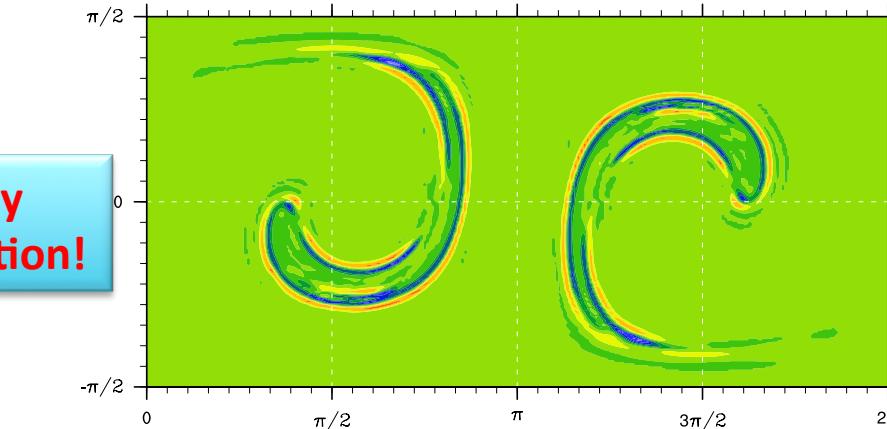
(right) same as (left) but using a fixer:

- (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

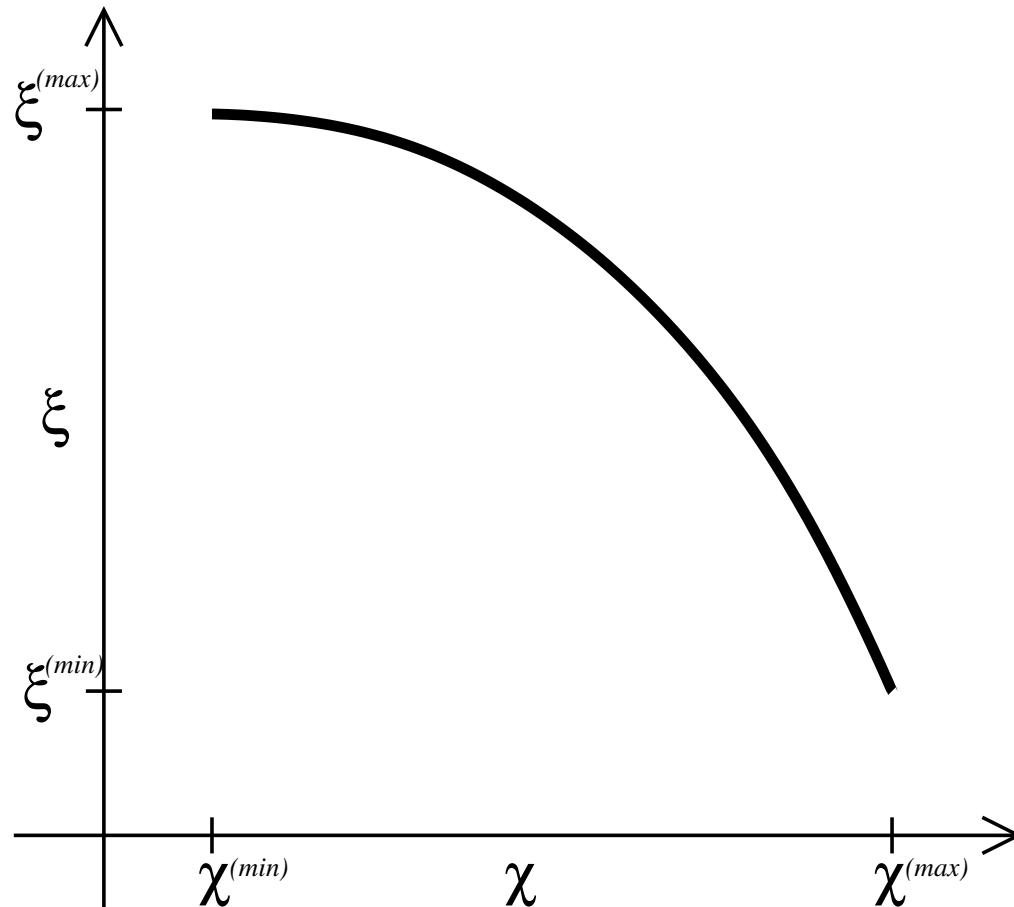


This test does not rely  
on an analytical solution!



Lauritzen and  
Thuburn (2010)

# Analyzing scatter plots

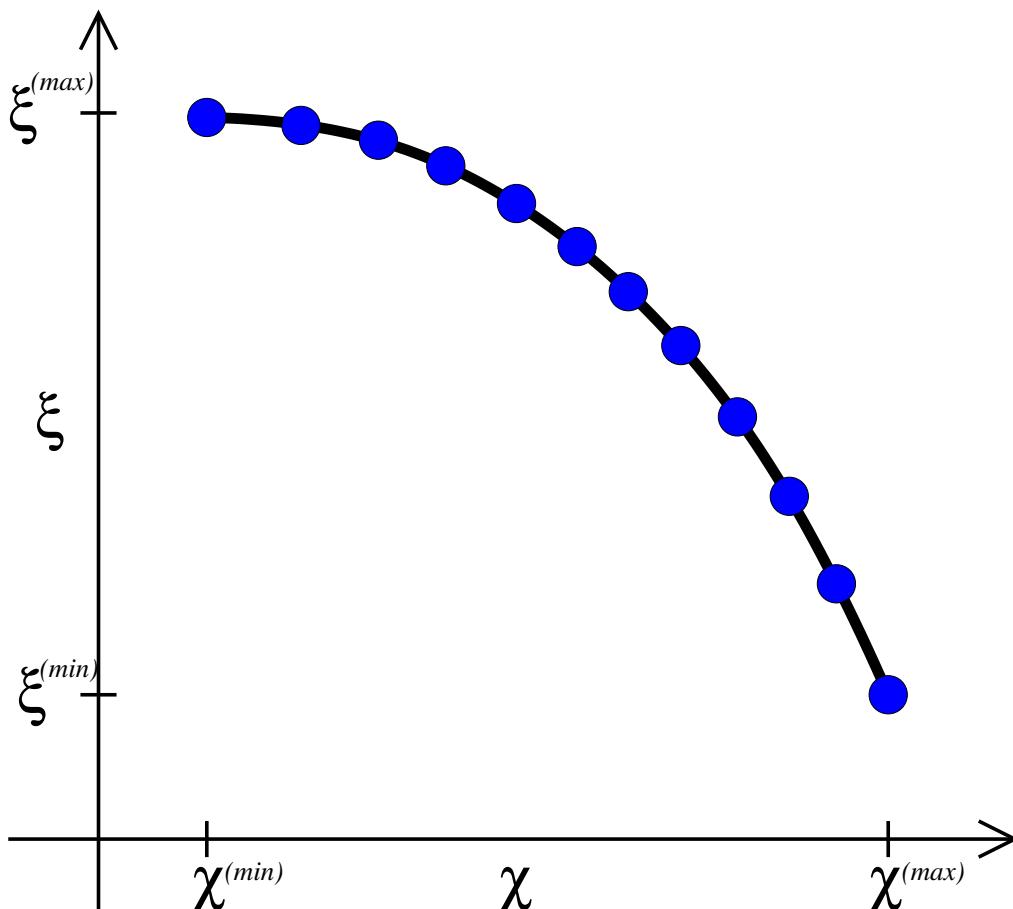


Analytical pre-existing functional relationship curve  $\psi$

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

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

# Analyzing scatter plots

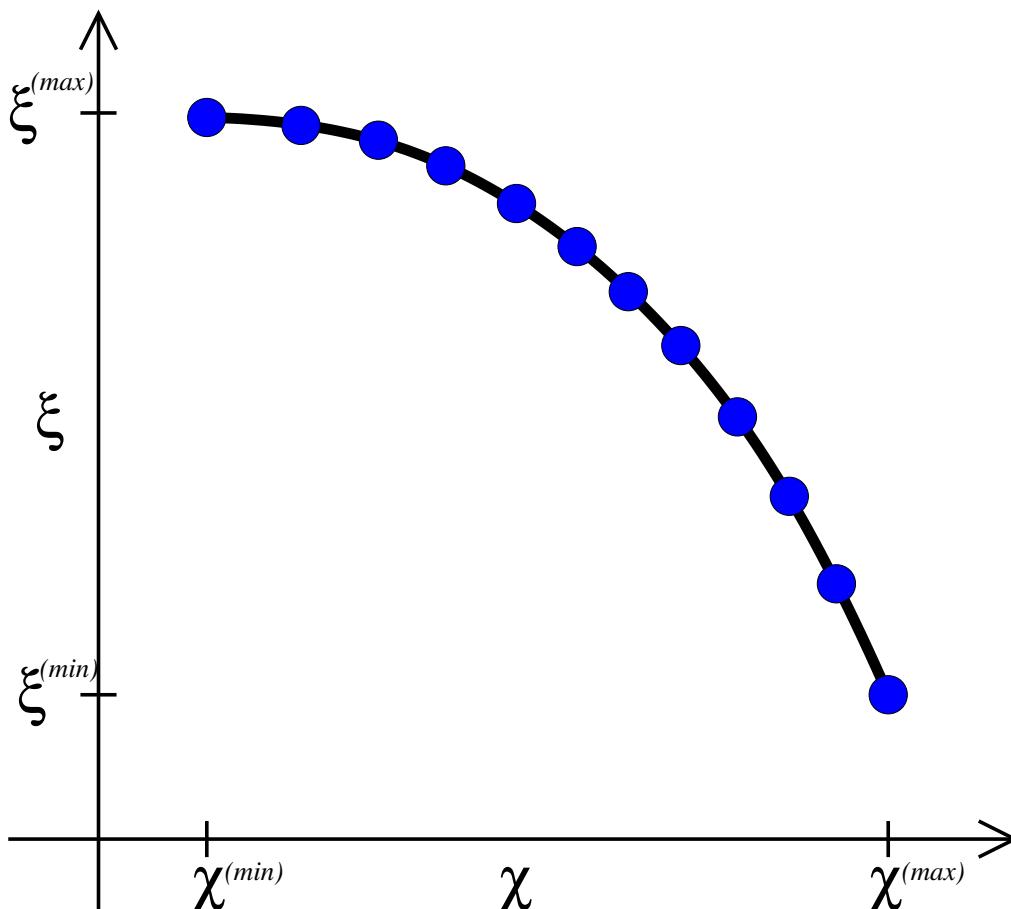


Discrete pre-existing functional relation (initial condition)

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

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

# Analyzing scatter plots

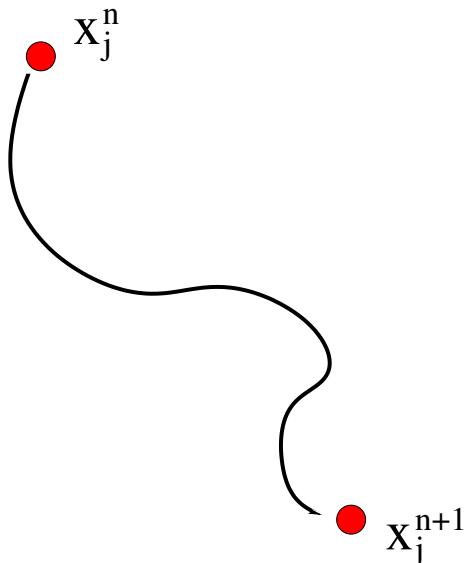


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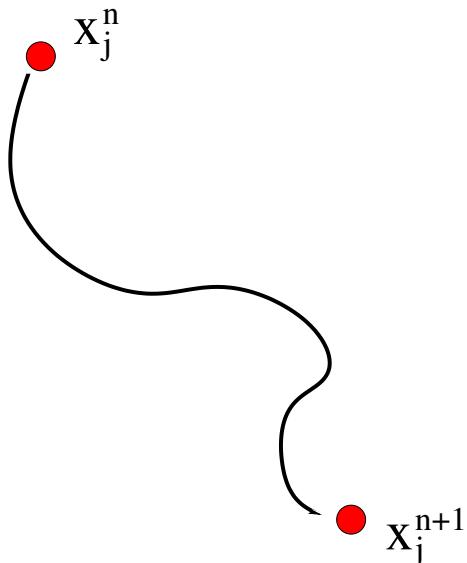


A fully Lagrangian model will maintain pre-existing functional relation

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

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

# Analyzing scatter plots

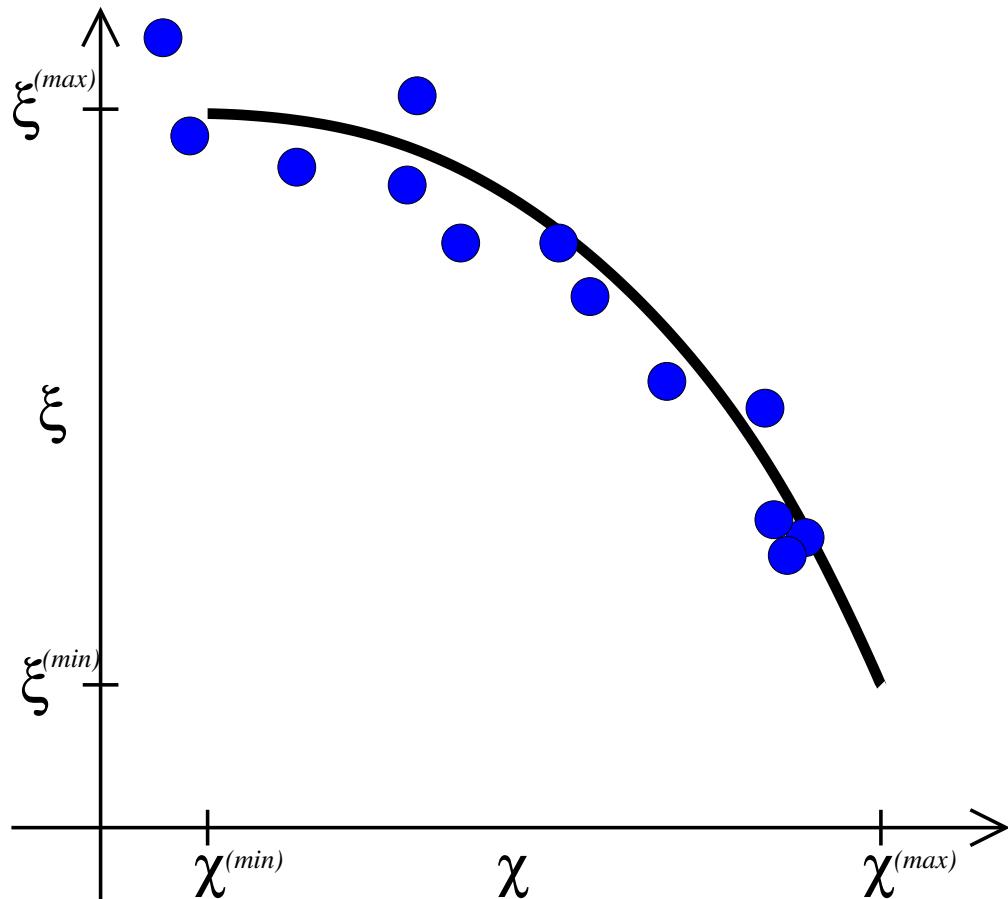


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# Analyzing scatter plots

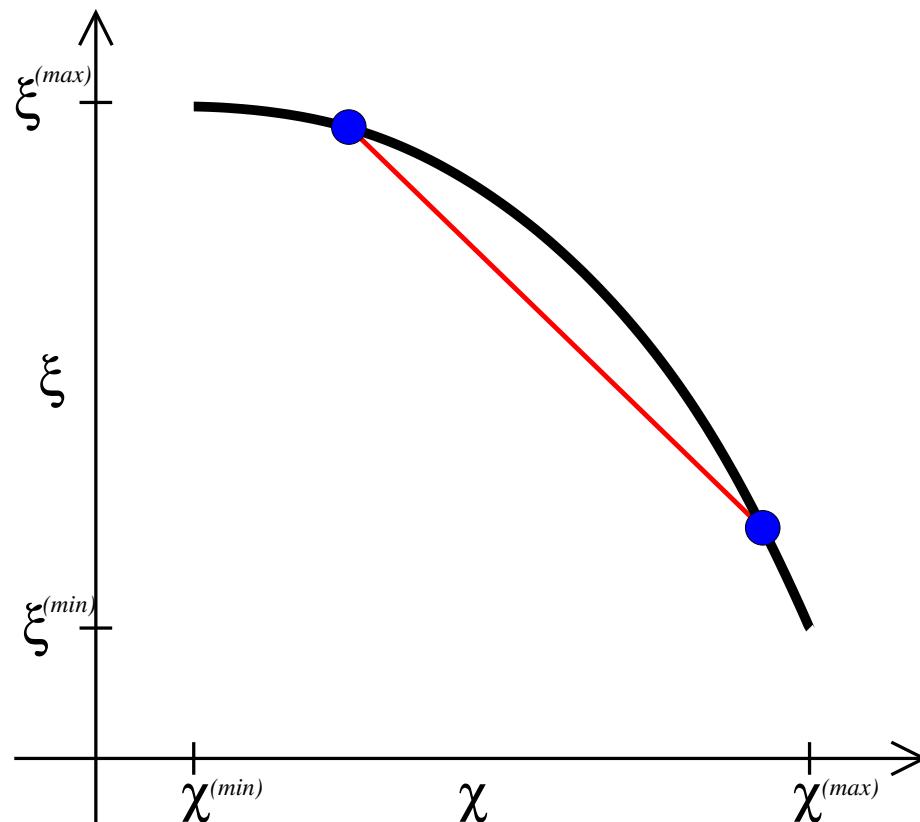


Any Eulerian/semi-Lagrangian scheme will disrupt pre-existing functional relation

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

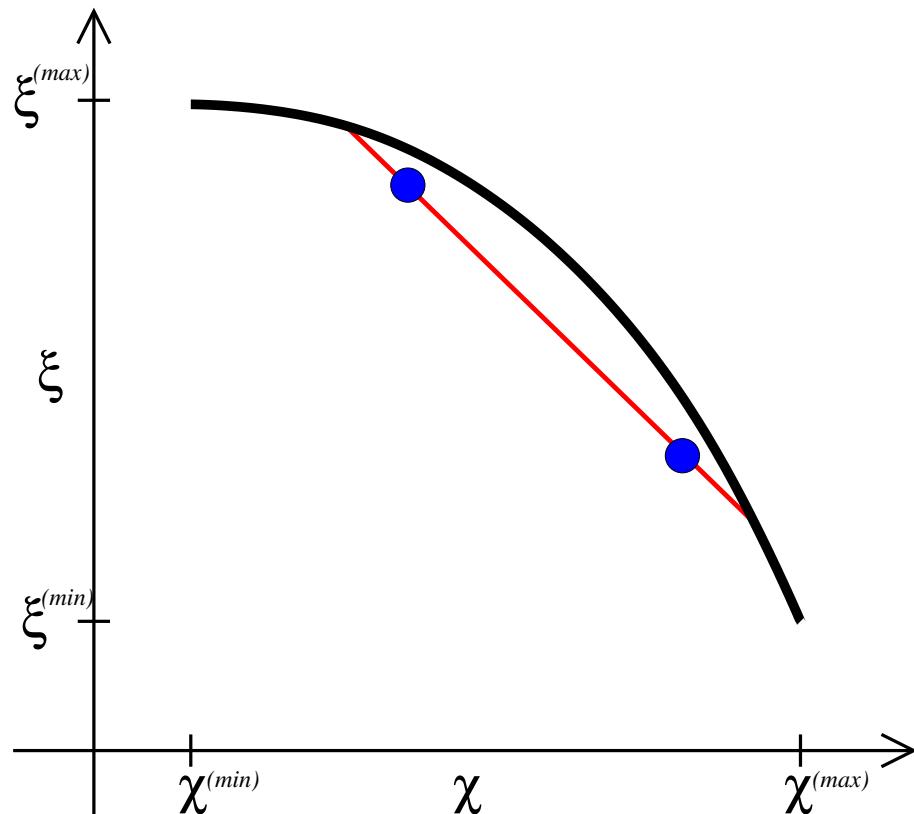
where  $\mathcal{T}$  is the transport operator and  $\mathcal{H}$  the set of indices defining the ‘halo’ for  $\mathcal{T}$ .

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

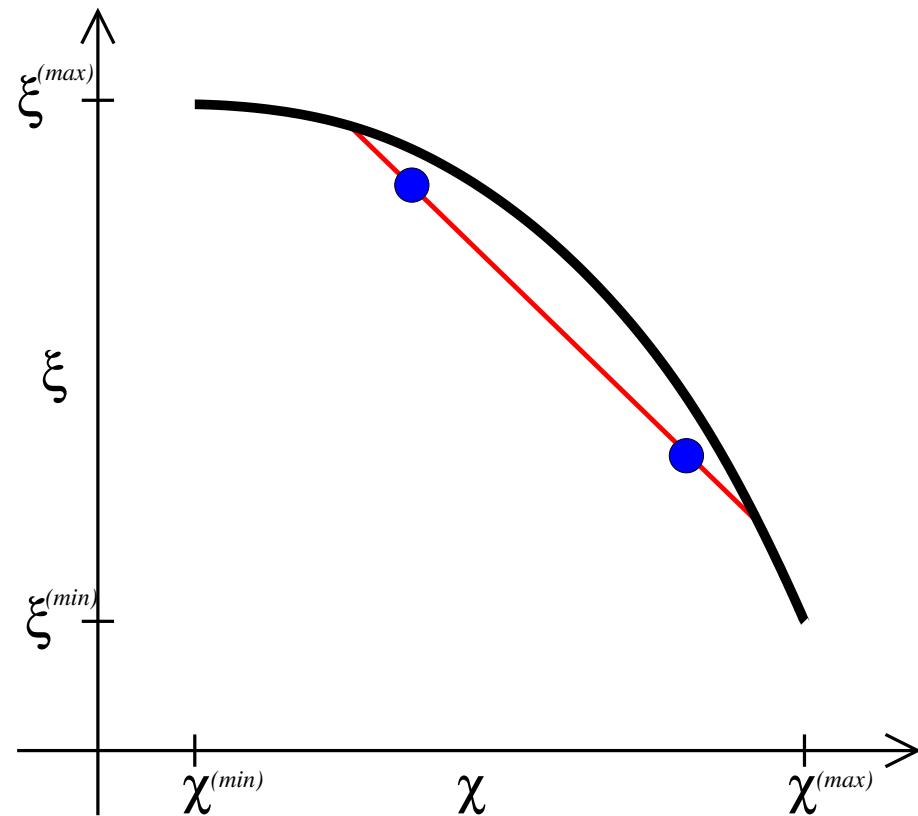
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→ Ideally numerical mixing should = 'real mixing'!

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

# Classification of numerical mixing on scatter plots



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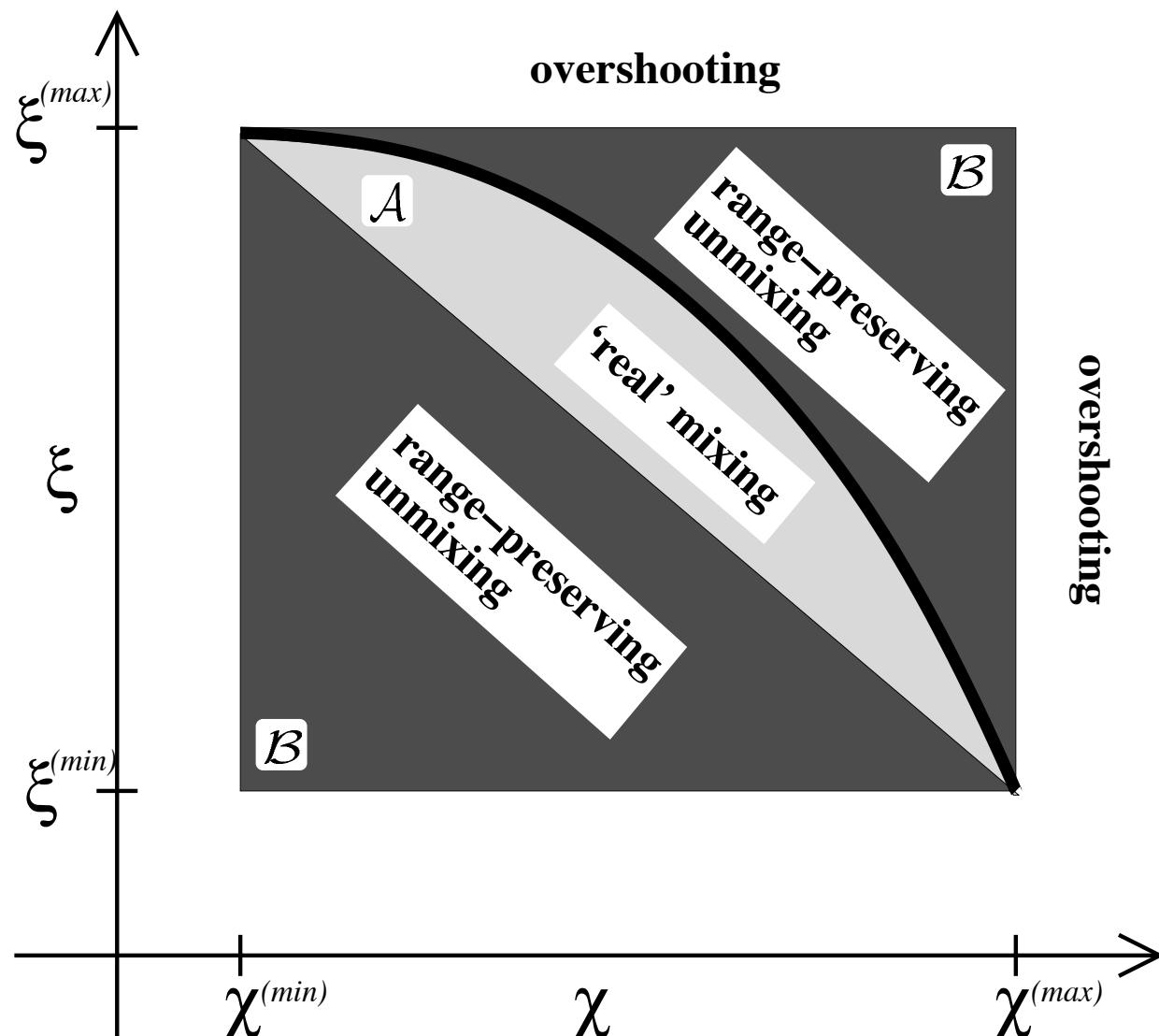
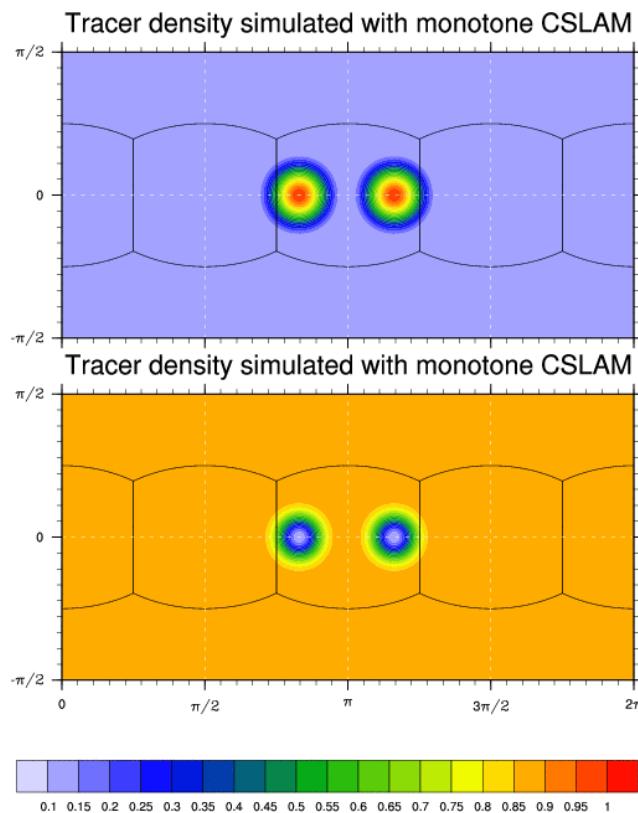


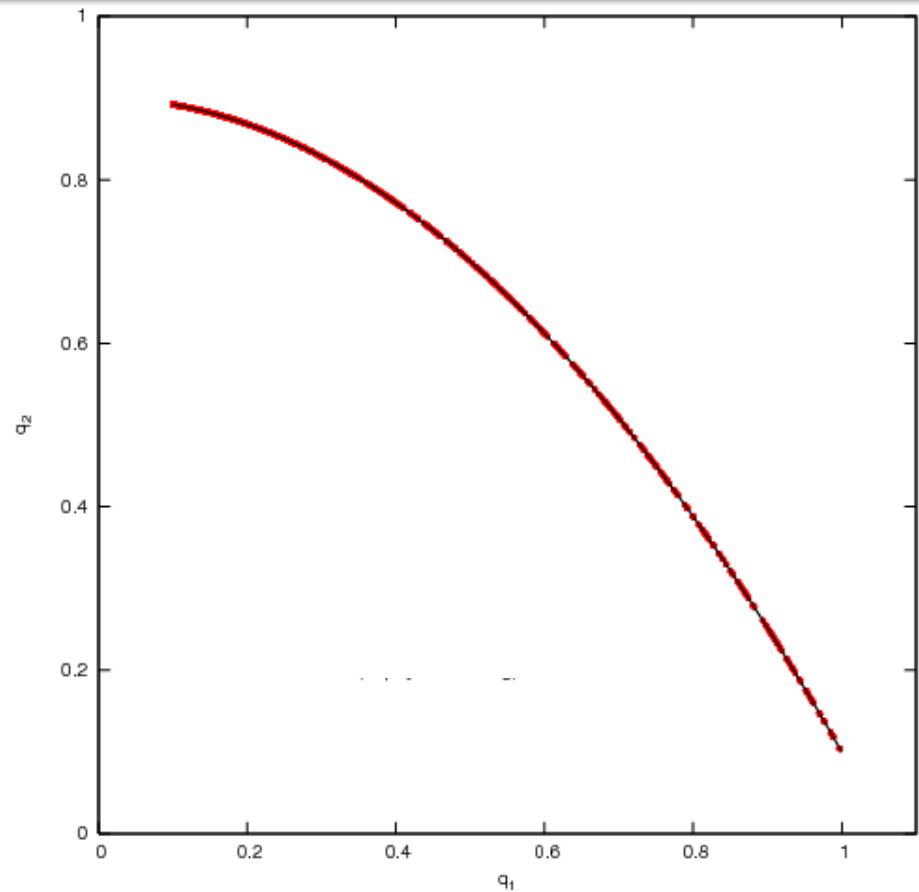
Figure from (Lauritzen and Thuburn, 2012)

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

## First-order scheme: only ‘real mixing’

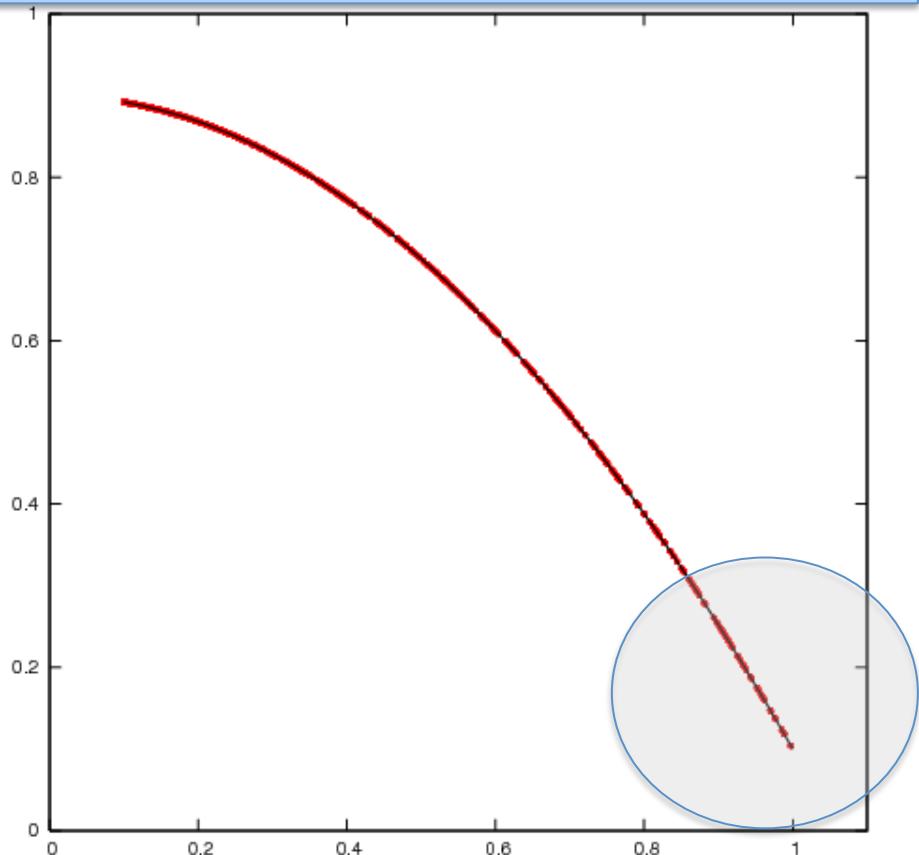
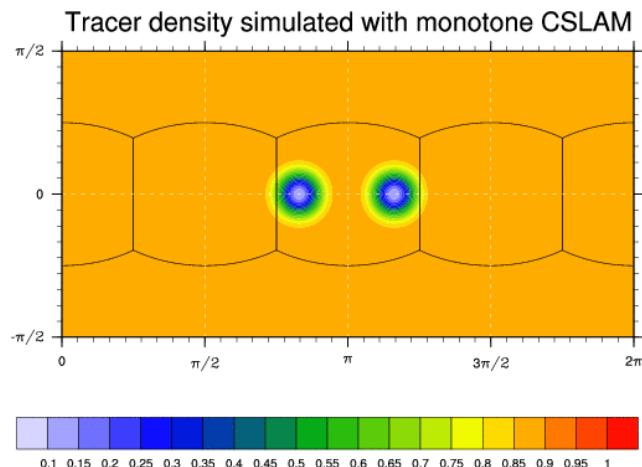
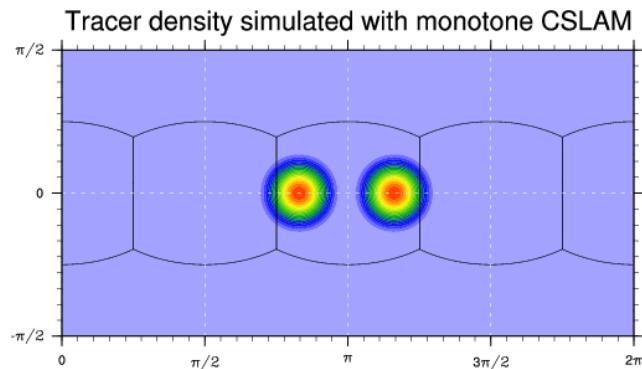


Nair and Lauritzen (2010) flow field



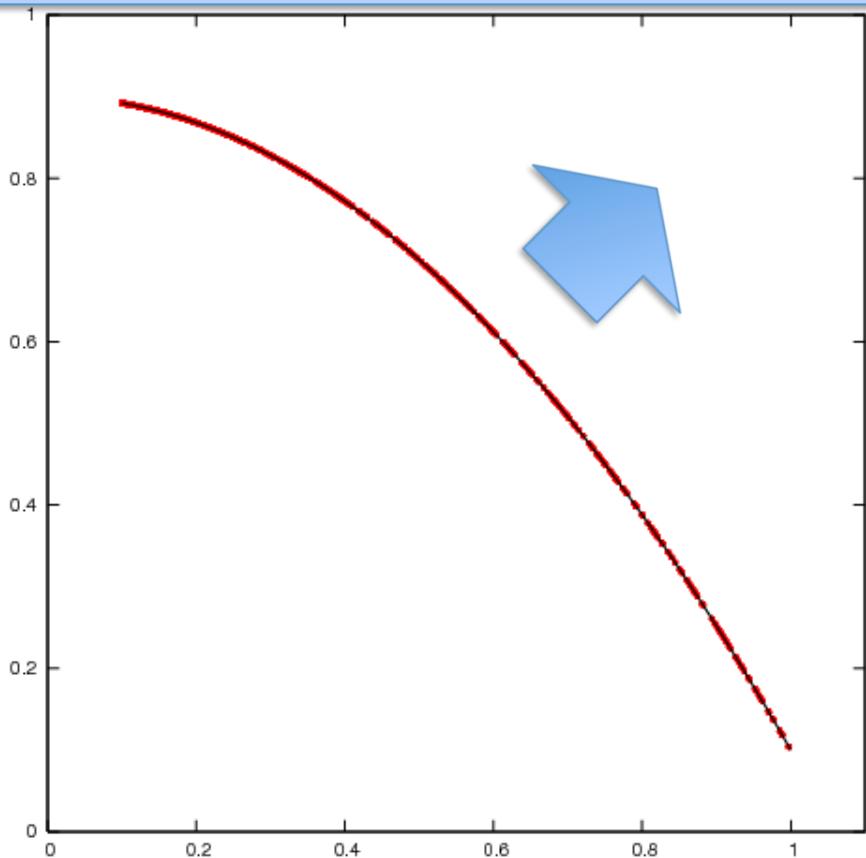
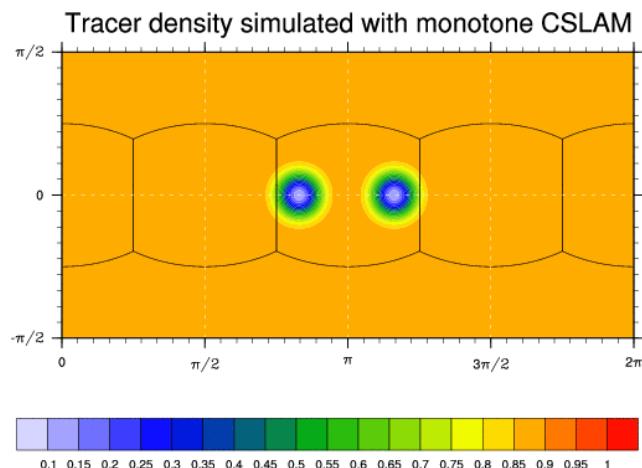
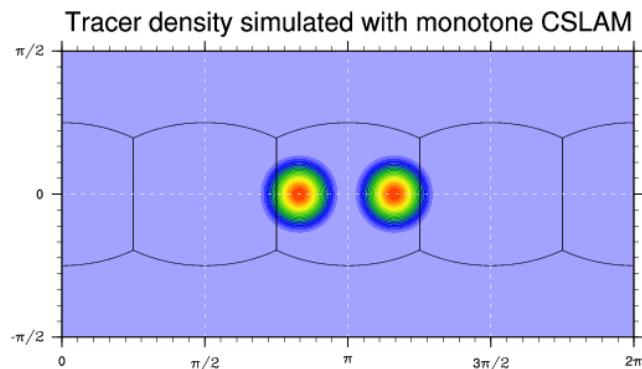
# Preserving pre-existing functional relation between tracers under challenging flow conditions

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



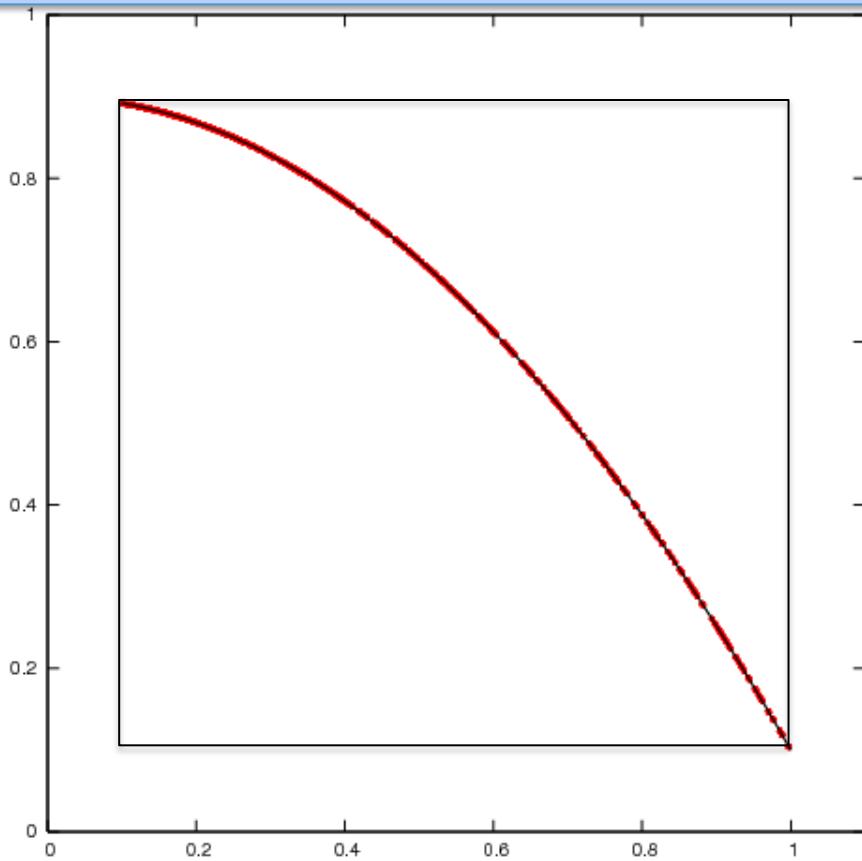
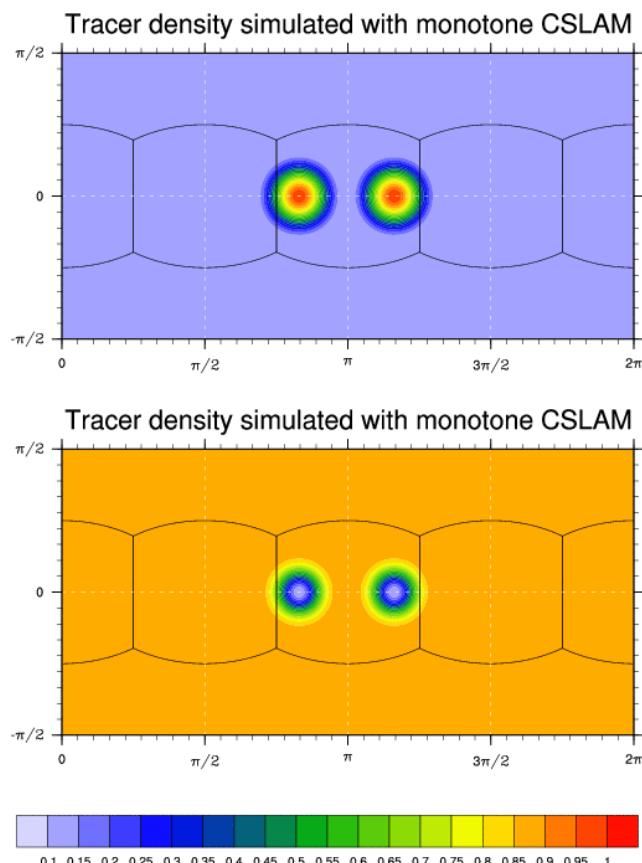
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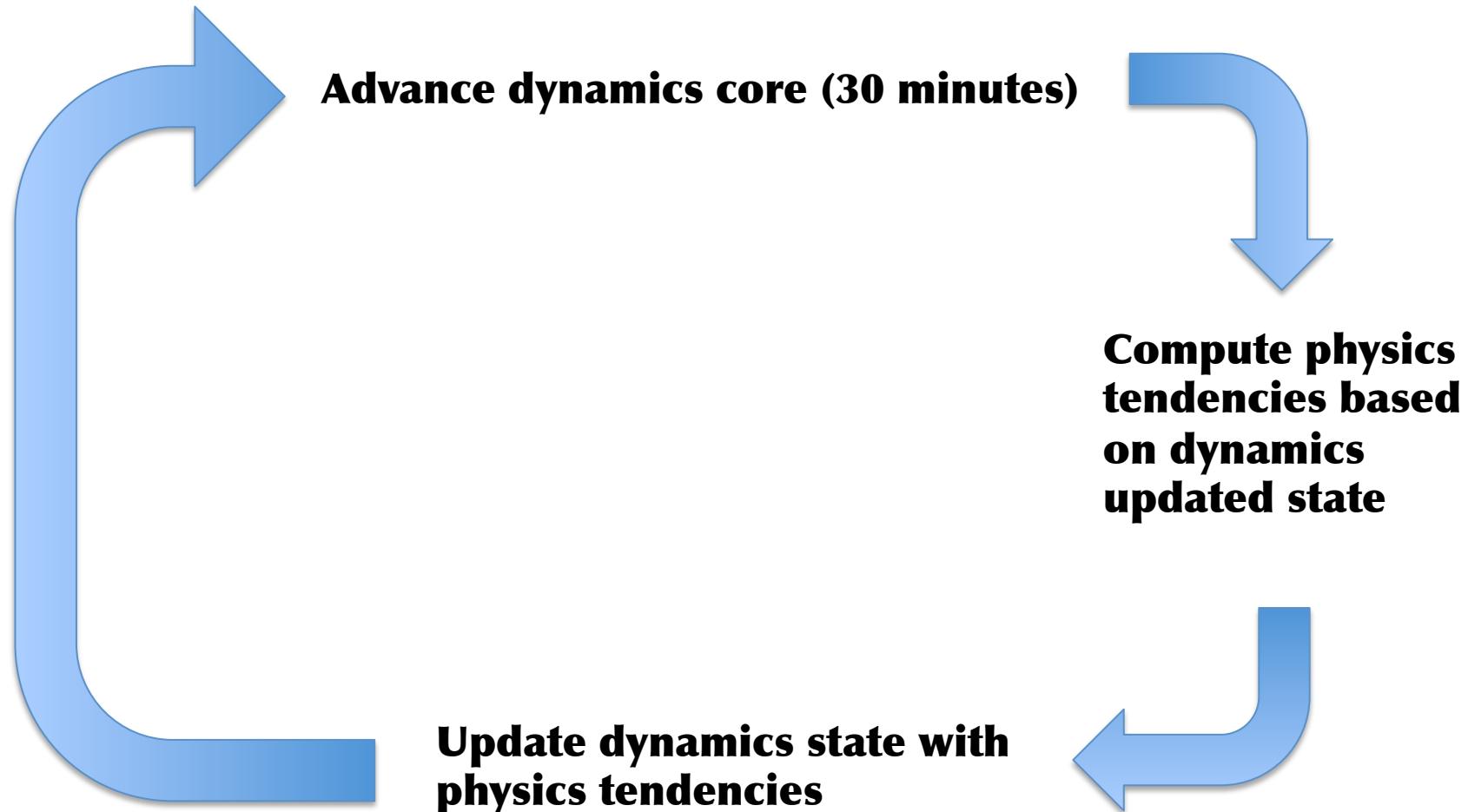


# Preserving pre-existing functional relation between tracers under challenging flow conditions

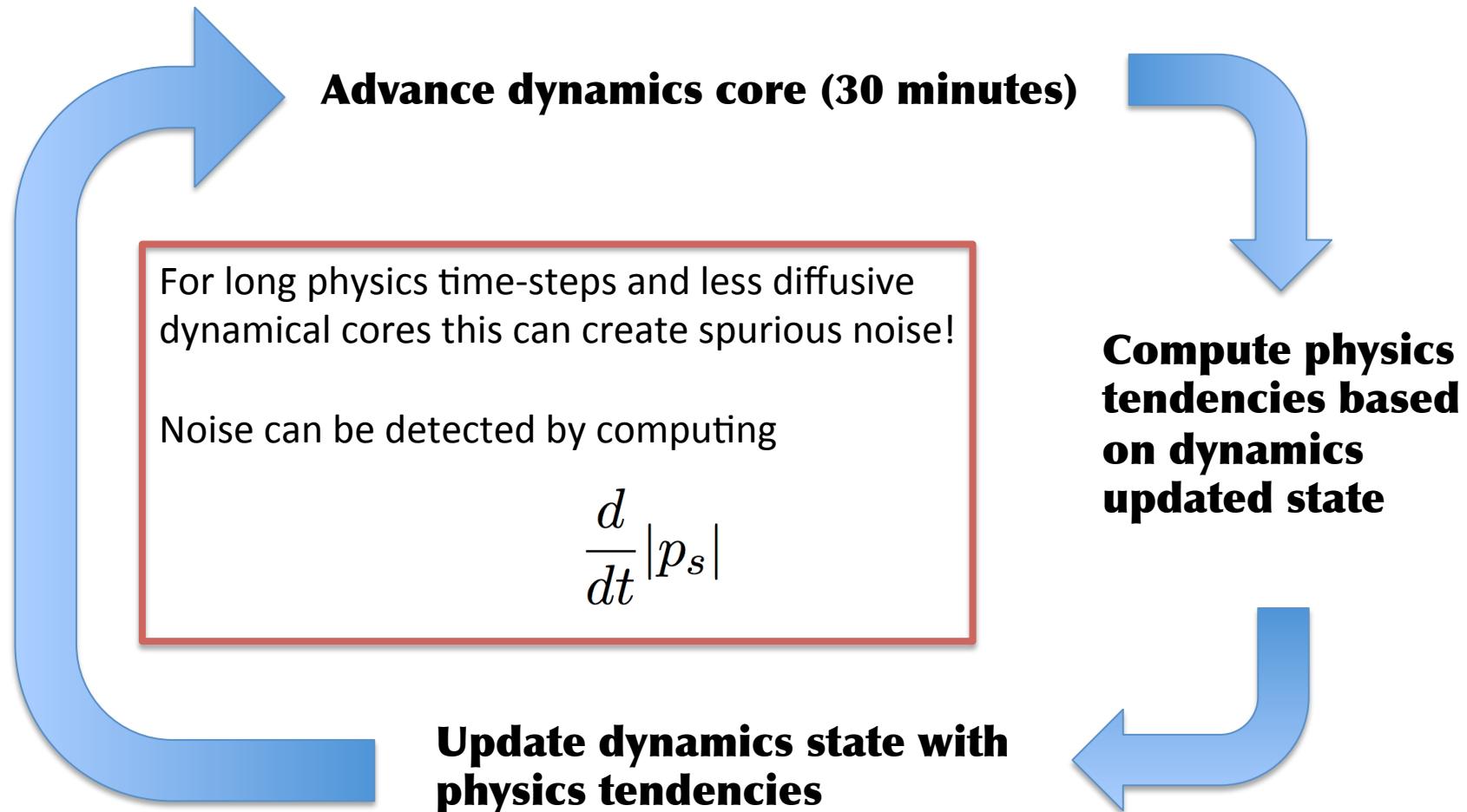
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# Physics dynamics coupling methods

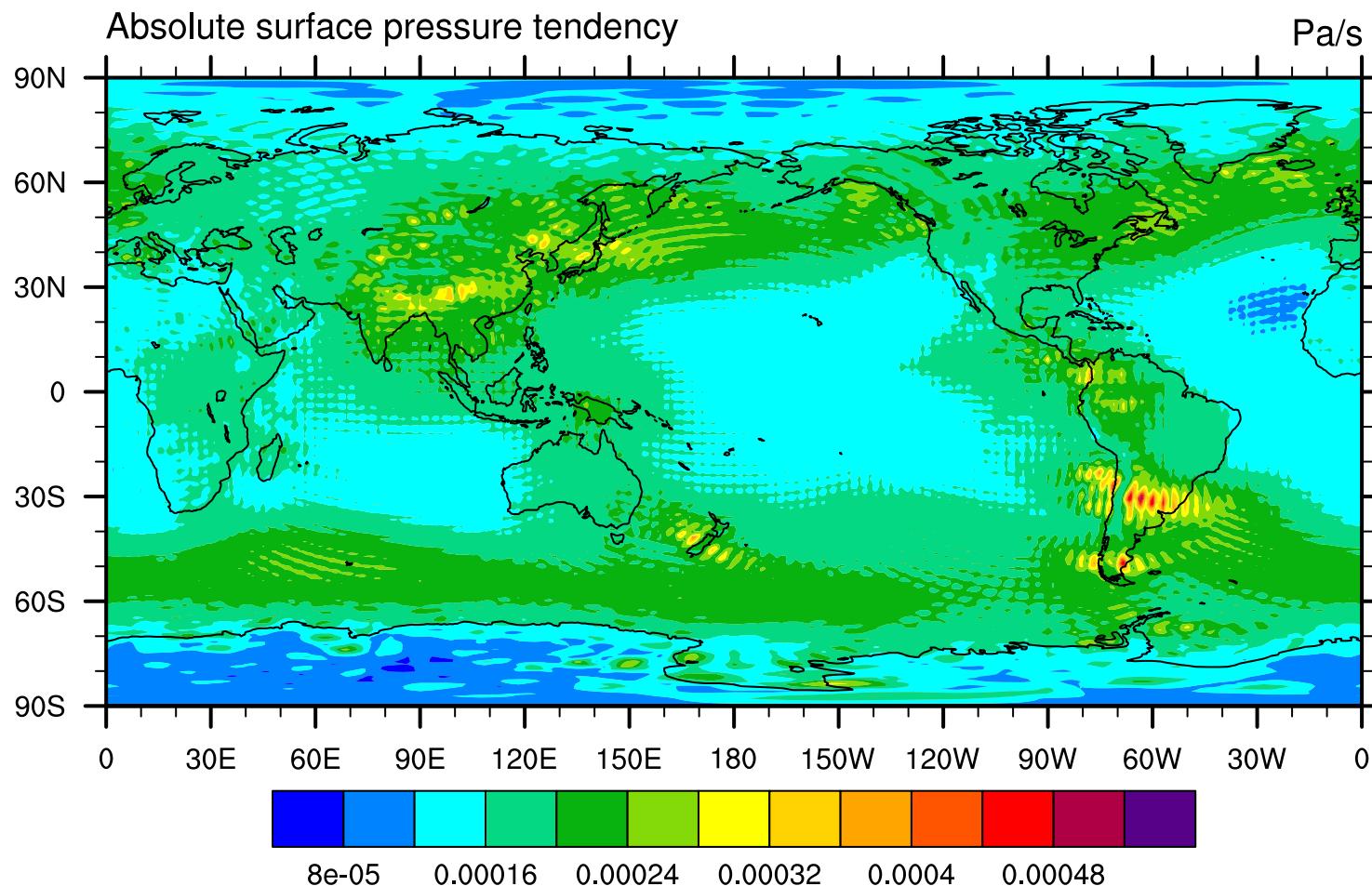


# Physics dynamics coupling methods

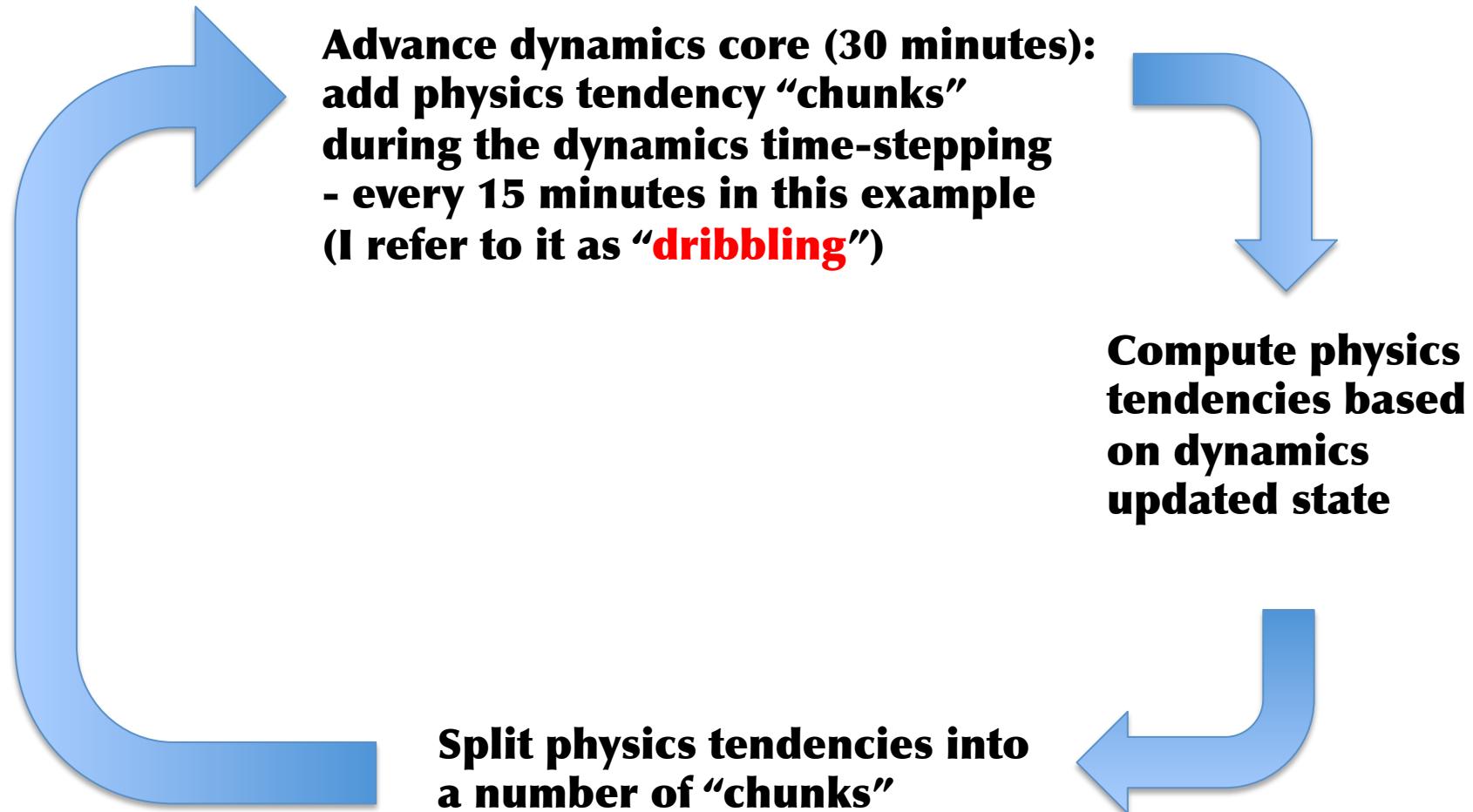


# Physics dynamics coupling methods

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



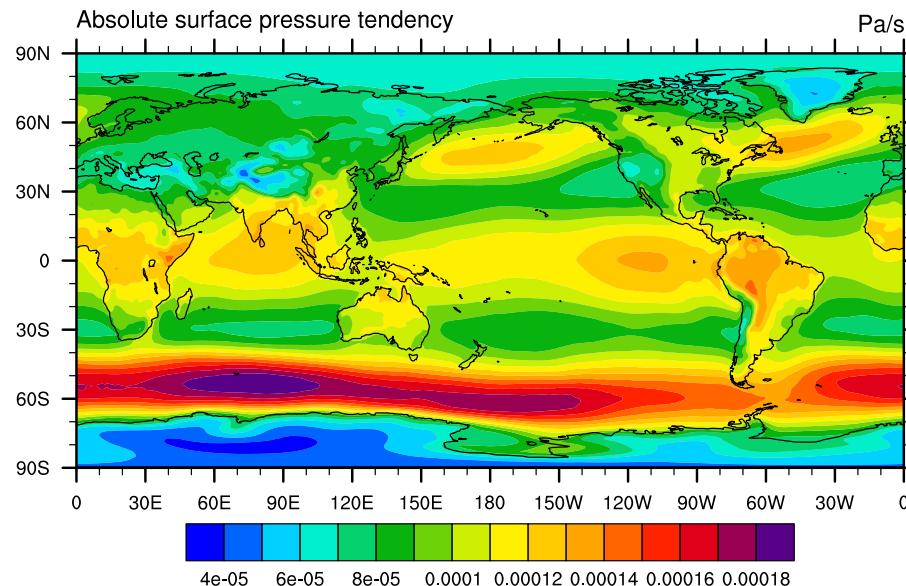
# Physics dynamics coupling methods



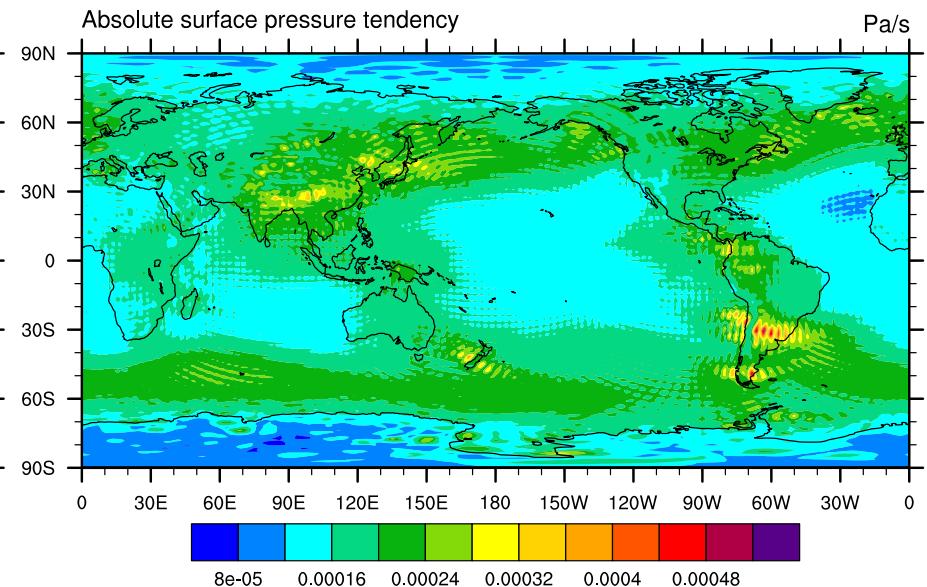
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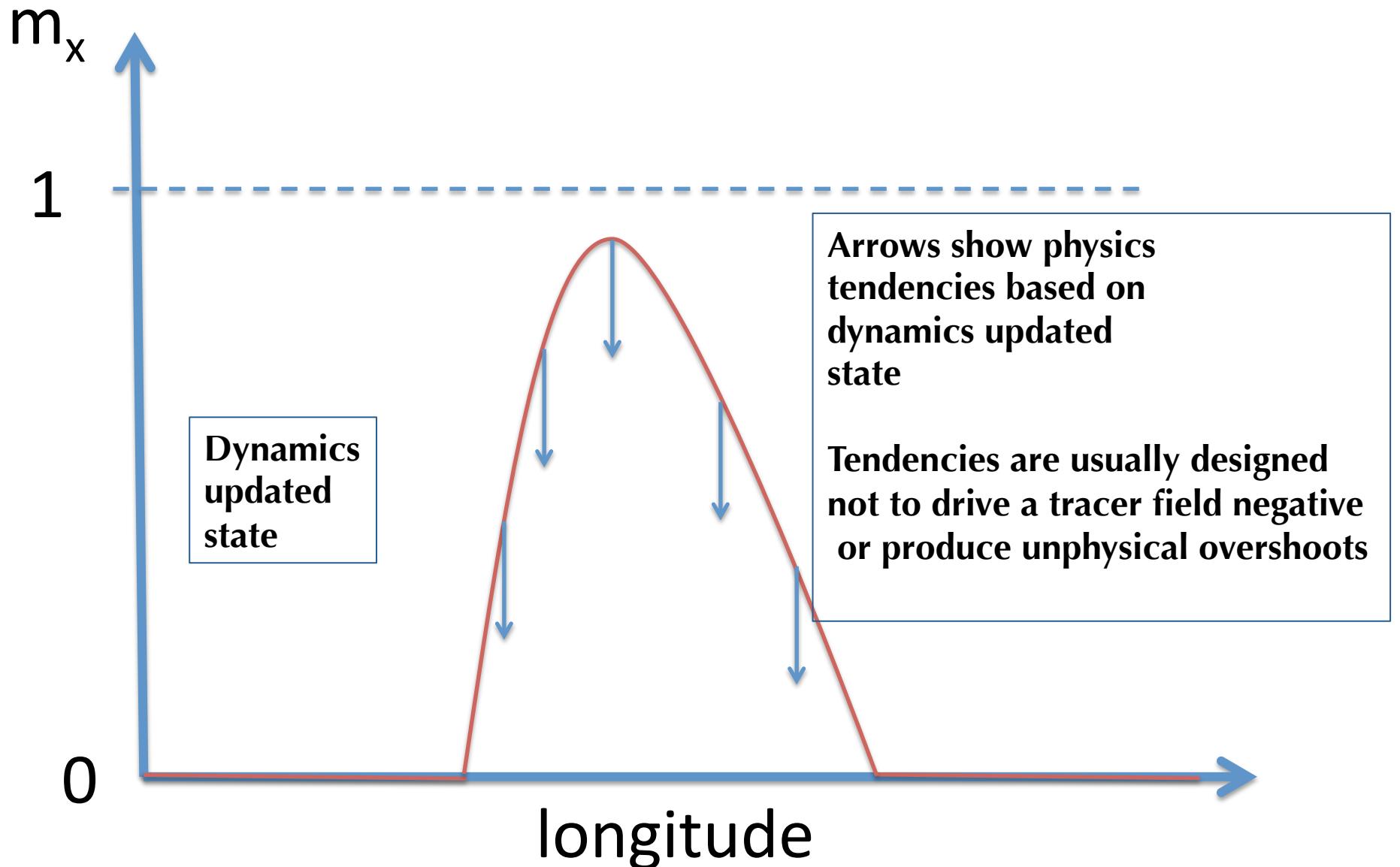
## “Dribbling” physics tendencies



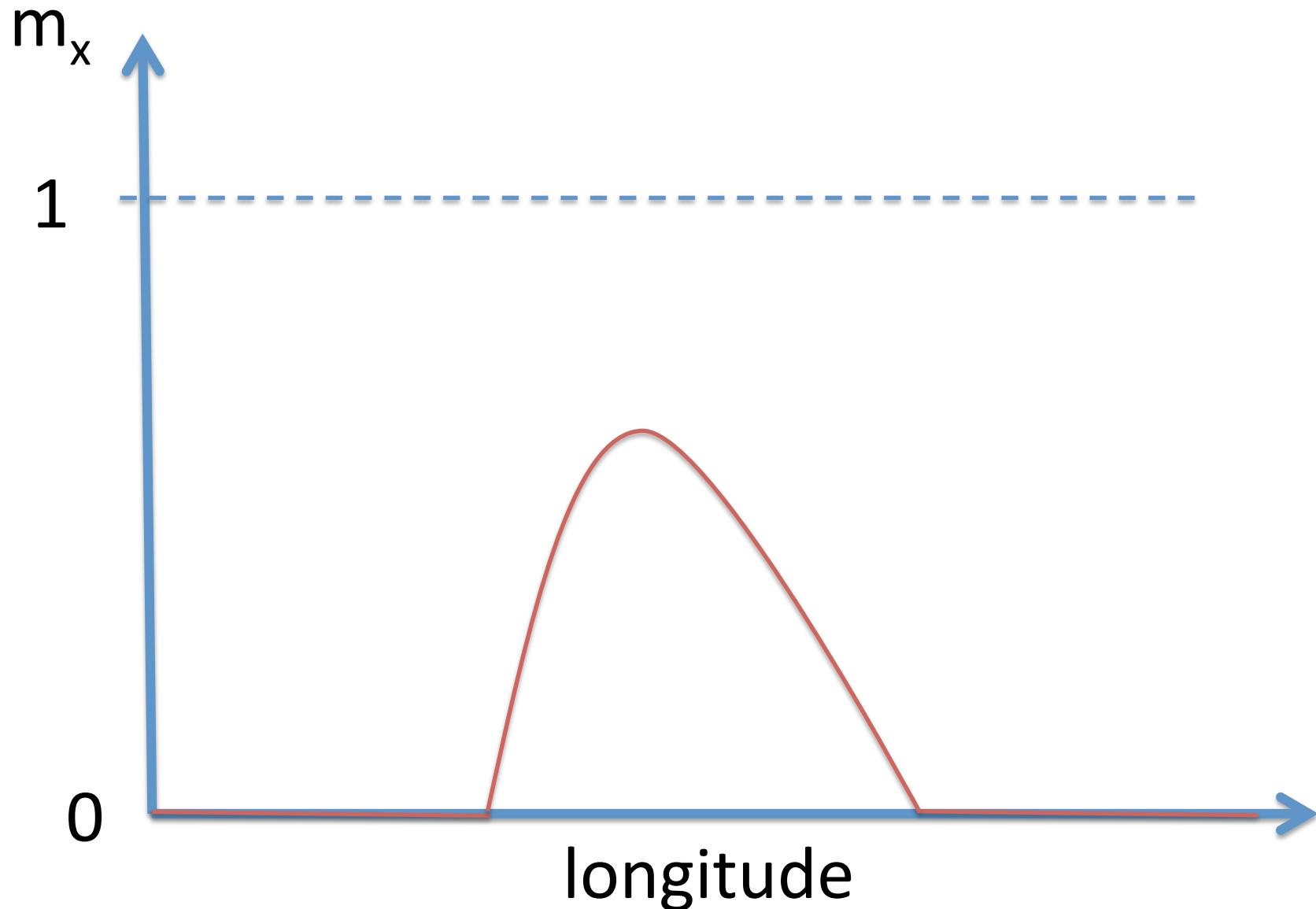
## State updated every 30 minutes



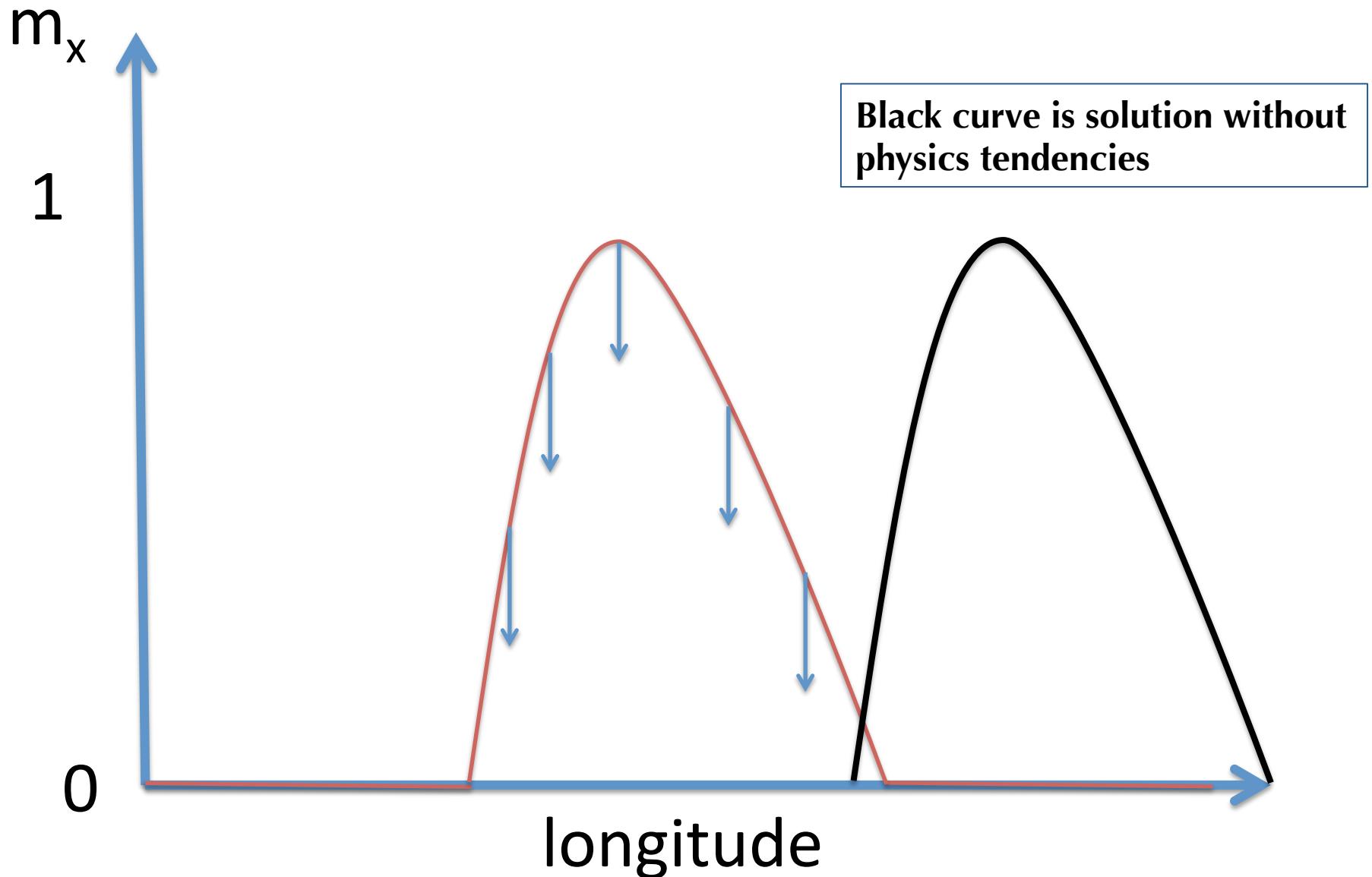
# Physics-dynamics coupling: state update



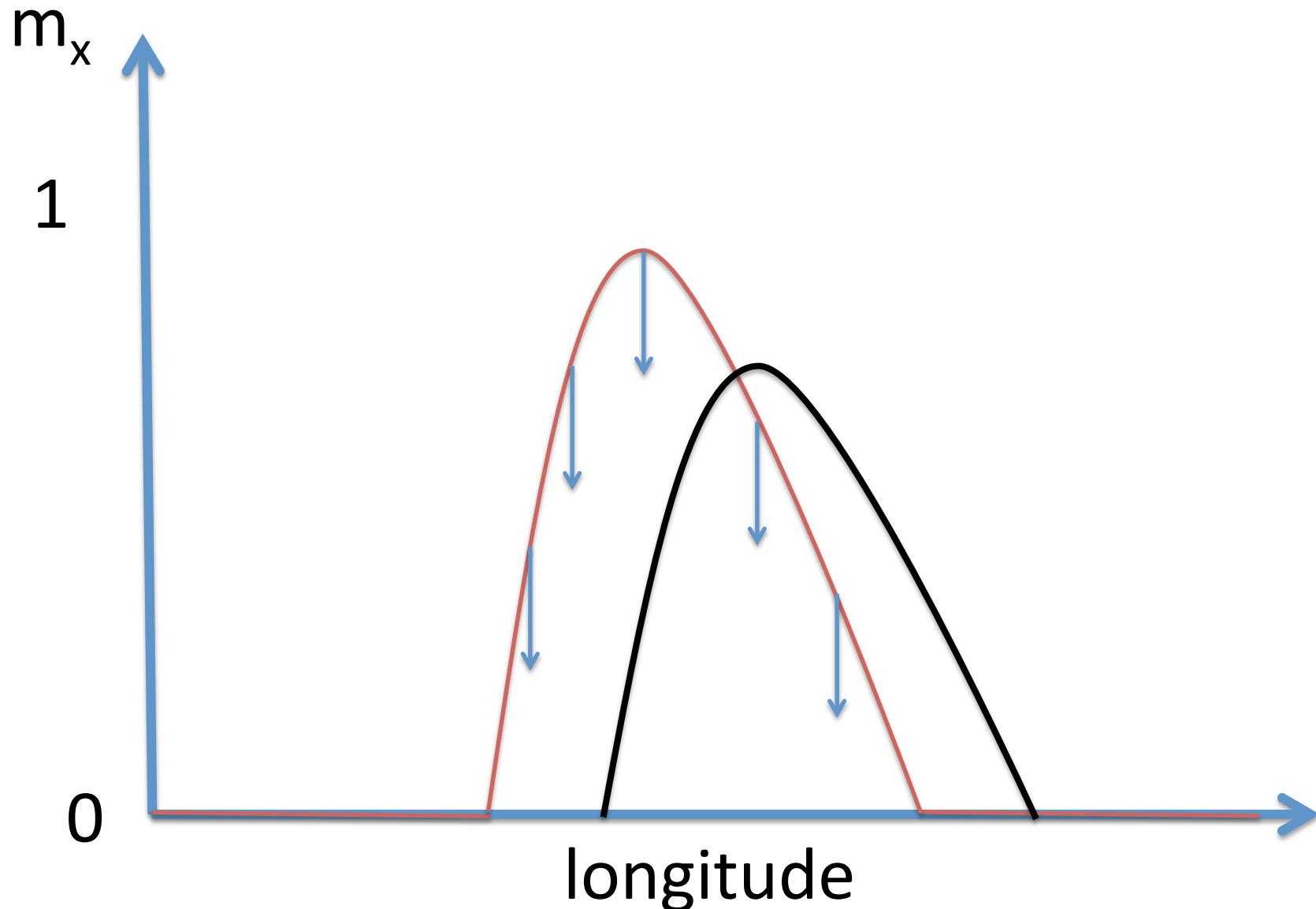
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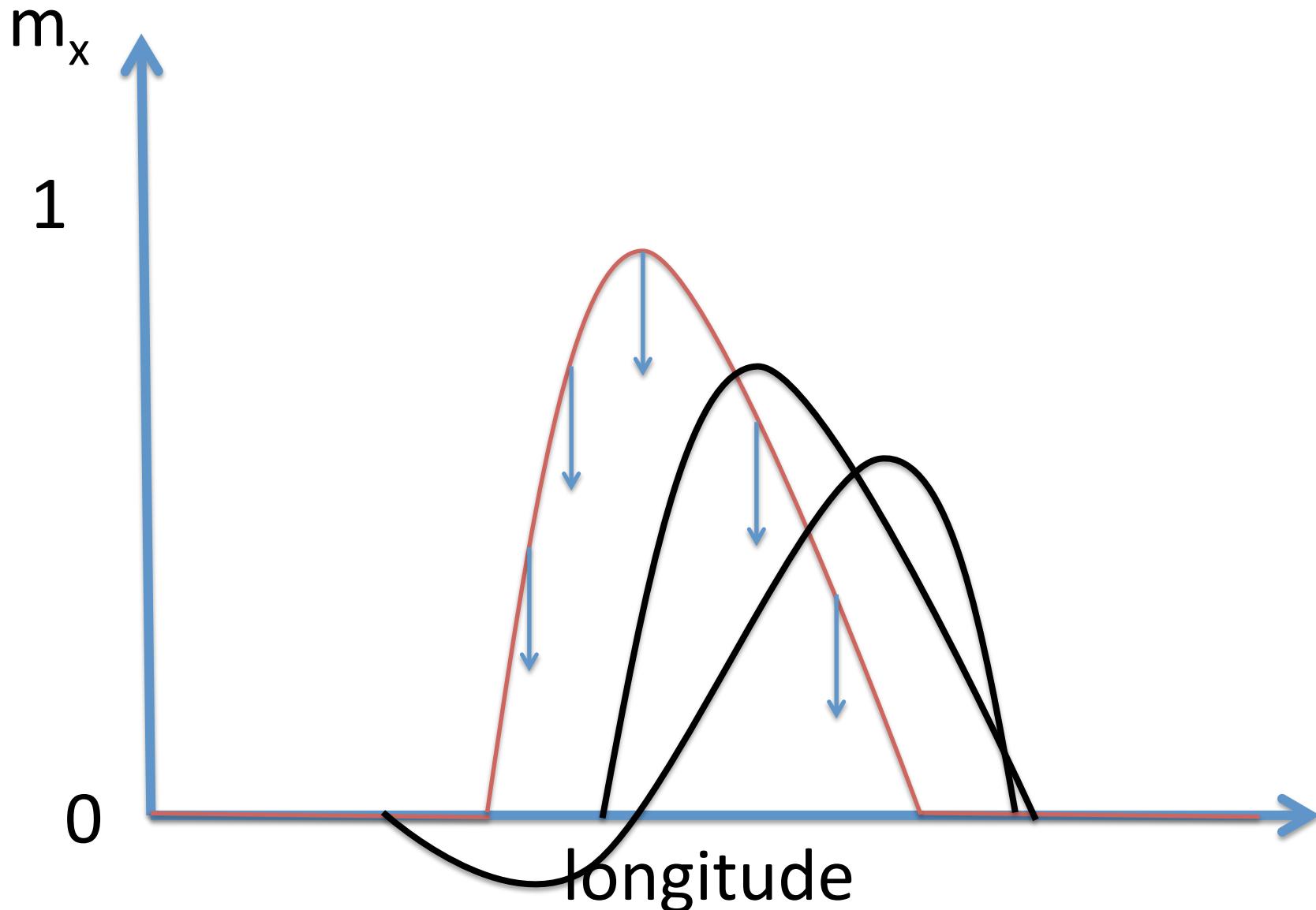
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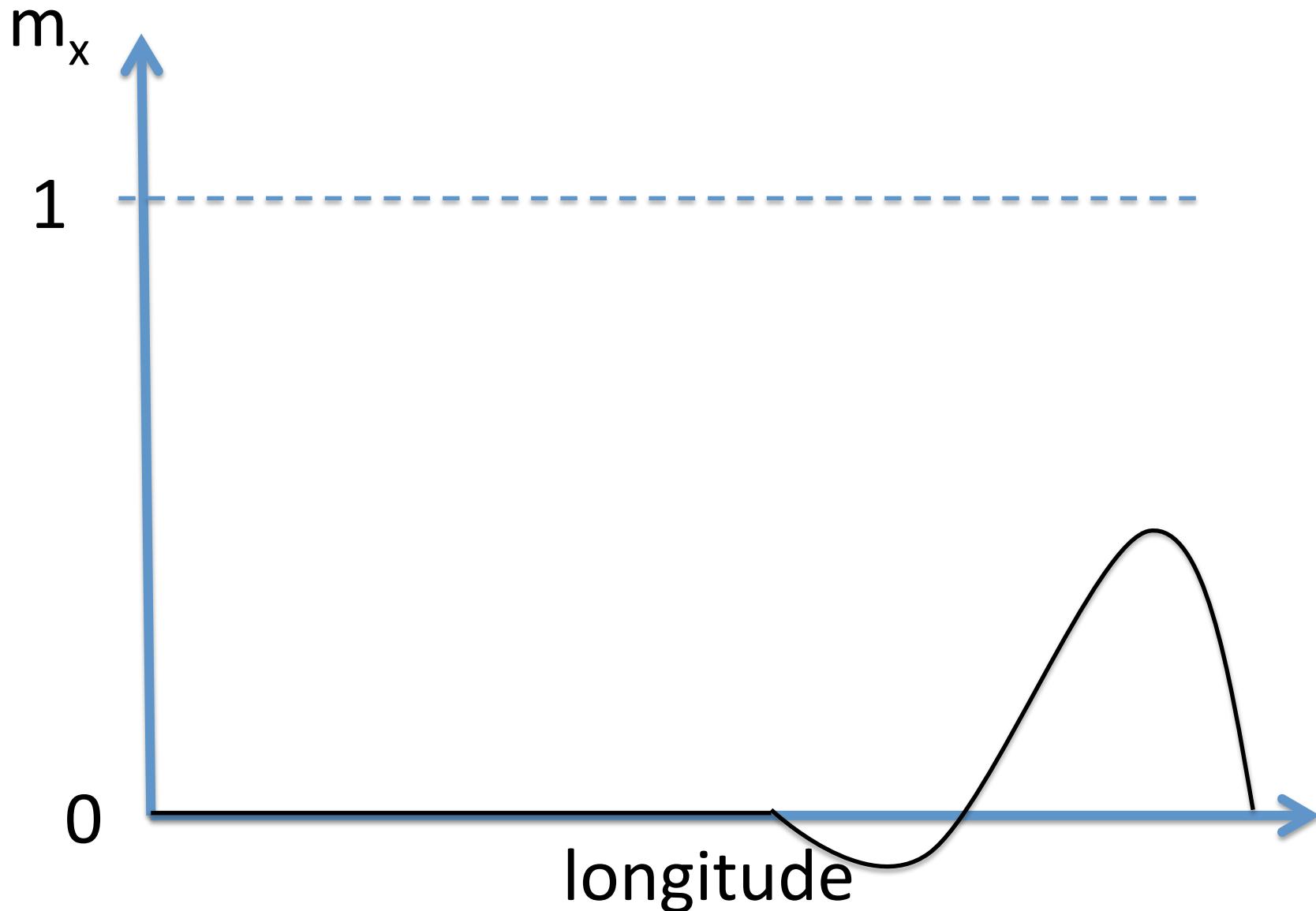
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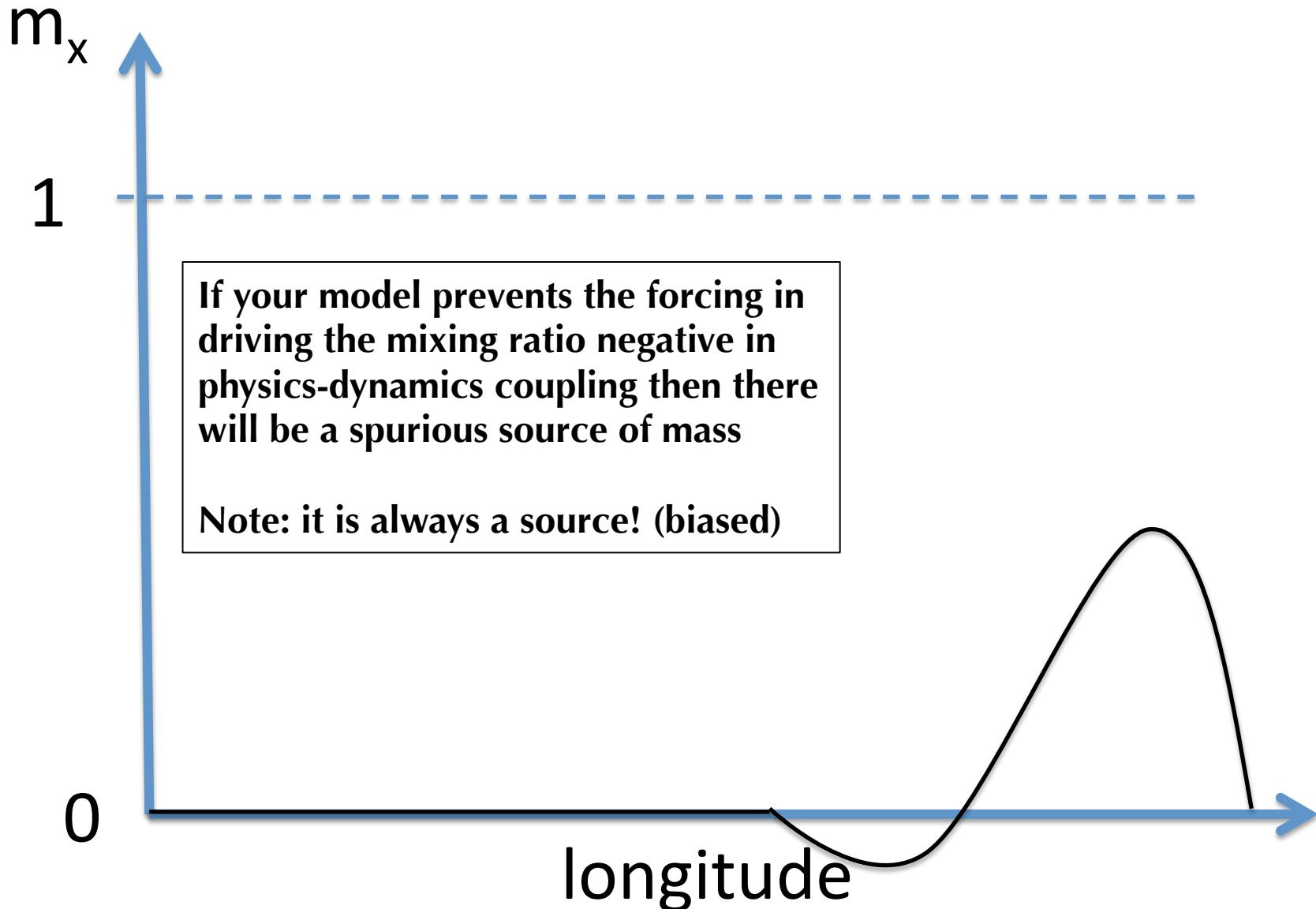
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# Physics-dynamics coupling: “dribbling” tendencies





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

Email: [pel@ucar.edu](mailto:pel@ucar.edu)