Desirable properties of transport schemes

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2nd WCRP Summer School on Climate Model Development: Scale aware parameterization for representing sub-grid scale processes
January 23, 2018
National Institute for Space Research, Center for Weather Forecasting and Climate Studies,
Cachoeira Paulista,São Paulo, Brazil.

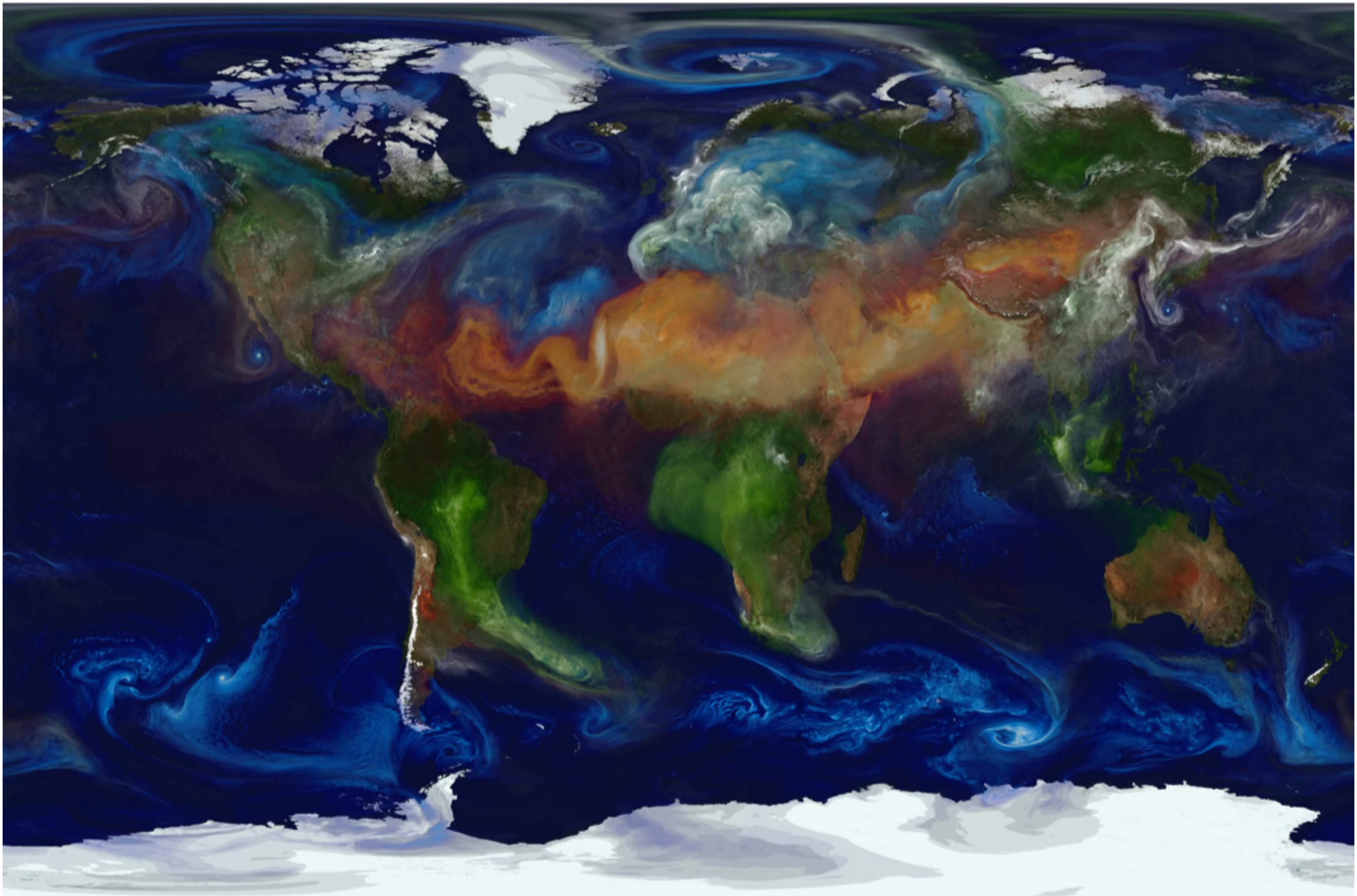
Desirable properties of transport schemes

What physical properties of the continuous equation of motion are important to respect in discretization schemes?

Here I'll focus on the continuity equation …

GEOS-5 simulation: winds transporting aerosols (5/2005-5/2007)

In general, dust appears in shades of orange, sea salt blue, sulfates white, and carbon green



The most important continuity equation in modeling

Consider the continuity equation for dry air

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \qquad (1)$$

where ρ_d is the density of dry air (mass per unit volume of Earth's atmosphere) and $\mathbf{v}$ is a 3D velocity vector.

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Accurate to approximately 0.01hPa globally

where ρ_d is t dry air (mass per unit volume of Earth's atmosphere velocity vector.

Dry air makes up 99.75% of the mass of the atmosphere:

mean mass of dry air = 5.1352 ± 0.0003 x 10^{18} kg

mean mass of atmosphere = 5.1480 x 10^{18} kg

Trenberth and Smith (2005)

The most important continuity equation in modeling

Consider the continuity equation for dry air

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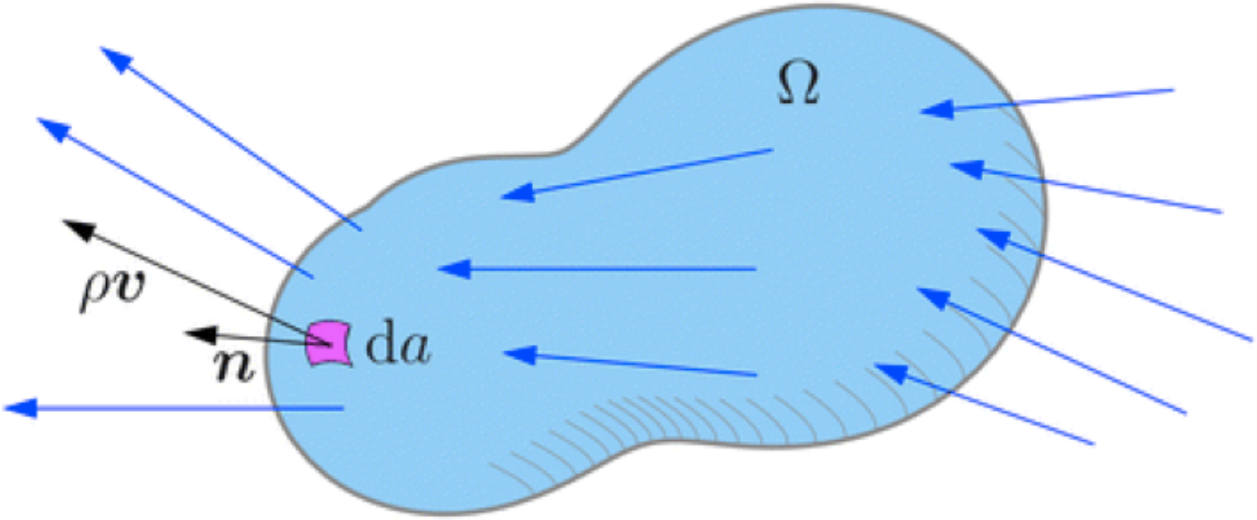
where ρ_d is the density of dry air (mass per unit volume of Earth's atmosphere) and $\mathbf{v}$ is a 3D velocity vector.

Note that the continuity equation for air is "tightly" coupled with momentum and thermodynamic equations

To solve (1) we need to know the velocity field!



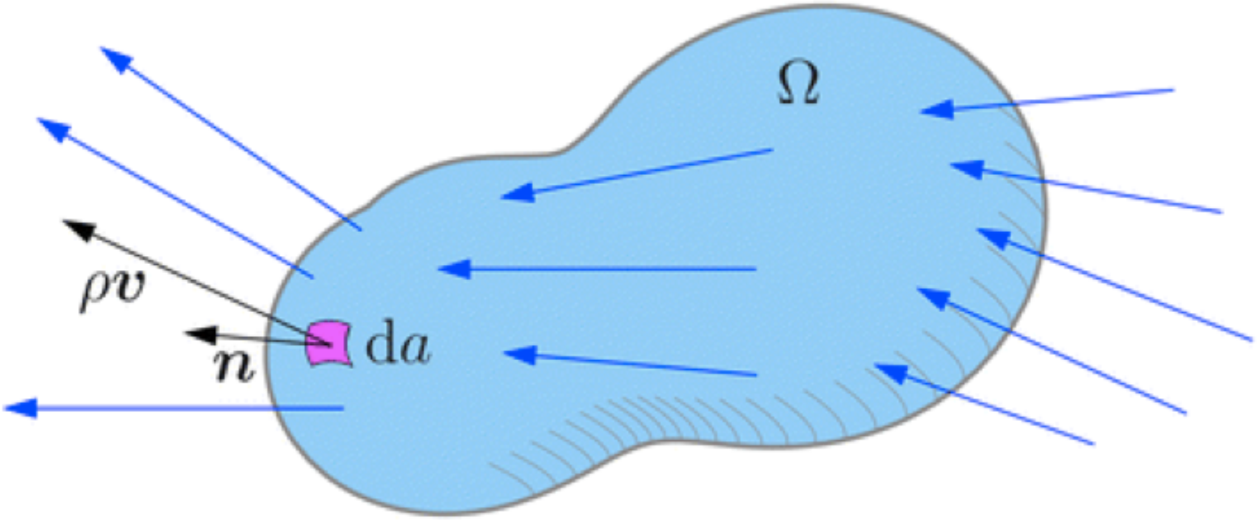
Eulerian version:

Ω stays fixed
in local coordinate system

- The continuity equation is a conservation law for mass:

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

where Ω is a fixed volume, $\partial\Omega$ the surface of Ω and $\mathbf{n}$ is outward pointing unit vector normal to the local surface.
$\Rightarrow$ The flux of mass through the area da is da times $\rho_d \mathbf{v} \cdot \mathbf{n}$.



Lagrangian version:

Ω moves with the flow

- The continuity equation is a conservation law for mass:

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

Conservation of mass

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

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

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

Integrate (1) over entire atmosphere Ω_{tot}

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

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?

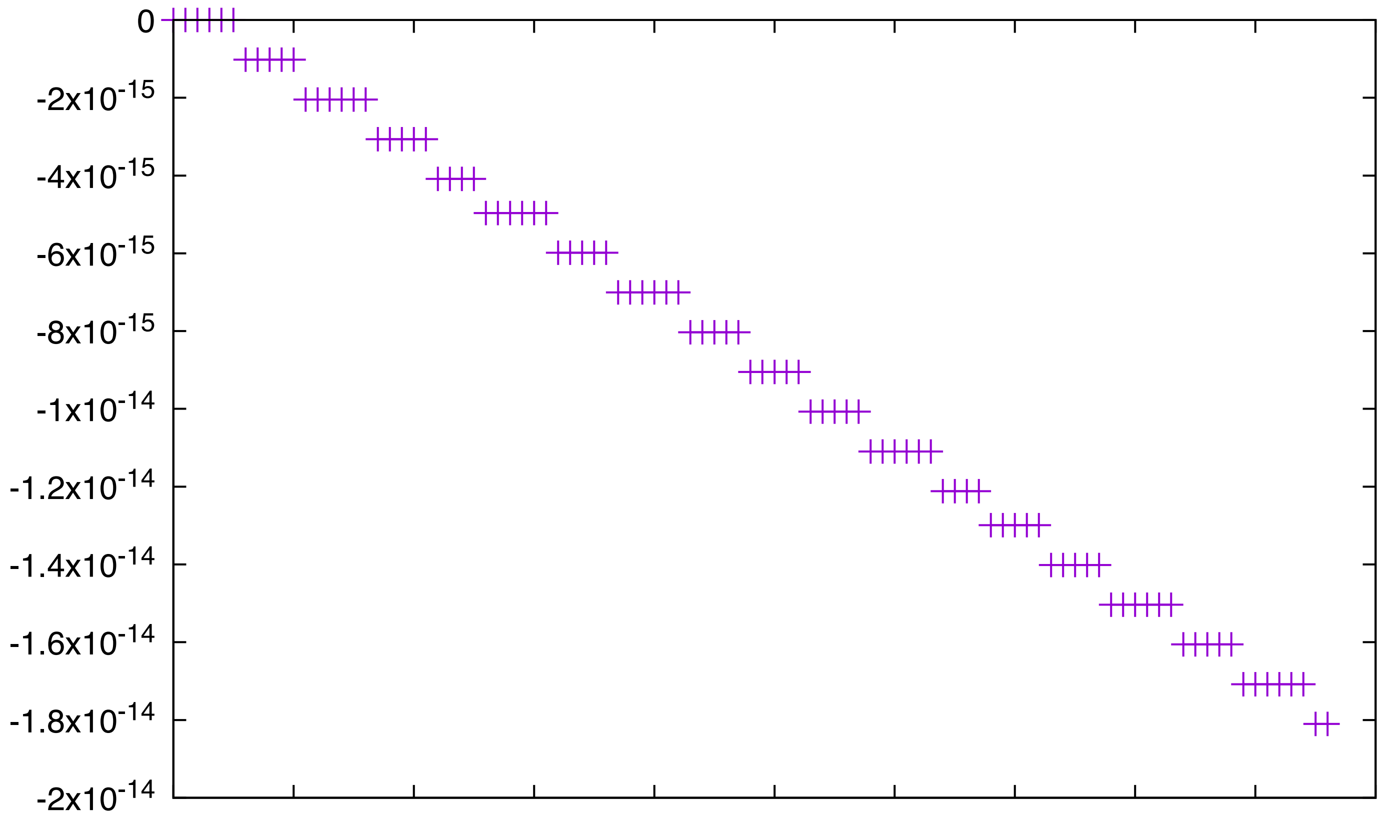
Integrate (1) over entire atmosphere Ω_{tot}

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

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

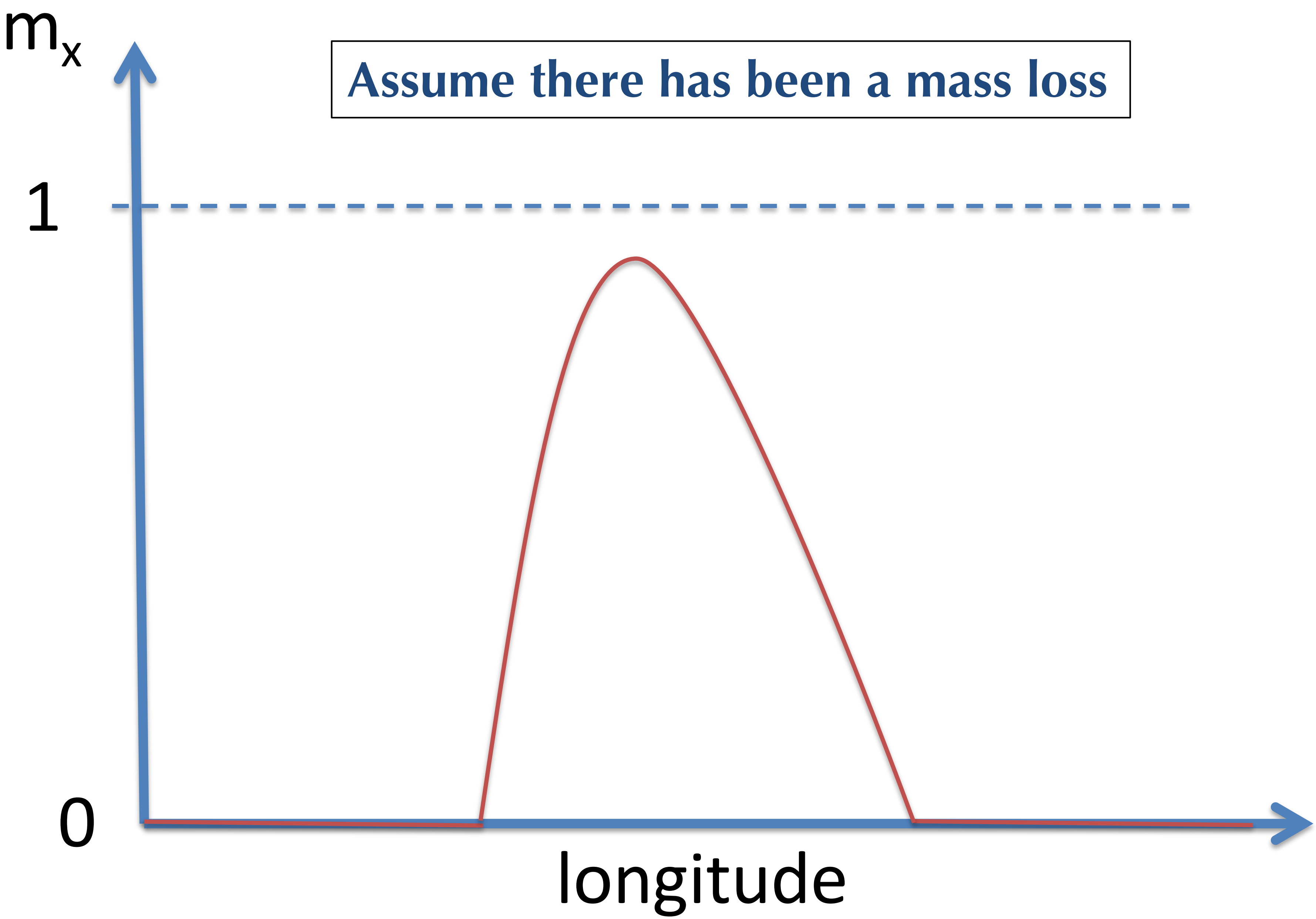
Accumulation of error

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



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

Ad hoc mass fixers are inherently problematic



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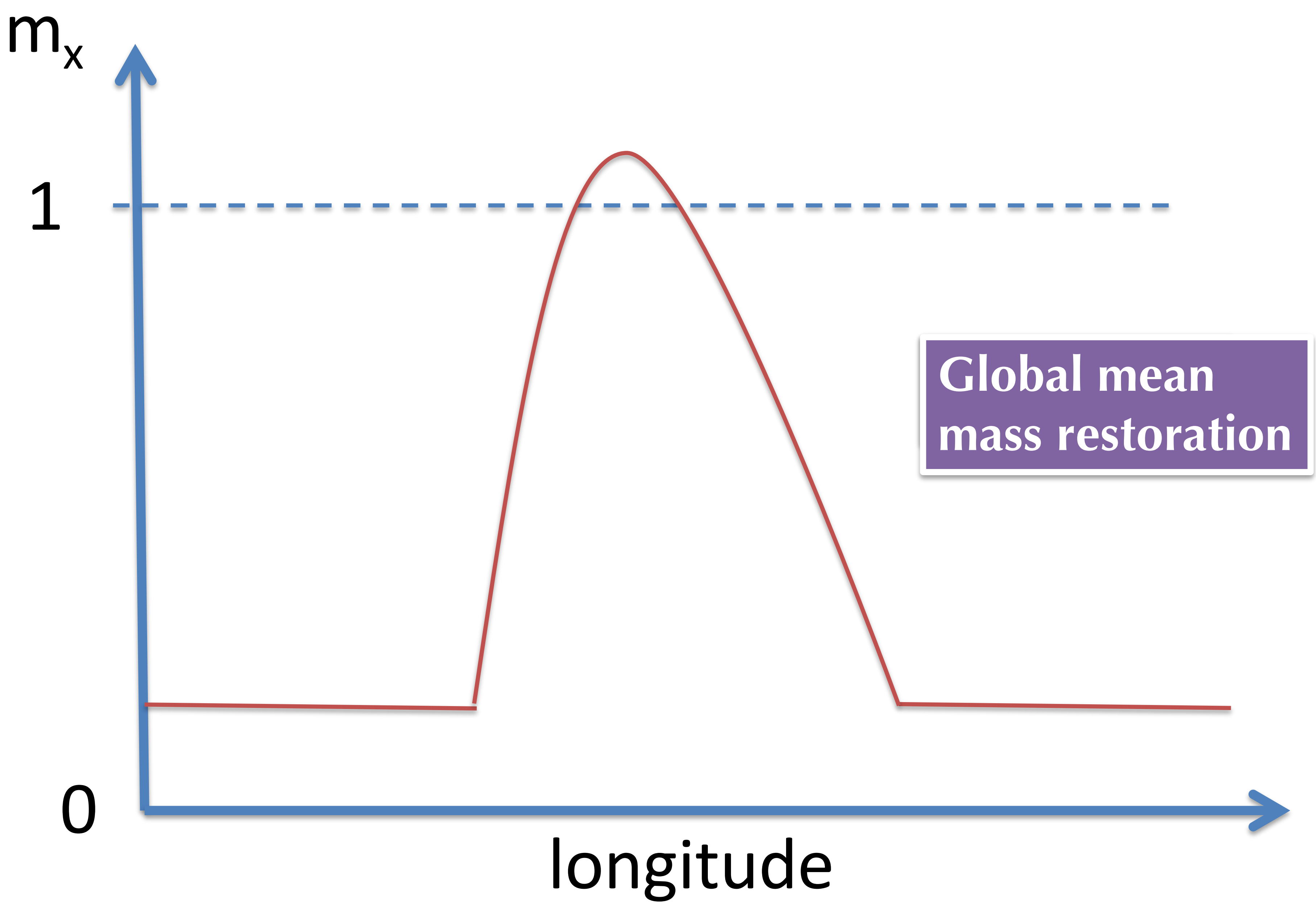

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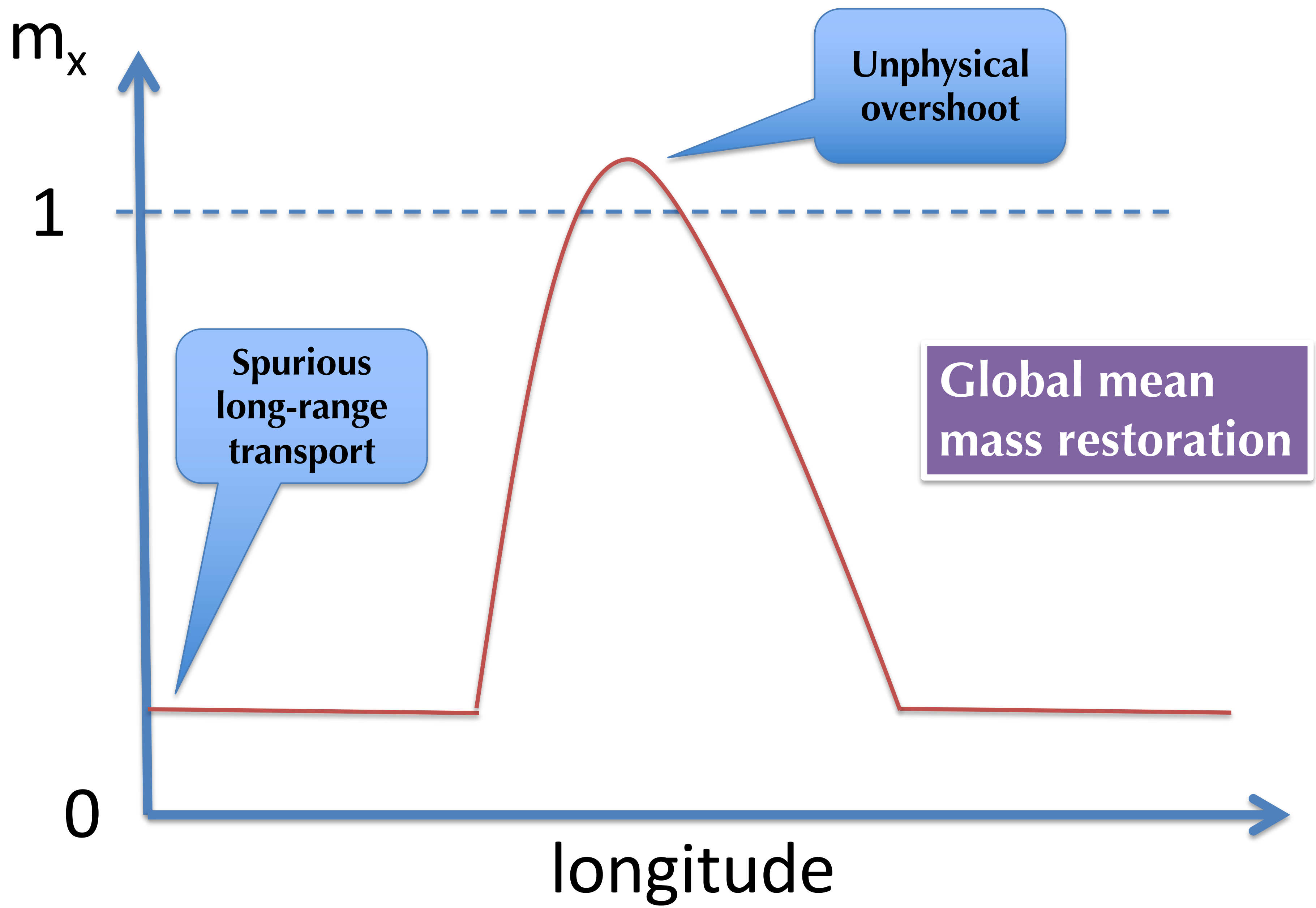

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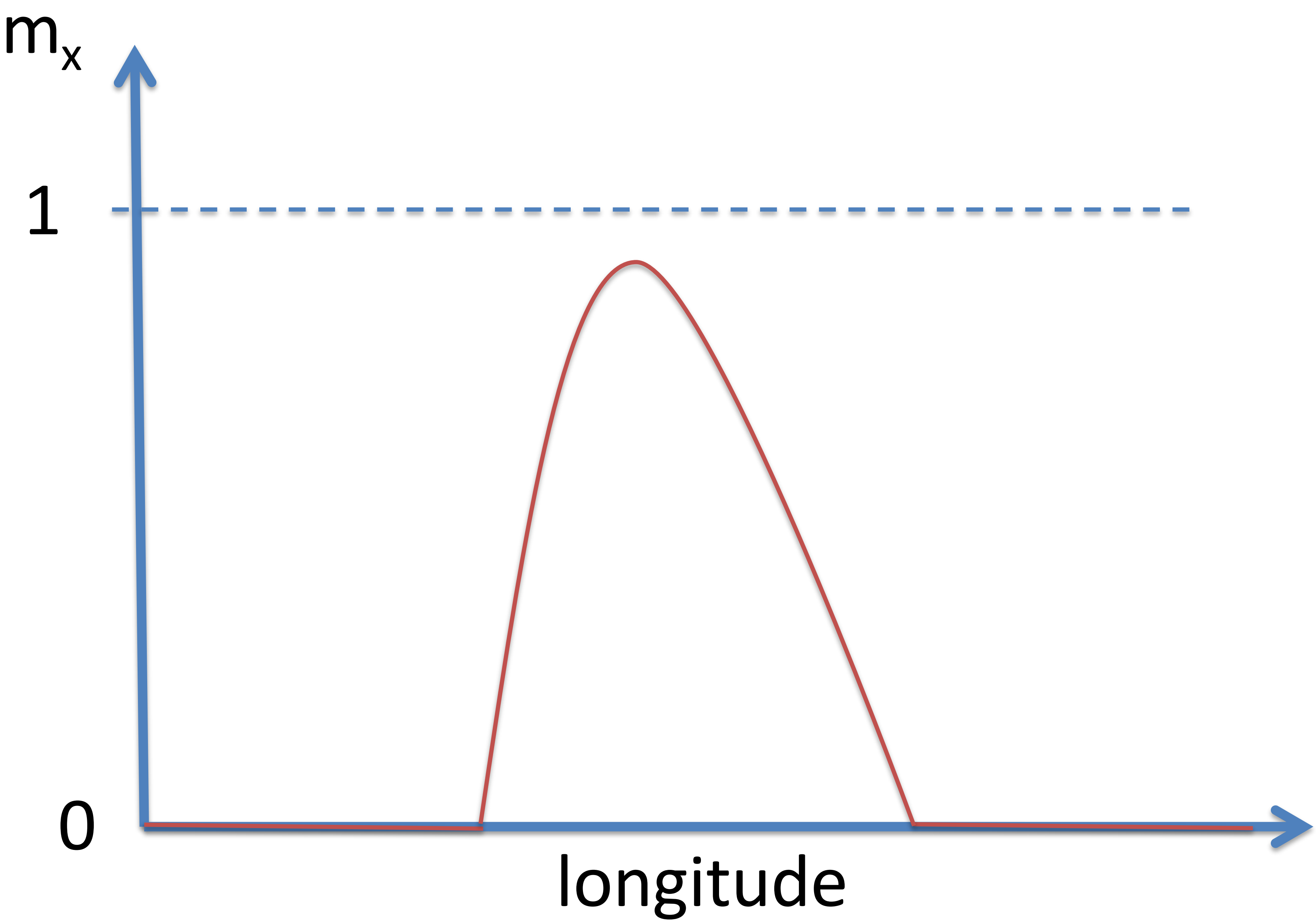

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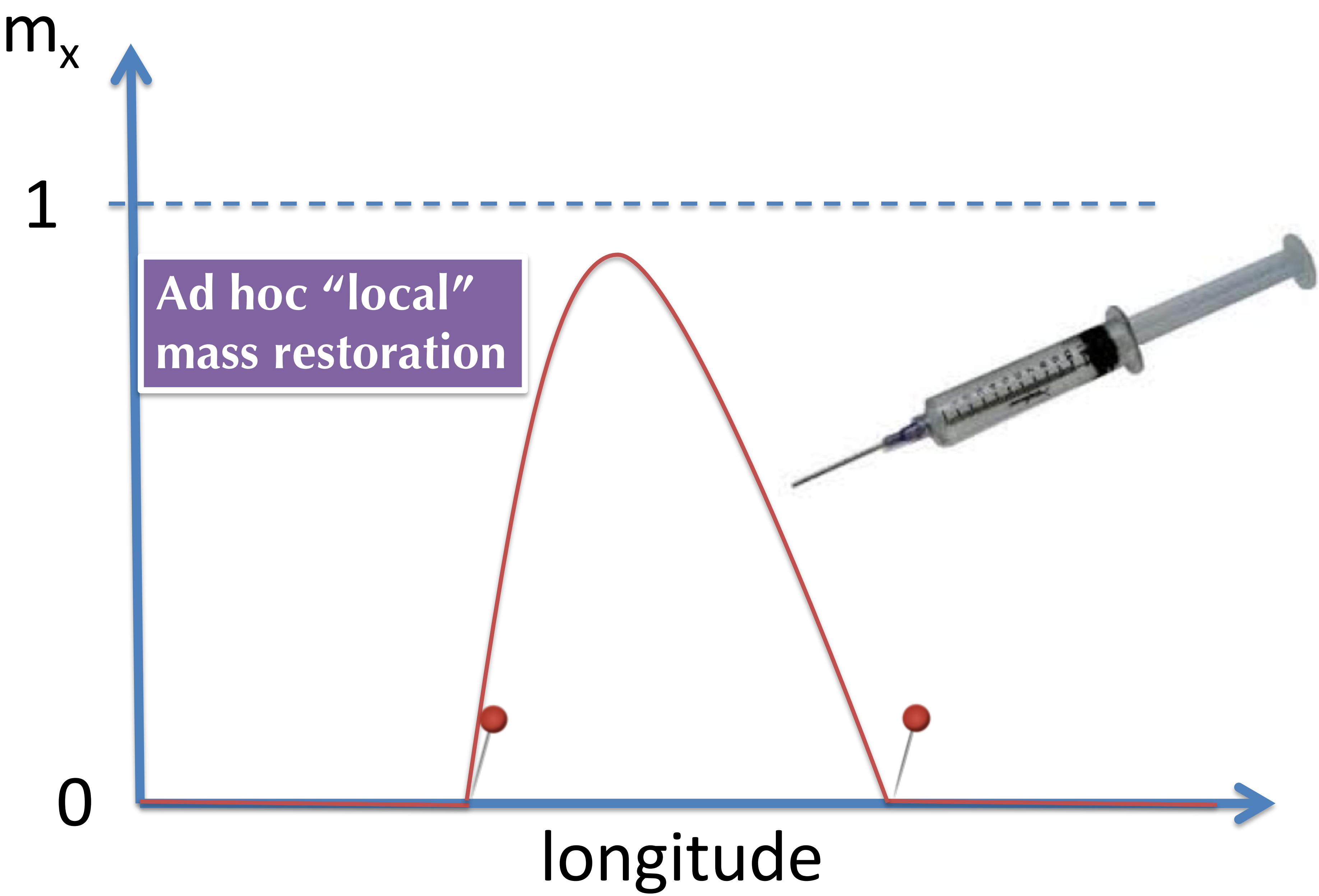

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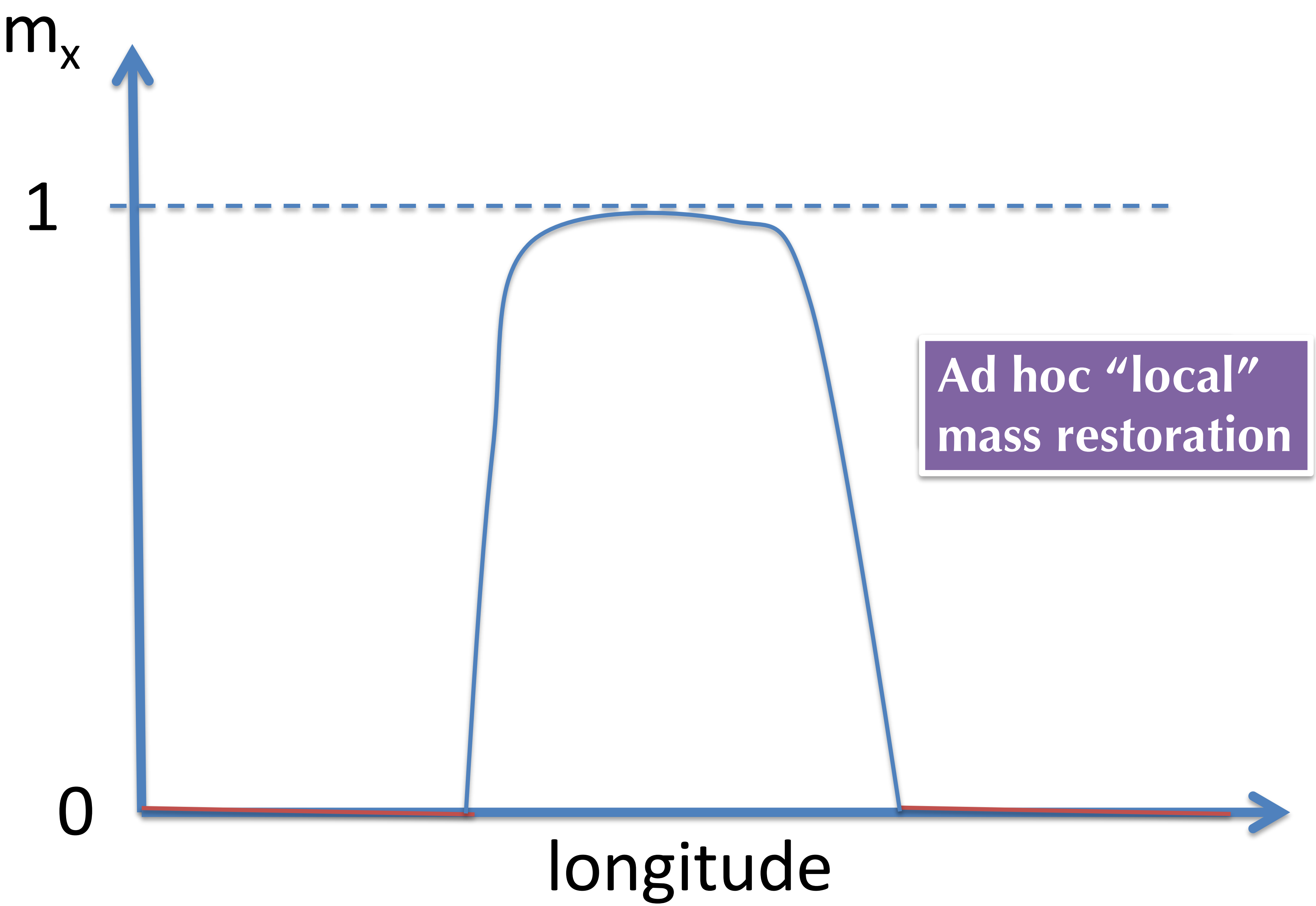

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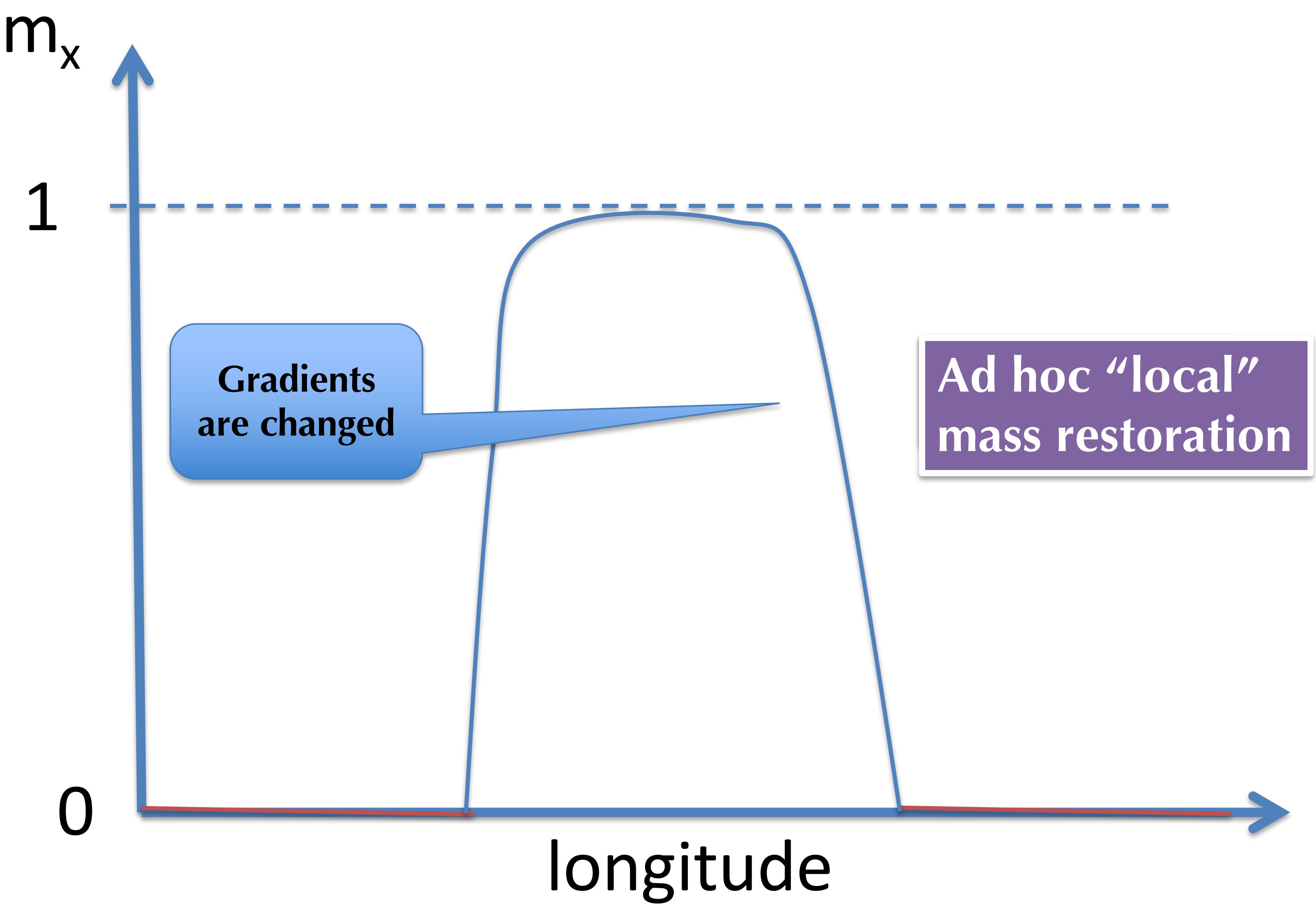
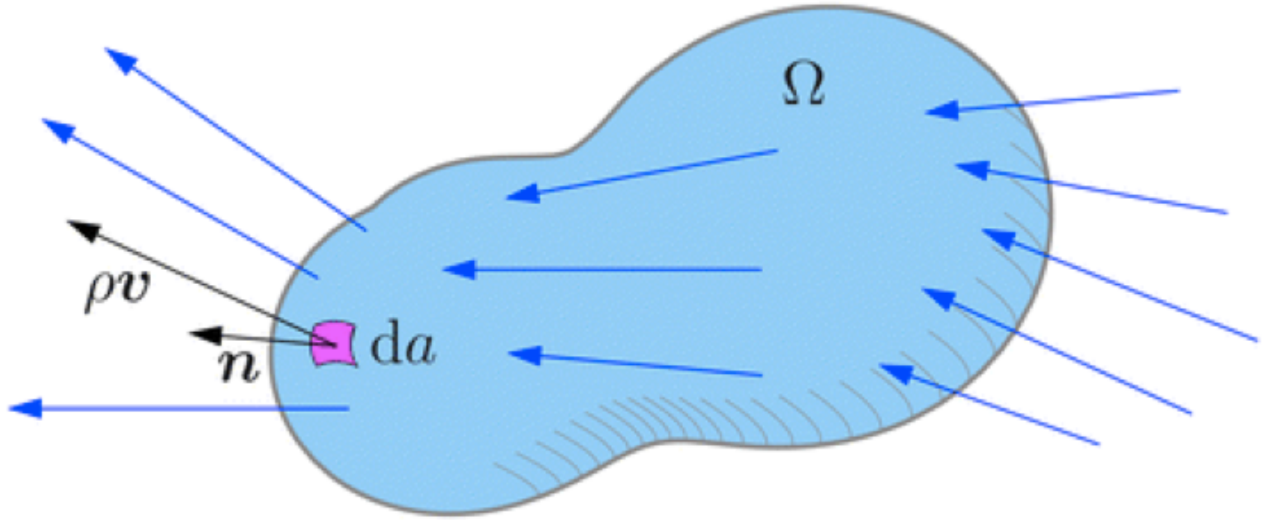


Inherent local mass-conservation is desirable



- The continuity equation is a conservation law for mass:

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

Conservation of $\mathbf{m_x}$ 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

Consider the continuity equation for dry air and X

$$\frac{\partial \rho_d}{\partial t} + \nabla \quad (2)$$

$$\frac{\partial}{\partial t}(m_x \rho_d) + \nabla \cdot (\quad (3)$$

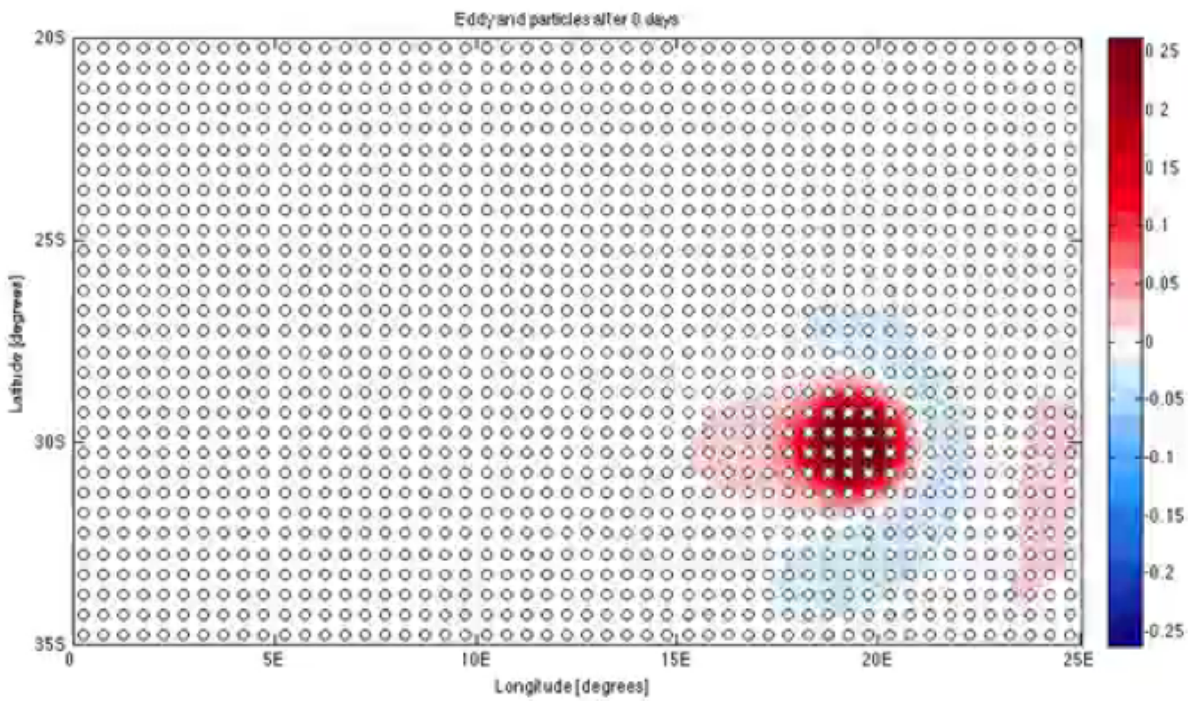
respectively. Applying the chai
substituting (2) implies

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.

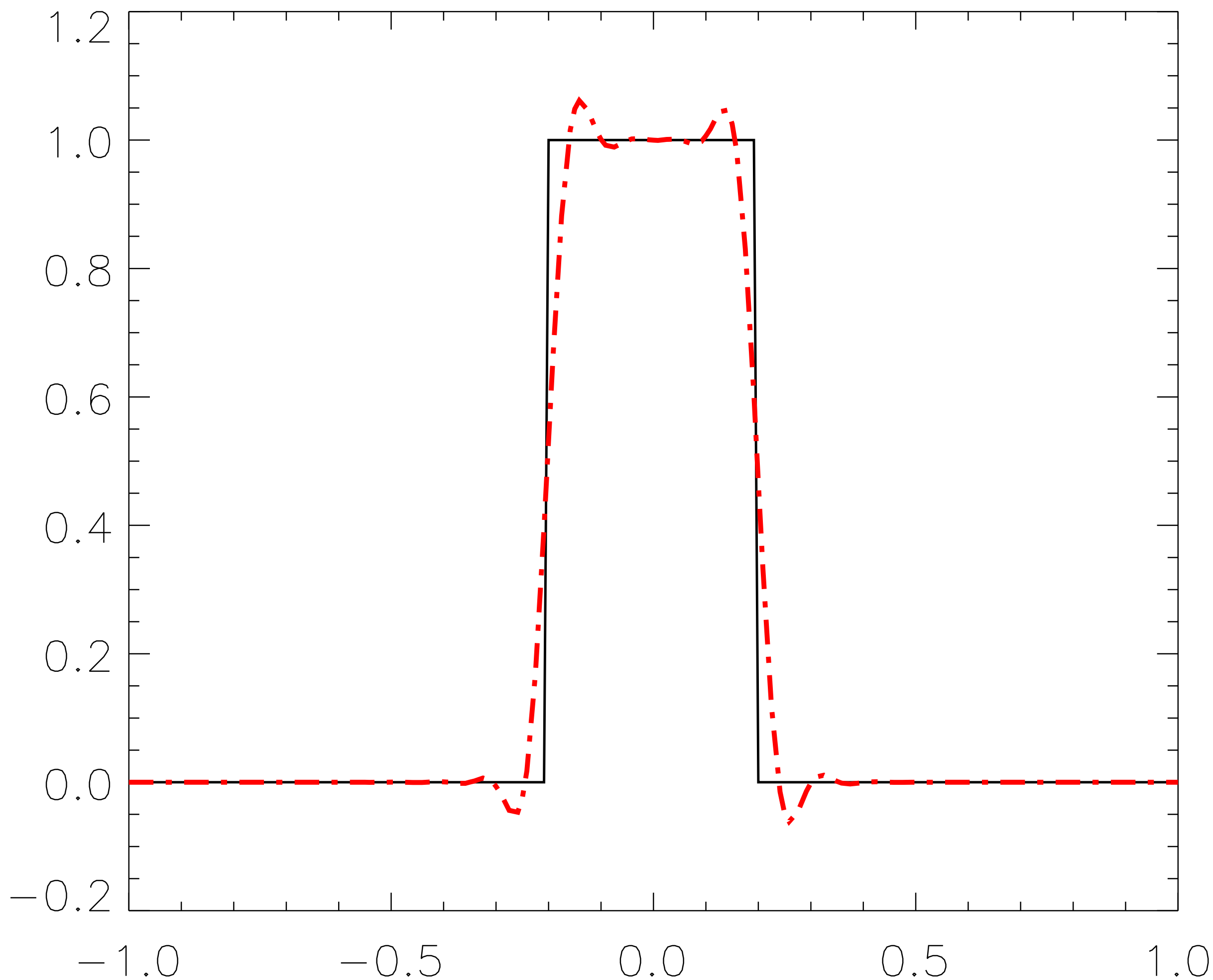
Conservation of m_x along parcel trajectories (if no sources/sinks of m_x)



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

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'!

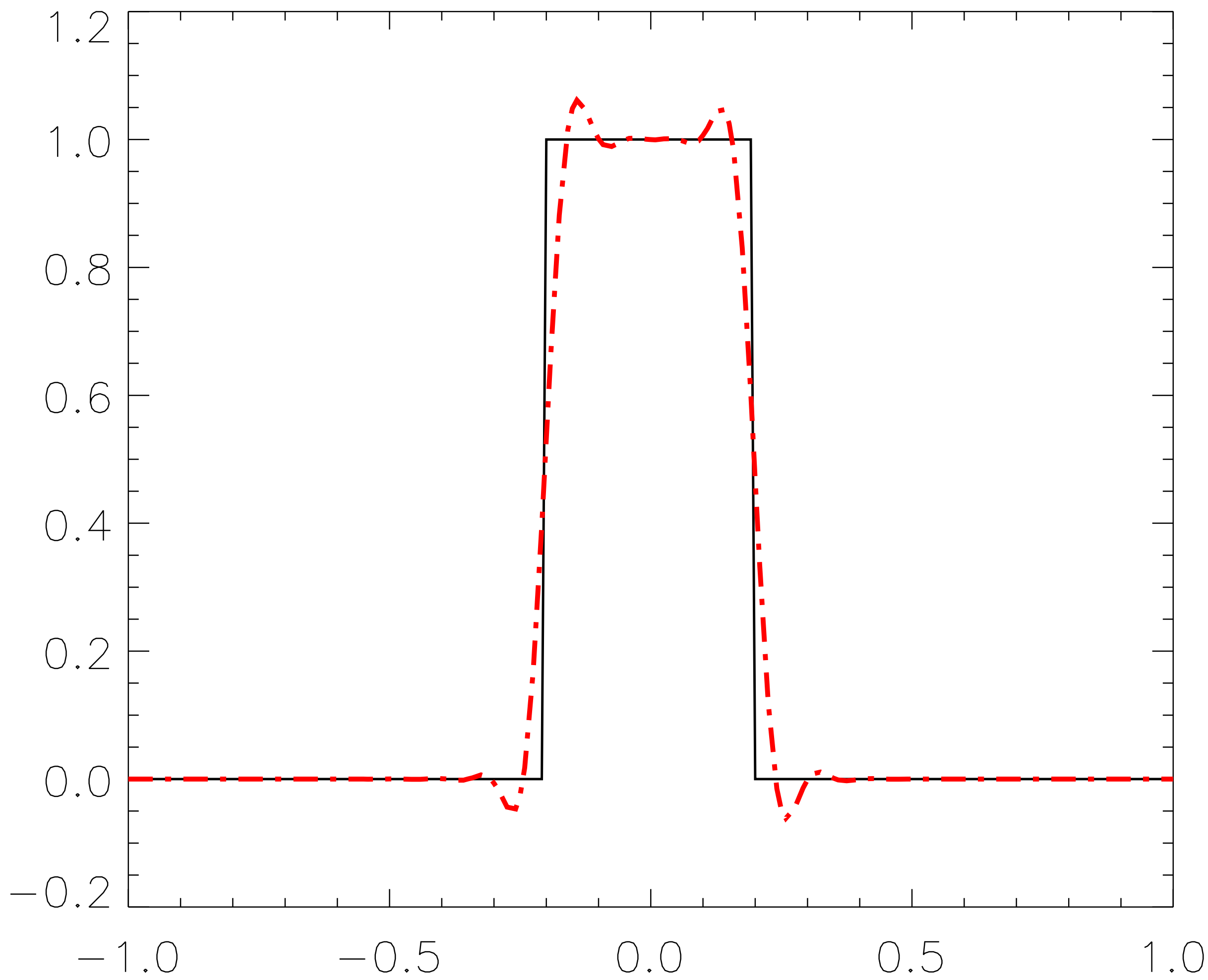
When modelers refer to "non-oscillatory", "shape-preserving", "physical realizable" or "monotone" they usually refer to the **monotonicity property** as defined by Harten (1983):

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



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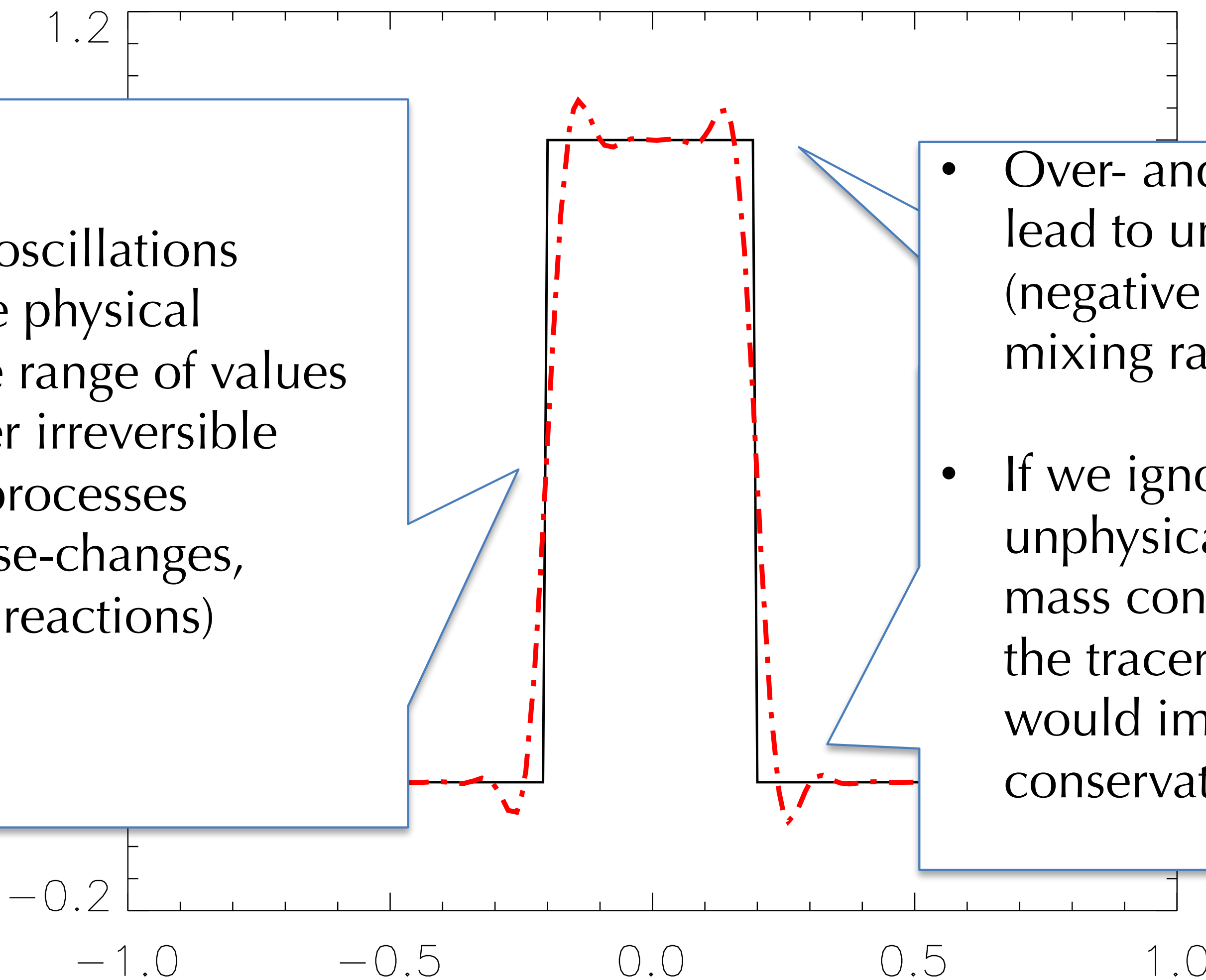


- Spurious oscillations within the physical realizable range of values can trigger irreversible diabatic processes (e.g., phase-changes, chemical reactions)

- Over- and undershoots can lead to unphysical values (negative mixing ratio or mixing ratio > 1)

- If we ignore ("chop") the unphysical values we loose mass conservation and if the tracer is humidity it would impact energy conservation

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

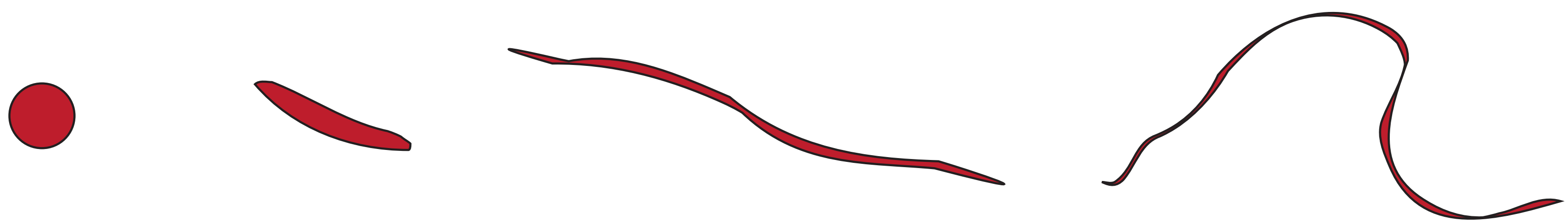
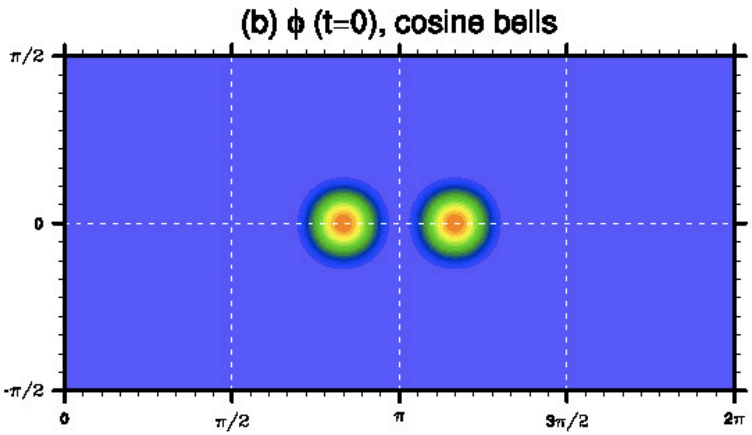
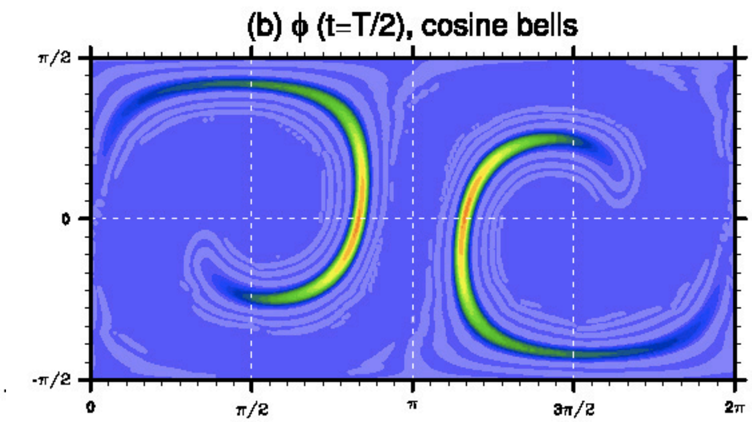


Fig. 2: In the highly nonlinear flows that characterize fluid motion in the atmosphere and ocean, Lagrangian control volumes are rapidly distorted due the presence of strong shear, rotation and dilation. The rapid distortion of Lagrangian control volumes makes the formulation of numerical models within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

$$\phi(\lambda,\theta) \geq \tau, \tag{27}$$

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

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

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

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

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

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

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

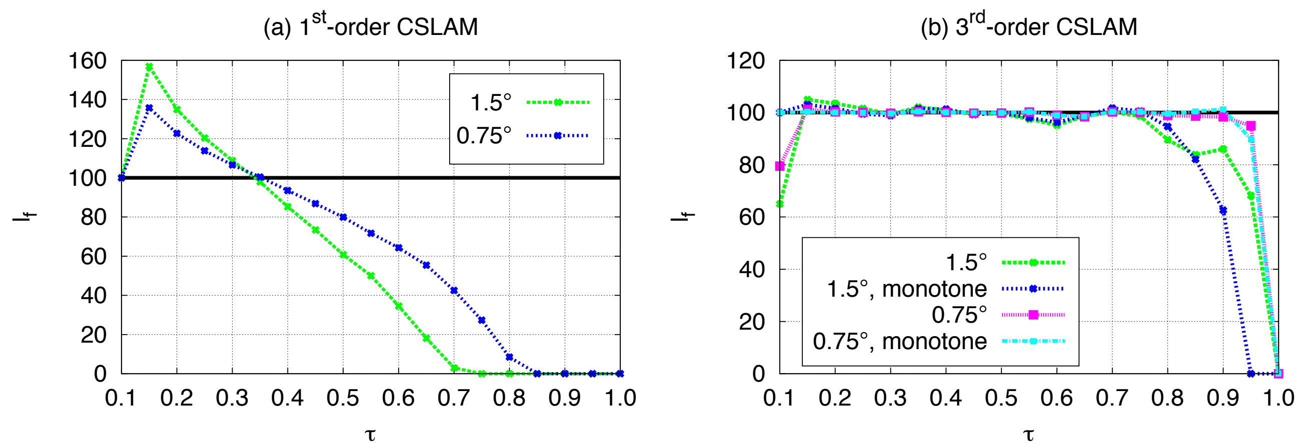


Fig. 6. Filament diagnostics $\ell_f(t=T/2)$ as a function of threshold value τ for different configurations of the CSLAM scheme with Courant number 5.5. (a) 1^{st}-order version of CSLAM at $\Delta\lambda = 1.5°$ and $\Delta\lambda = 0.75°$, and (b) 3^{rd}-order version of CSLAM with and without monotone/shape-preserving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

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.

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

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

respectively.

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

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 sources/sinks)

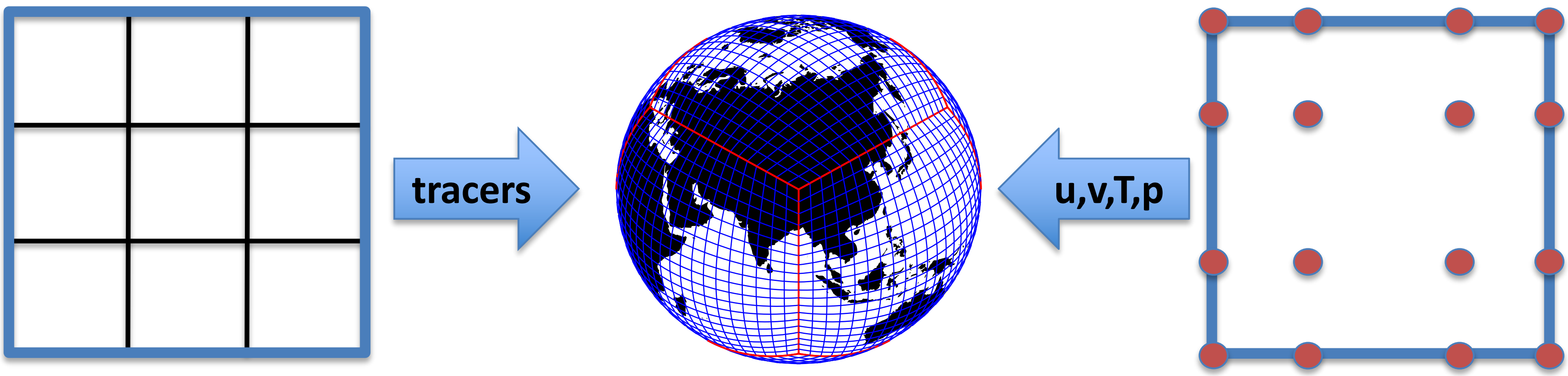
$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0, \qquad (4)$$

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

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



Finite-volume method

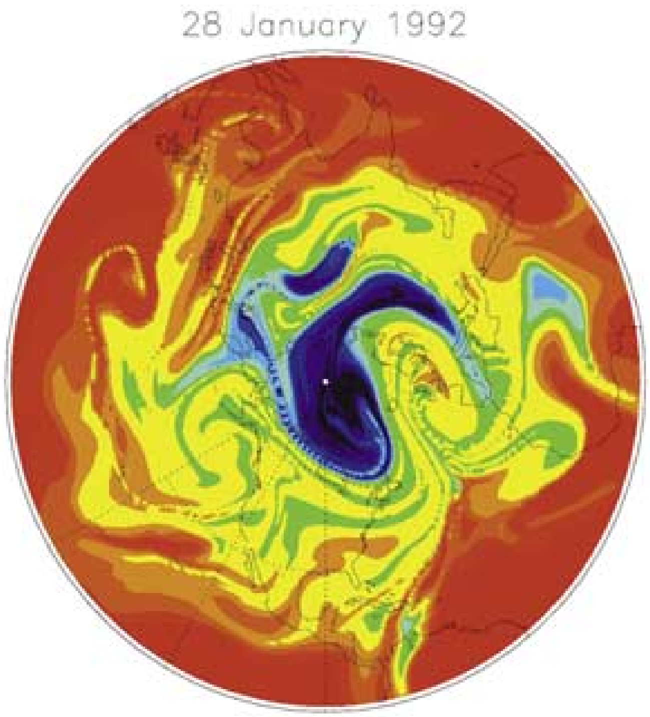
Spectral-element method

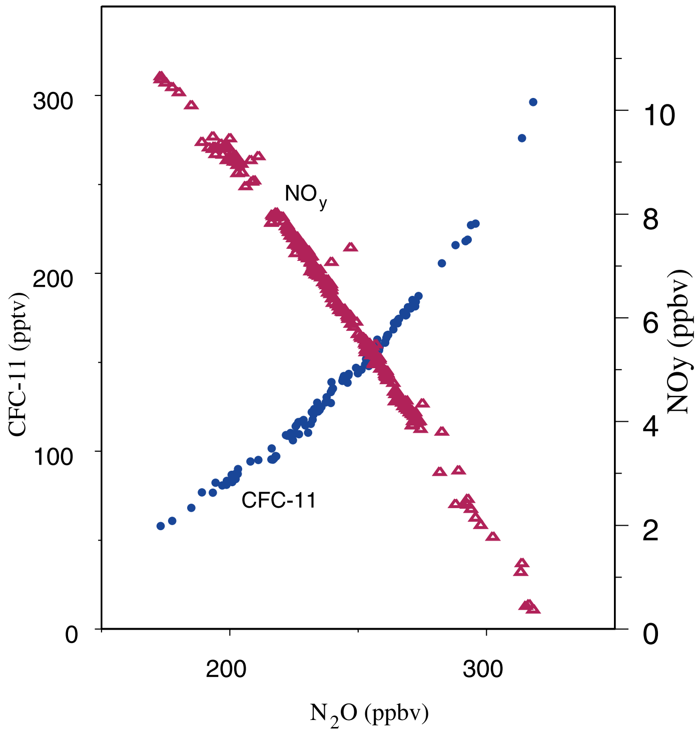
We need to couple without violating mass-conservation, shape-preservation, and consistency

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).

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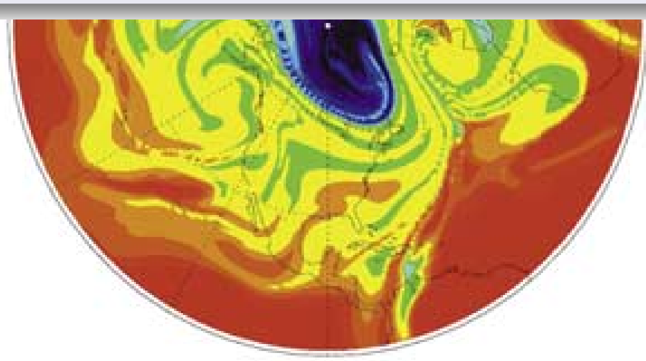
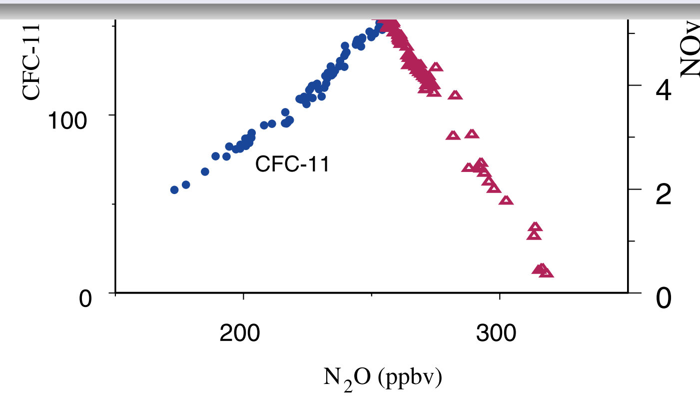
E.g., nitrous oxide (N_2O) against 'total odd nitrogen' (NO_y) or chlorofluorocarbon (CFC's)

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)

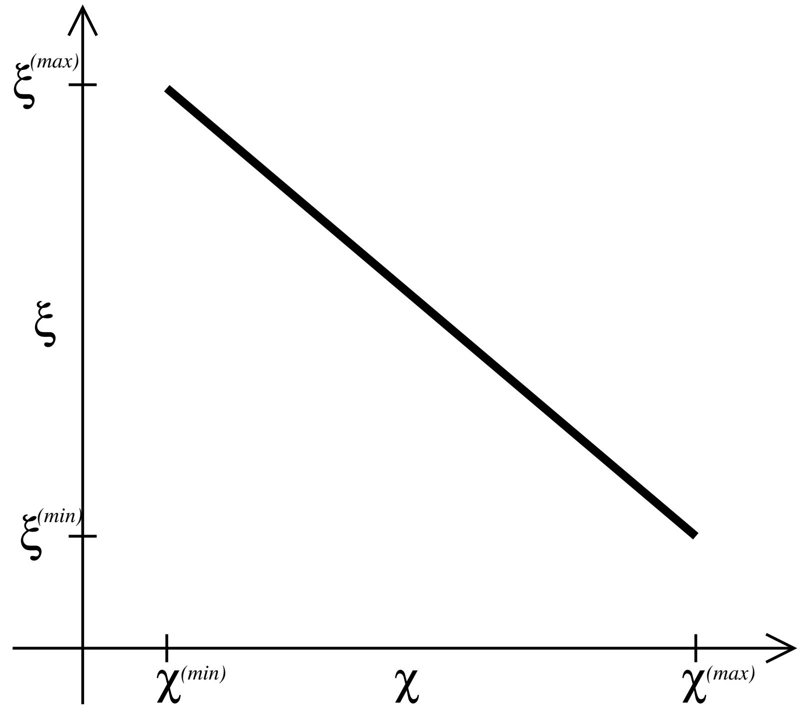
The transport operator should ideally not perturb pre-existing functional relationships





Figures from Plumb (2007).

Analyzing scatter plots

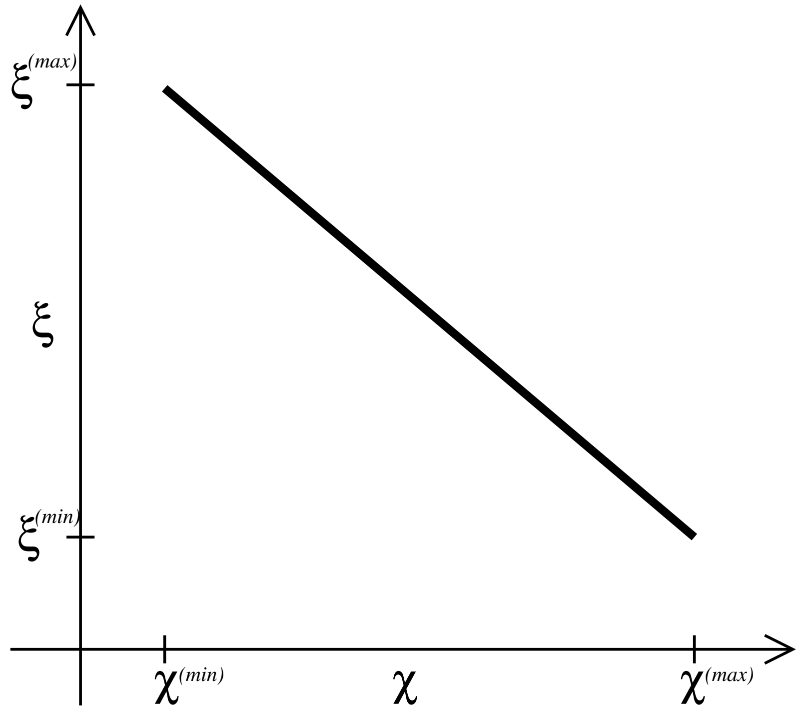


Analytical pre-existing functional relationship curve ψ (linear)

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

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

Analyzing scatter plots



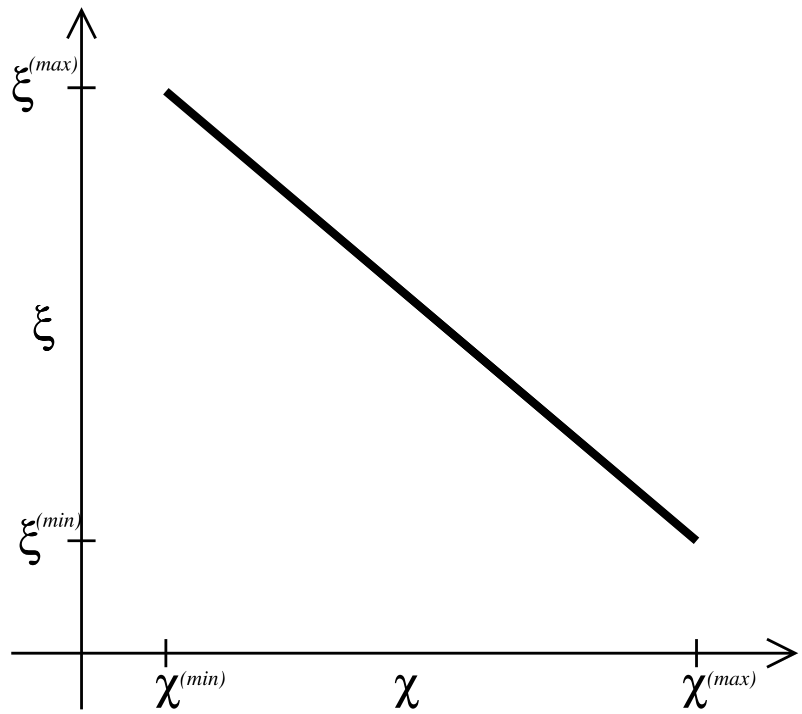
Analytical pre-existing functional relationship curve ψ (linear)

χ and ξ are transported separately by the transport scheme

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

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

Analyzing scatter plots



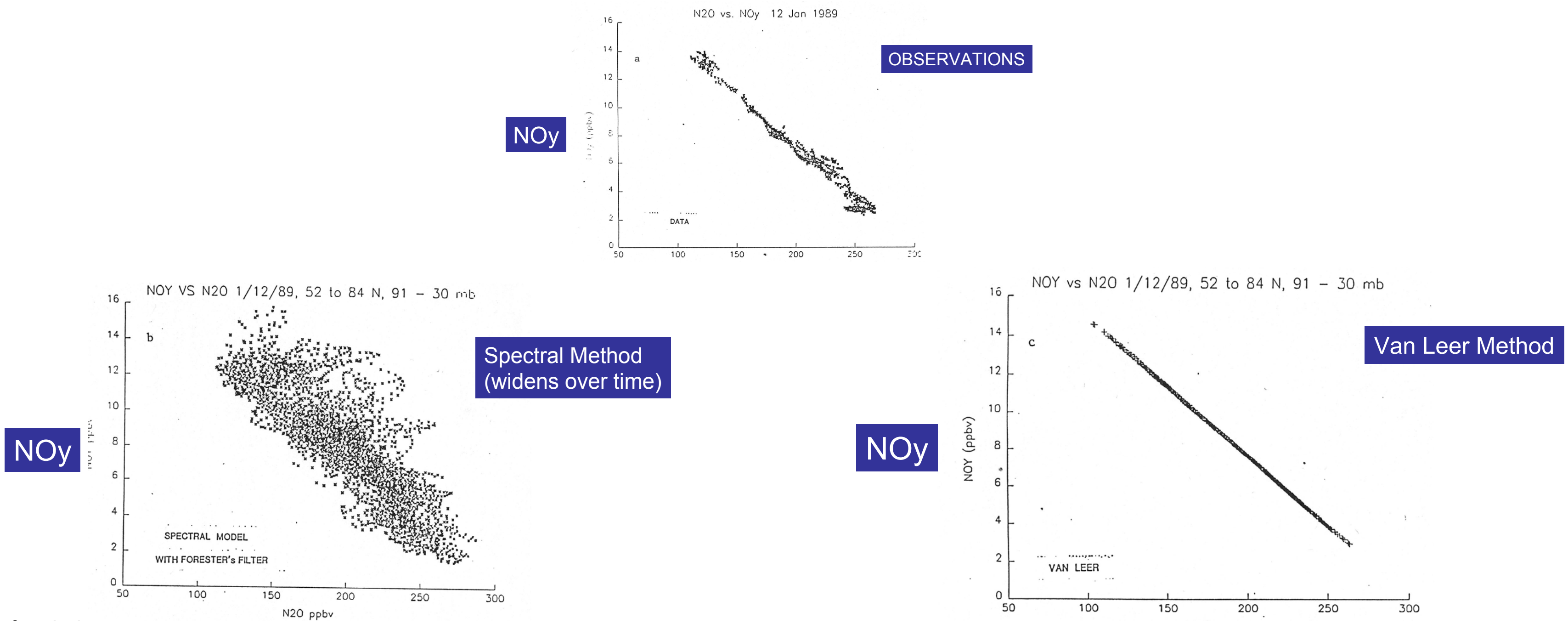
Analytical pre-existing functional relationship curve ψ (linear)

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

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

$\rightarrow$ 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)

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

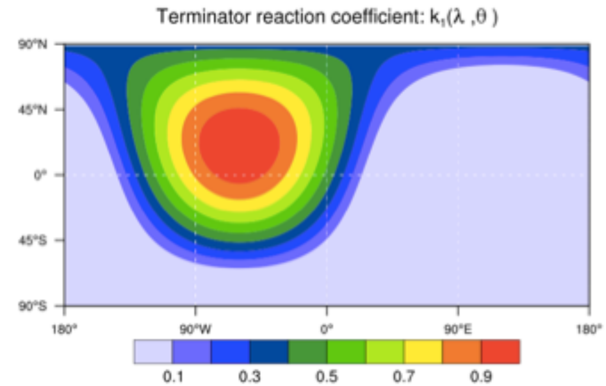
The terminator 'toy'-chemistry test: A simple tool to assess errors in transport schemes

(Lauritzen et al., 2015)

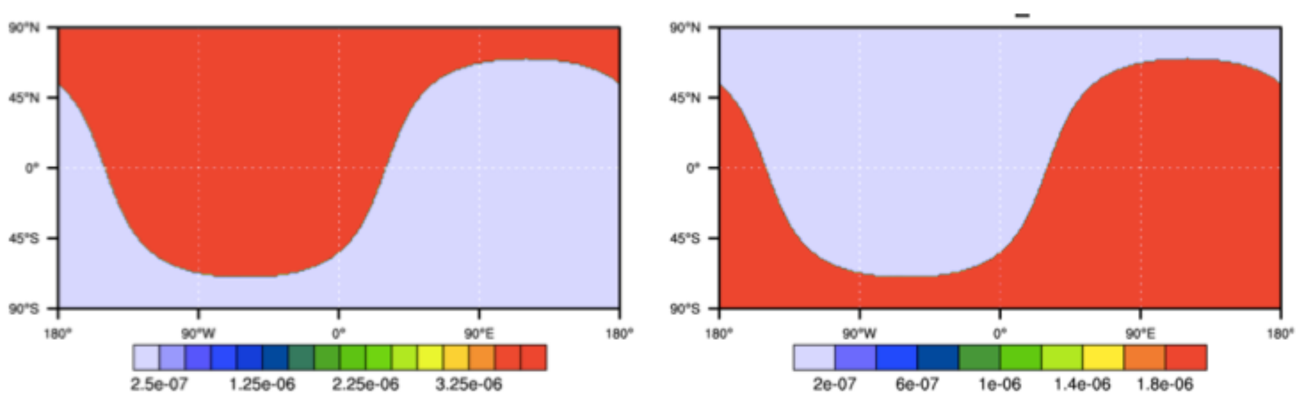
See: http://www.cgd.ucar.edu/cms/pel/terminator.html

- Consider 2 reactive chemical species, Cl and Cl_2 :

$$Cl_2 \rightarrow Cl + Cl : k_1$$
$$Cl + Cl \rightarrow Cl_2 : k_2$$



- Steady-state solution (no flow):



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

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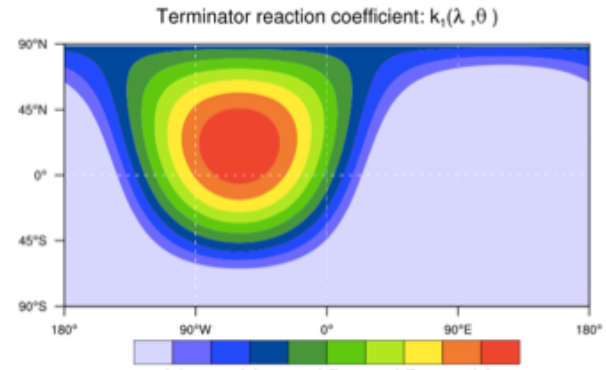
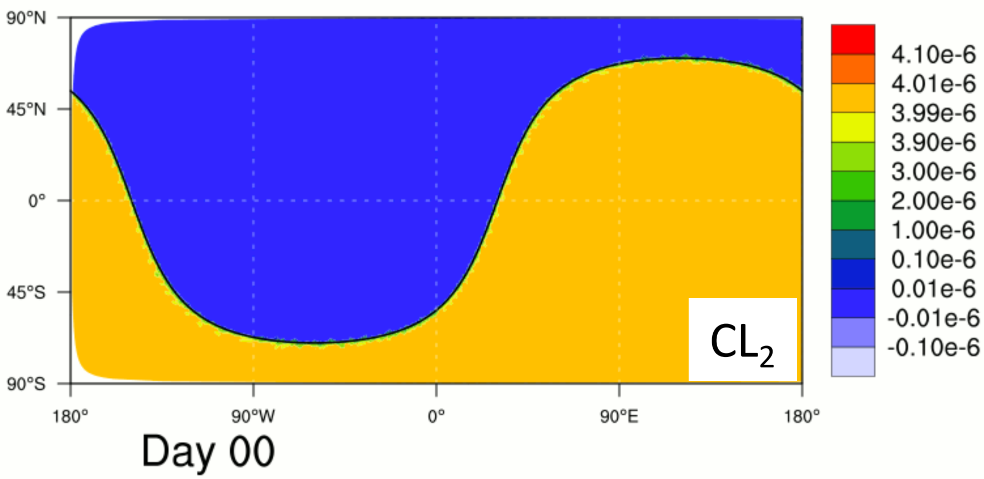
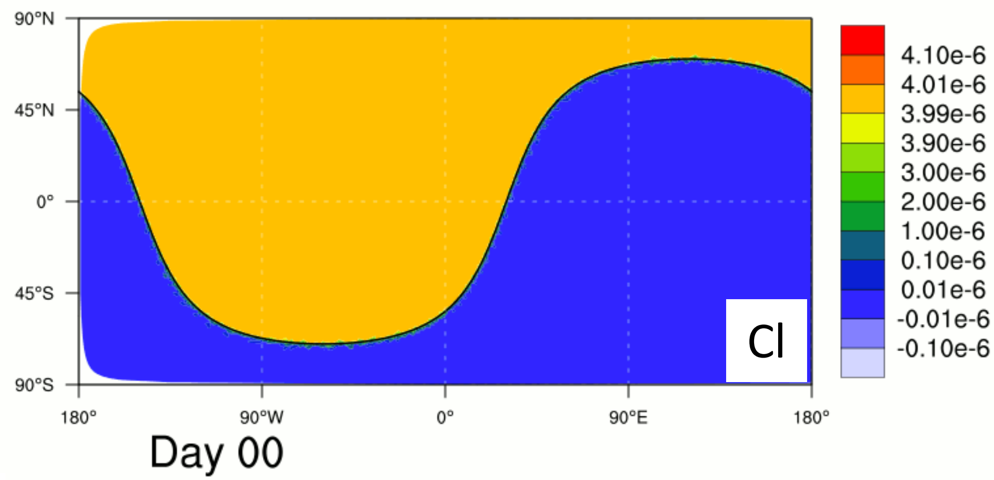






- In any flow-field Cl_y=Cl+2*Cl_2 should be constant at all times (linear correlation preservation).

SciDAC Scientific Discovery through Advanced Computing

National Center for Atmospheric Research Atmospheric Chemistry Observations & Modeling

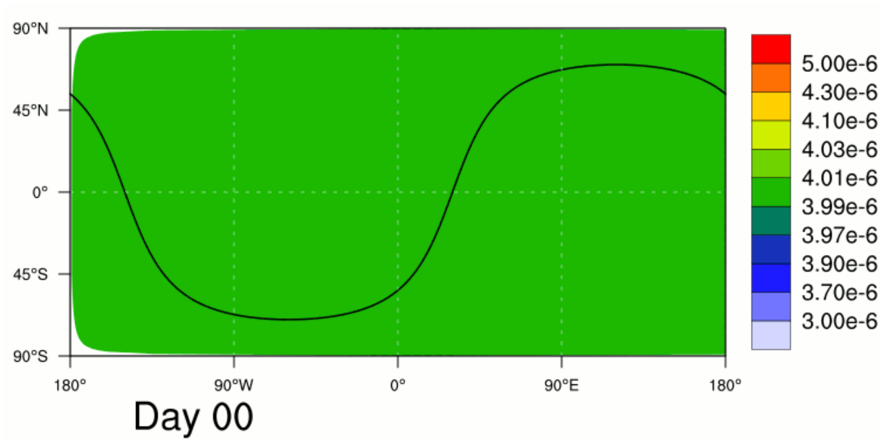
NCAR UCAR National Center for Atmospheric Research Climate & Global Dynamics climate • models • society

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

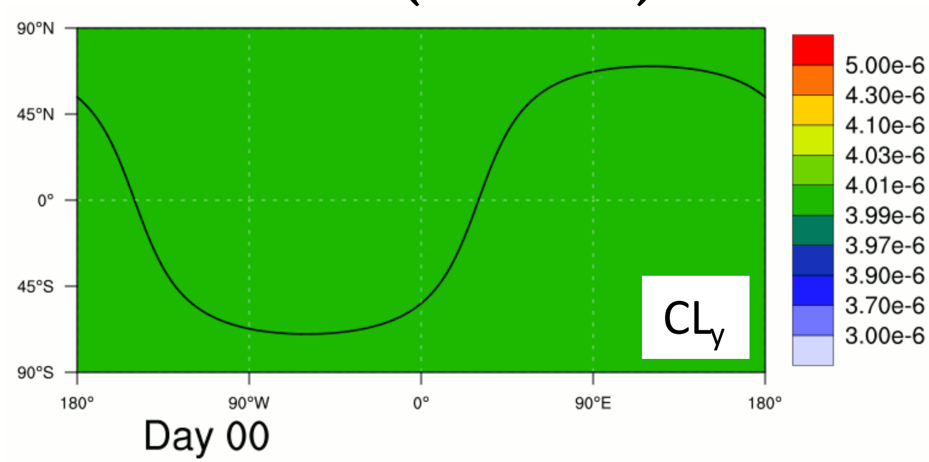
(Lauritzen et al., 2015)

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

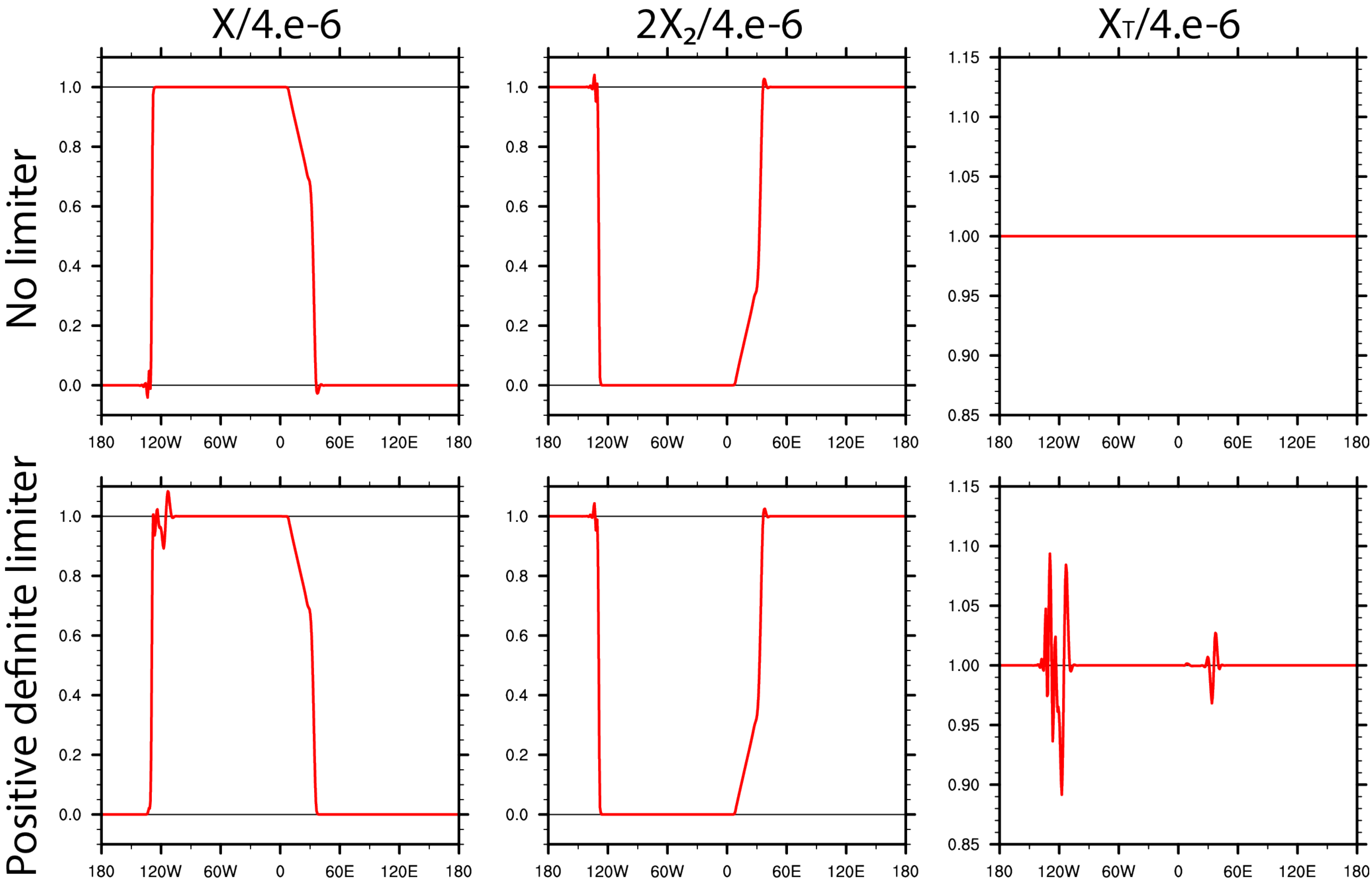
CAM-SE



CAM-FV (Lin 2004)

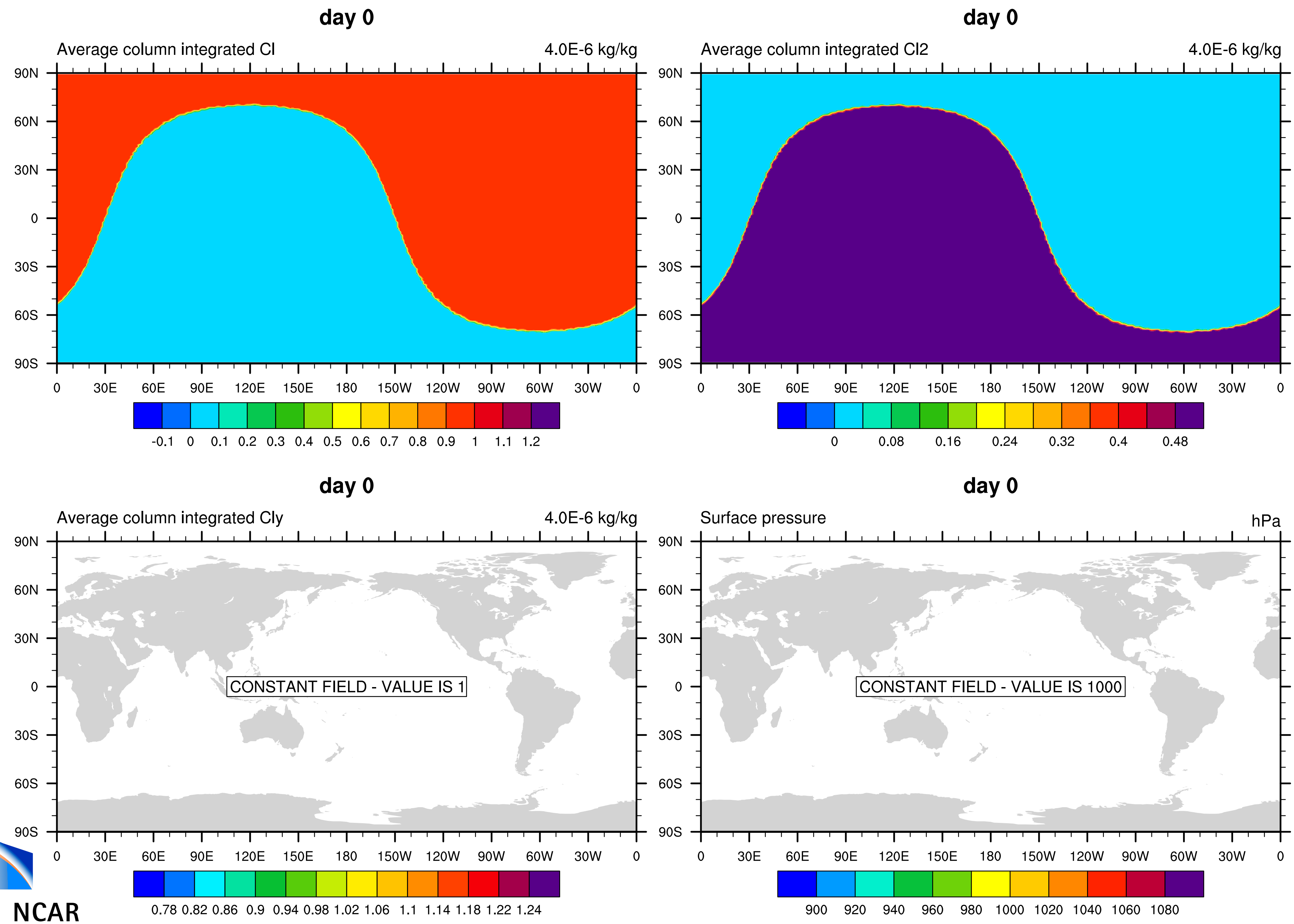


- **In any flow-field $Cl_y = Cl + 2*Cl_2$ should be constant at all times (correlation preservation).**



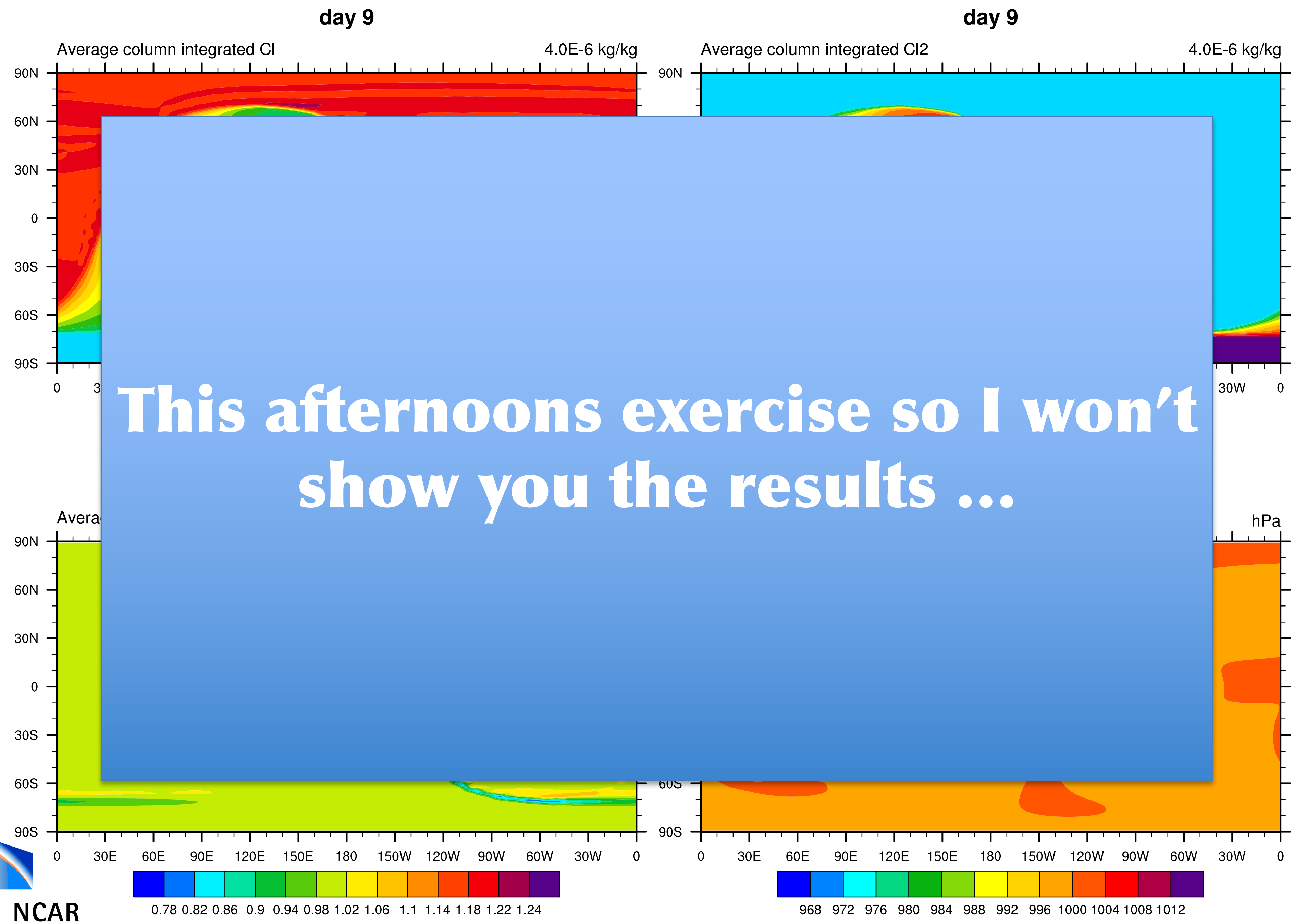
X/4.e-6
2X2/4.e-6
XT/4.e-6
No limiter
Positive definite limiter
1.0
0.8
0.6
0.4
0.2
0.0
1.15
1.10
1.05
1.00
0.95
0.90
0.85
180
120W
60W
0
60E
120E
180

3D version: Initial condition



NCAR

CAM-SE



This afternoons exercise so I won't show you the results …

NCAR

Conserving sum of “families” of species

Chlorine (in CAM-chemistry)

Total Organic Chlorine (set at the surface)

$$T_{C\ell}^{ORG} = CH_3C\ell + 3CFC\ell_3 + 2CF_2C\ell_2 + 3C\ell C\ell_2FCC\ell F_2 + HCF_2C\ell + 4CC\ell_4 + 3CH_3CC\ell_3.$$

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

$$T_{C\ell}^{INORG} = C\ell + C\ell O + OC\ell O + 2C\ell_2 + 2C\ell_2O_2 + HOC\ell + C\ell ONO_2 + HC\ell,$$

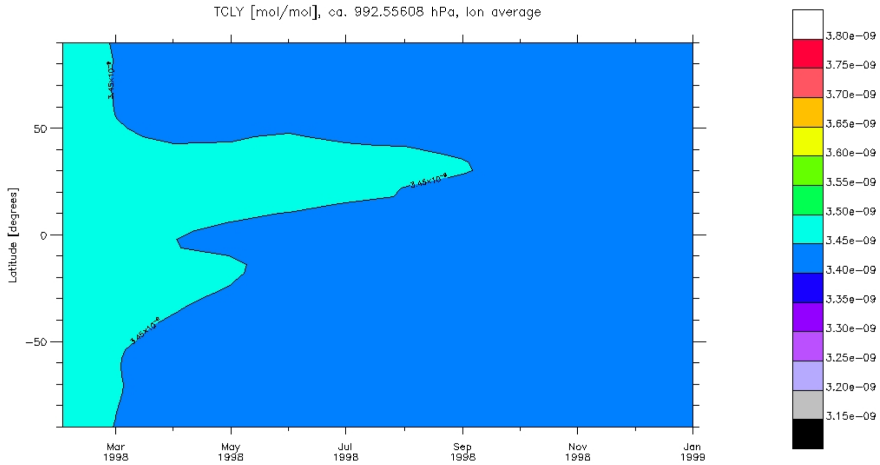
Total Chlorine

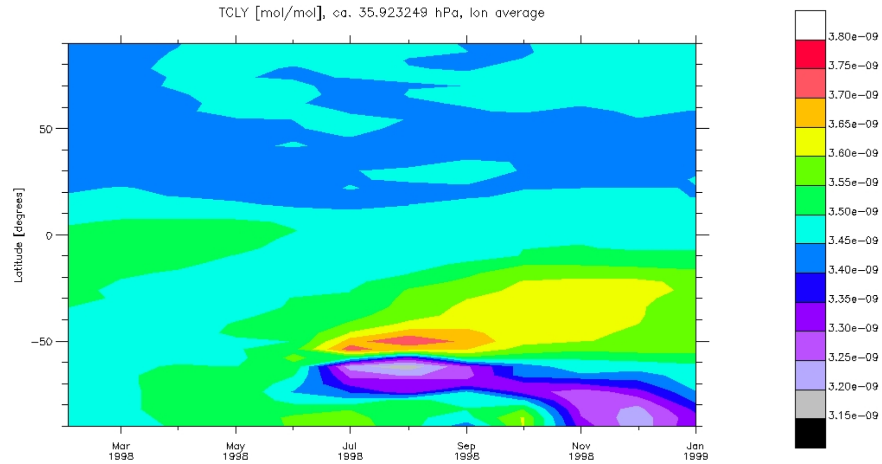
$$TCLY = T_{C\ell}^{ORG} + T_{C\ell}^{INORG}$$

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	→	CH3CO3 + NO2 + M	k(CH3CO3+NO2+M)·1.111E28 ·exp(–14 000/T)
CH3CO3 + CH3CO3	→	2·CH3O2 + 2·{CO2}	2.50E-12·exp(500/T)
GLYALD + OH	→	HO2 + .2·GLYOXAL + .8·CH2O + .8·{CO2}	1.00E-11
GLYOXAL + OH	→	HO2 + CO + {CO2}	1.10E-11
CH3COOH + OH	→	CH3O2 + {CO2} + H2O	7.00E-13
C2H5OH + OH	→	HO2 + CH3CHO	6.90E-12·exp(–230/T)
C3H6 + OH + M	→	PO2 + 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?

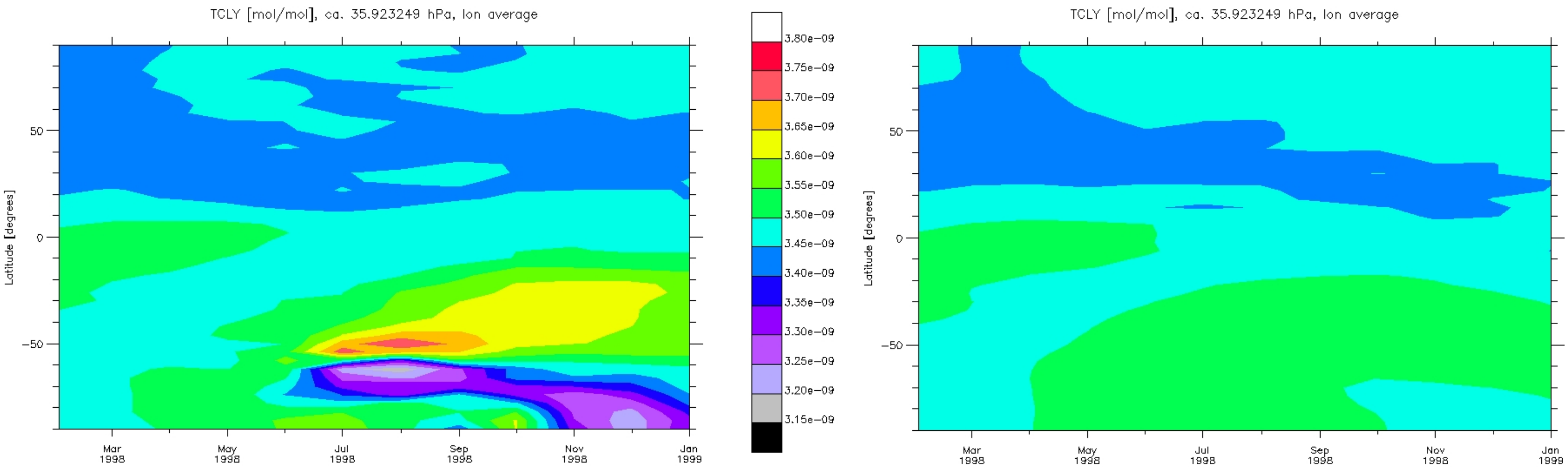
Transport scheme can not maintain the sum when transporting the species individually:

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

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

where N_χ is the number of species χ_i.

Conserving sum of "families" of species



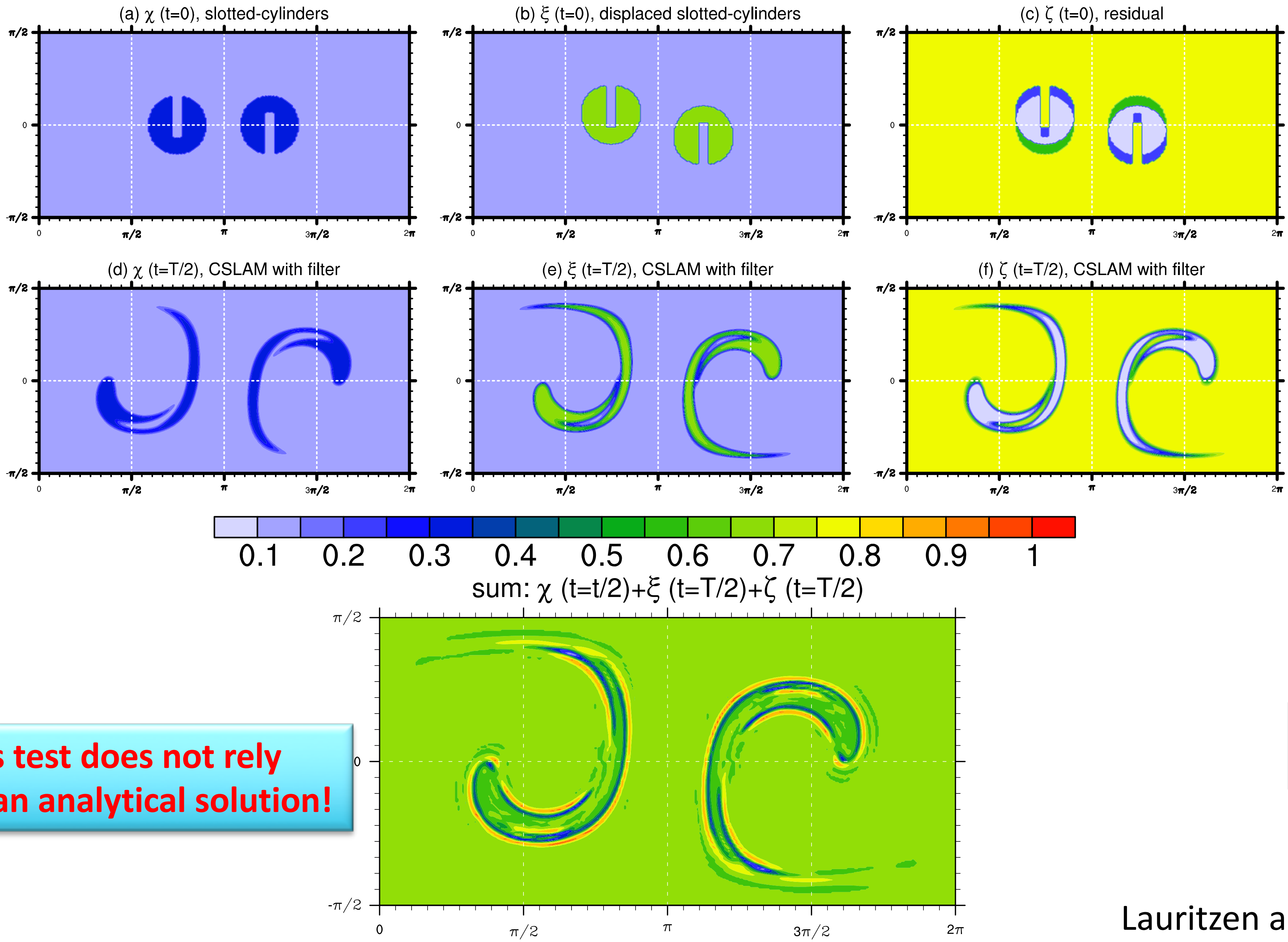
(left) same as previous slide:

- large unphysical deviations from constancy in TCLY near the edge of the polar stratospheric vortex ⇒ less TCLY over South pole ⇒ 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)

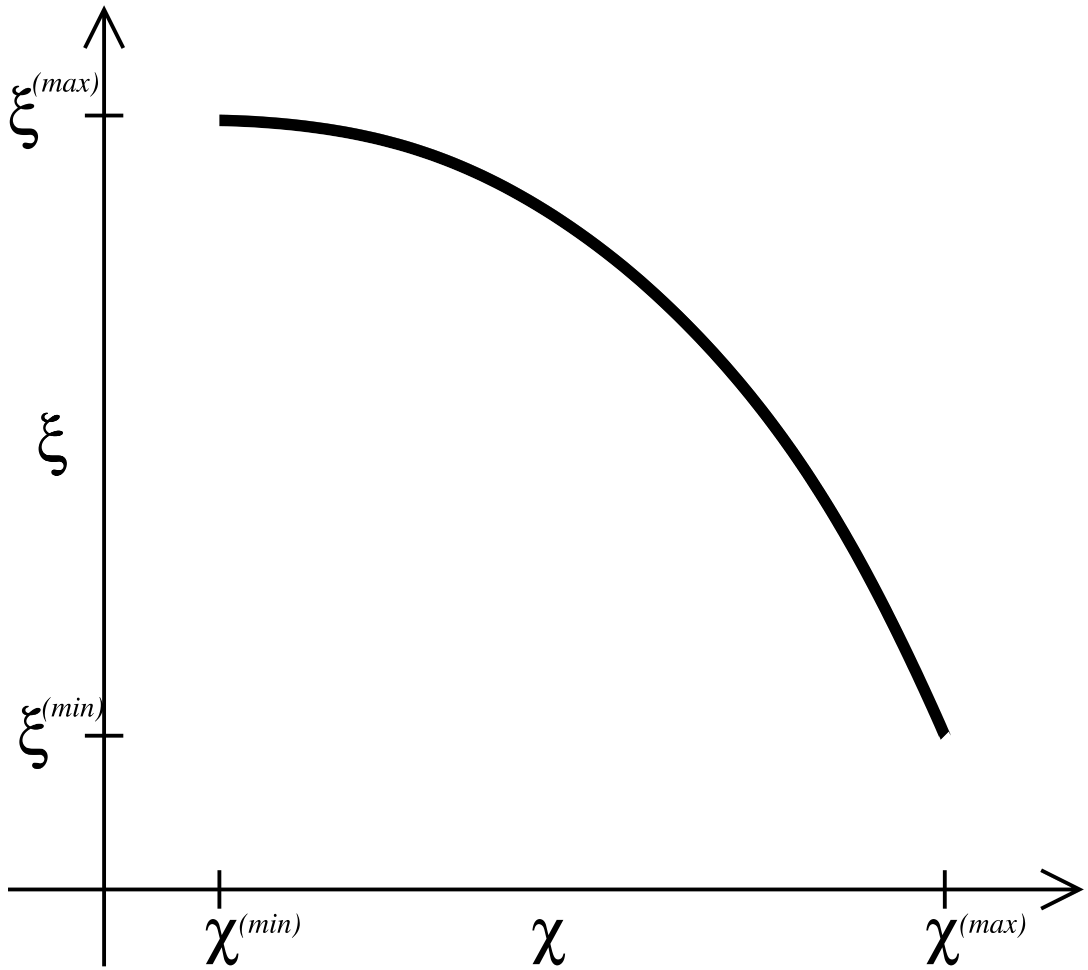
Simple idealized "family of species" test



This test does not rely on an analytical solution!

Lauritzen and Thuburn (2010)

Analyzing scatter plots

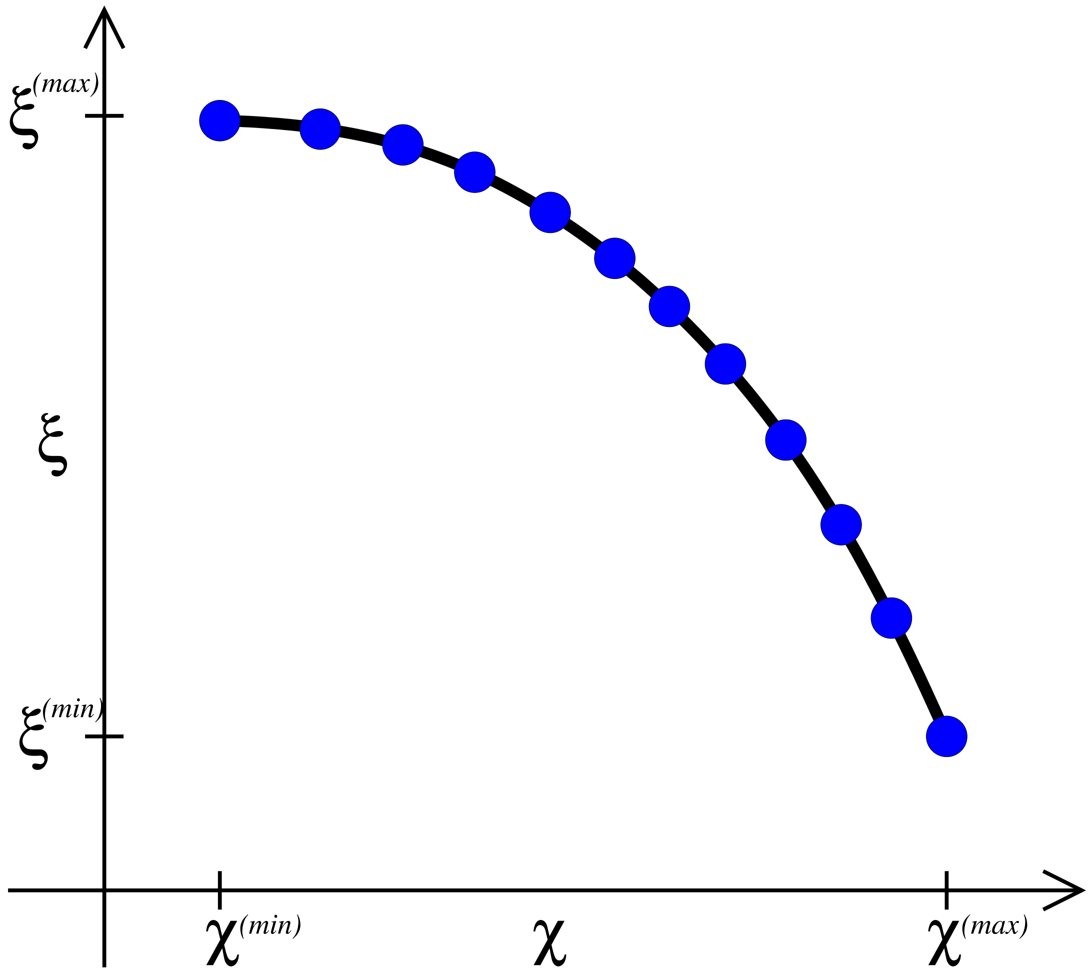


Analytical pre-existing functional relationship curve ψ

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

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

Analyzing scatter plots

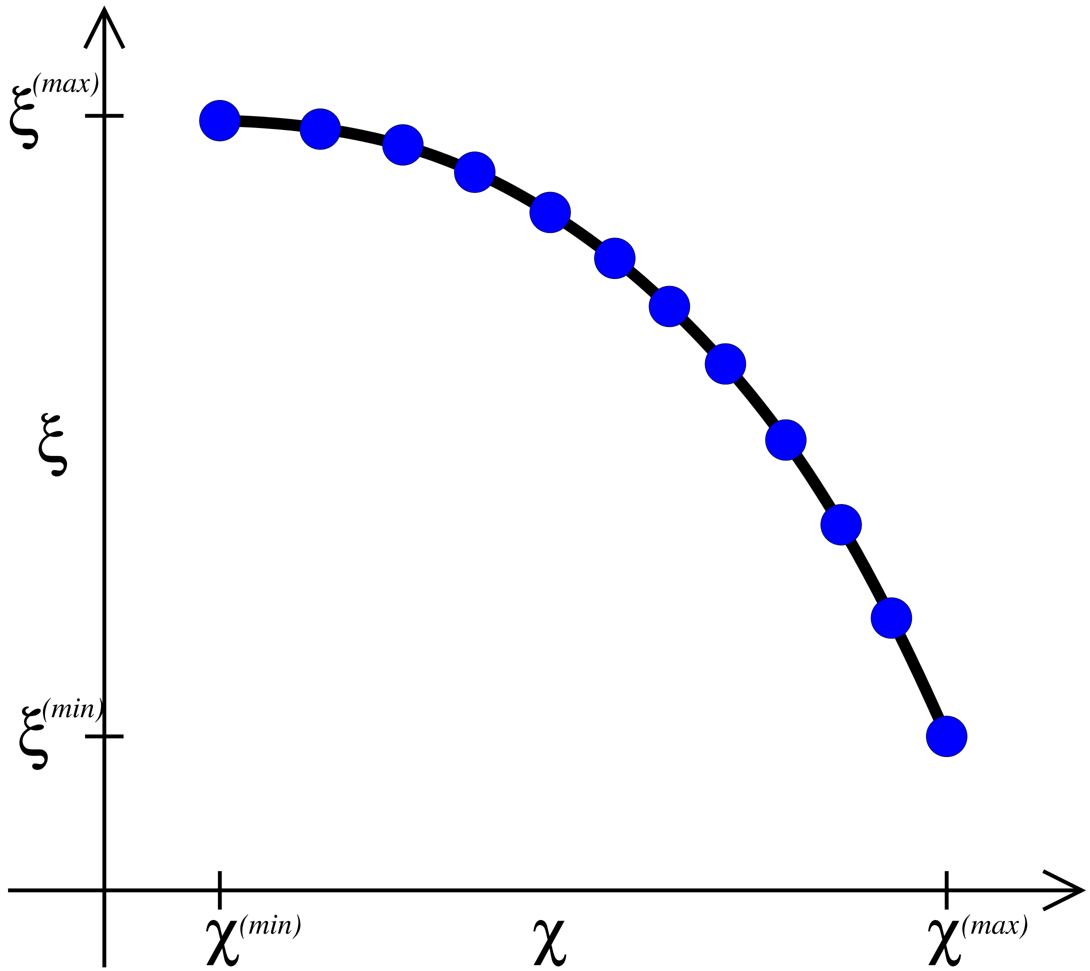


Discrete pre-existing functional relation (initial condition)

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

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

Analyzing scatter plots



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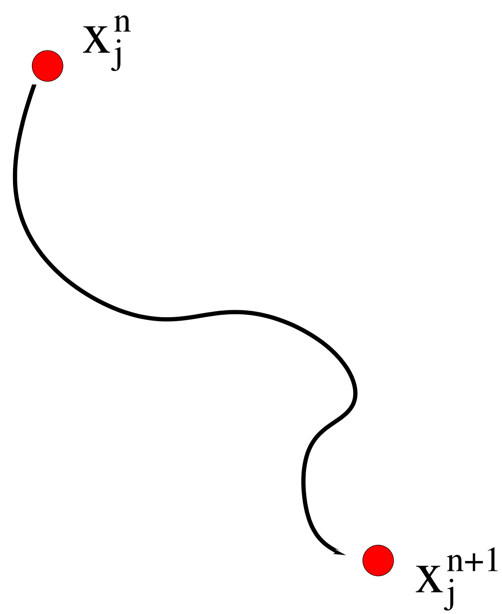
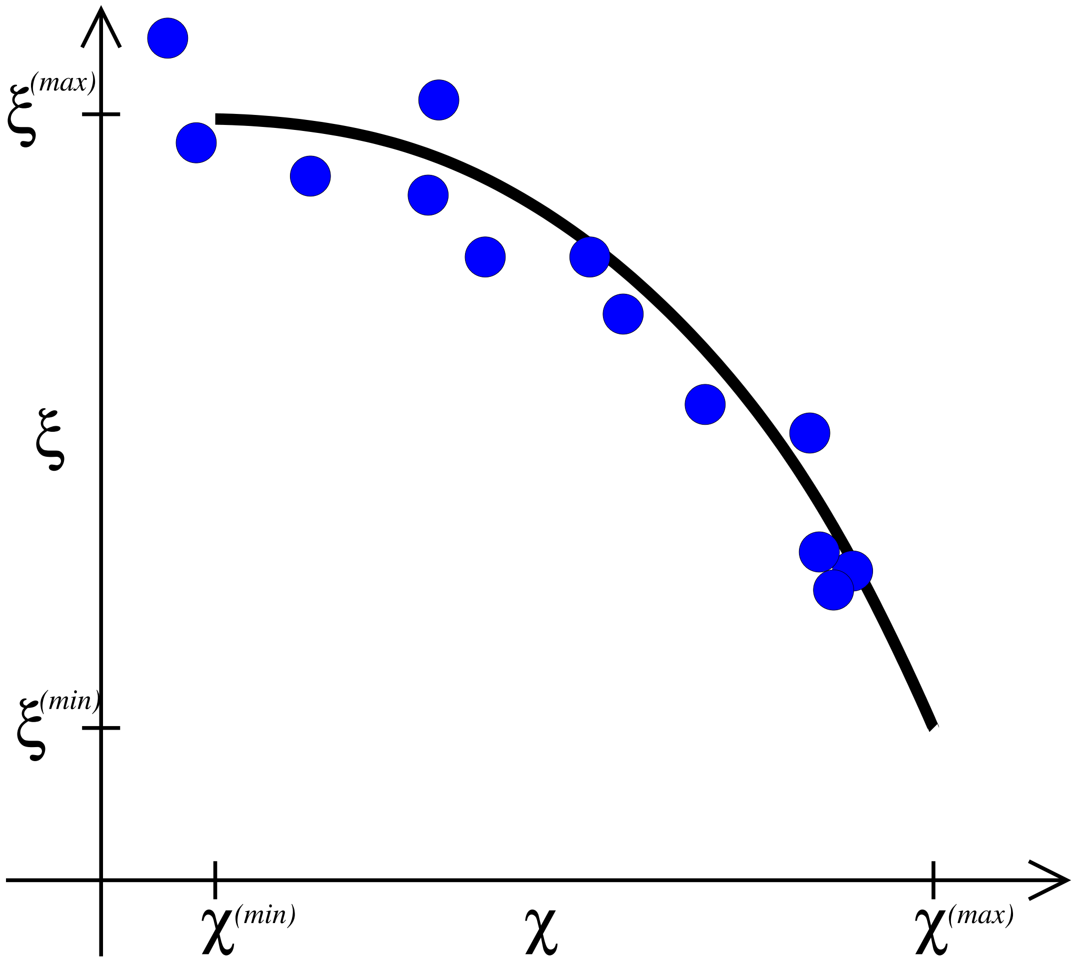


A fully Lagrangian model will maintain pre-existing functional relation

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

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

Analyzing scatter plots

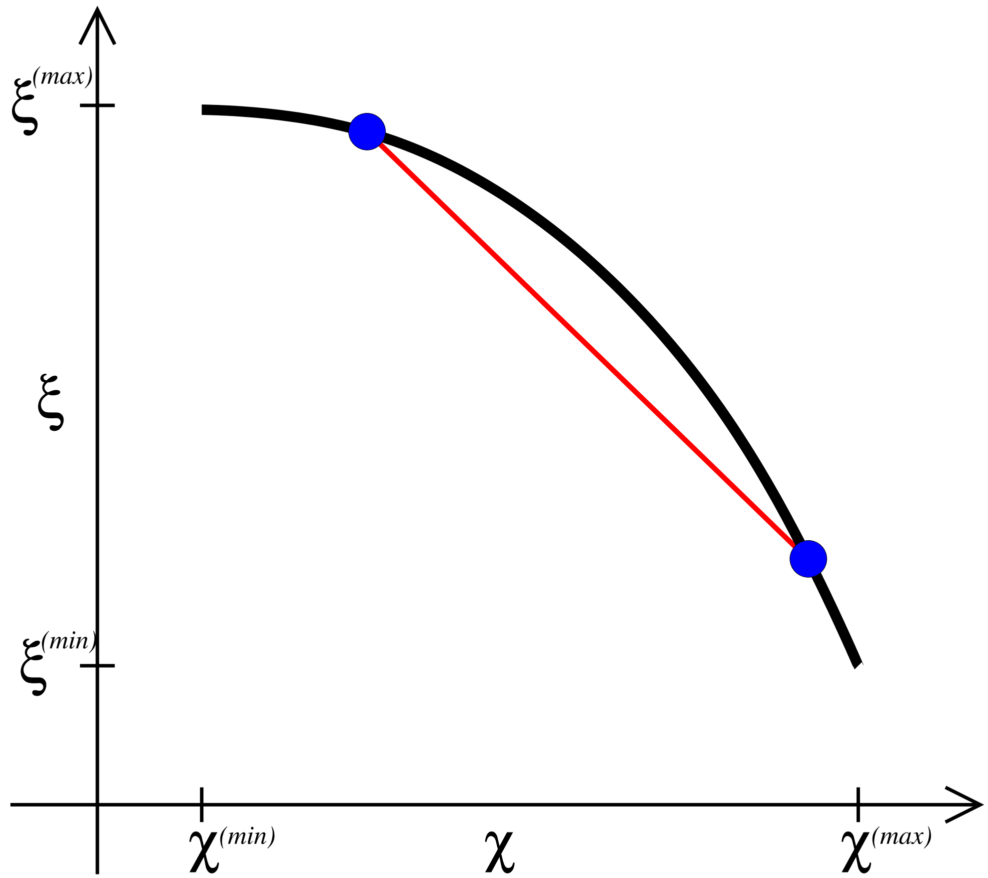


Any Eulerian/semi-Lagrangian scheme will disrupt pre-existing functional relation

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

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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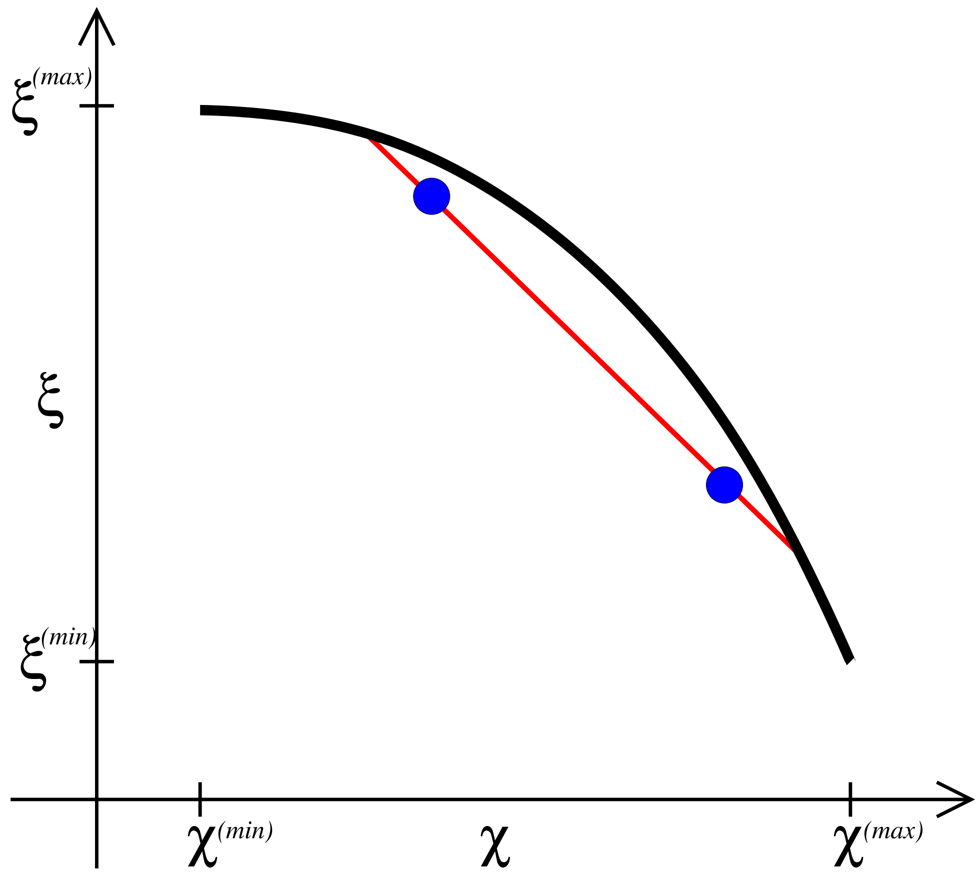
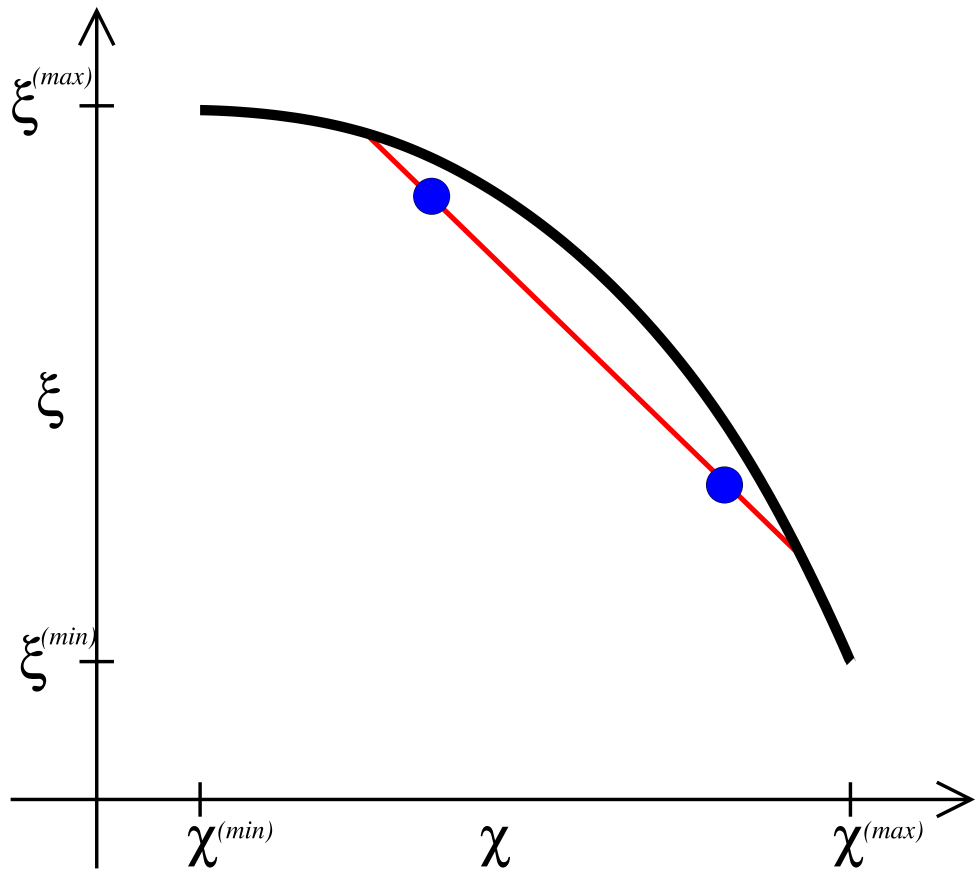


‘Real mixing’ (when occurring) will tend to replace the functional relation by a scatter by linearly interpolating along mixing lines between pairs of points
$\rightarrow$ Ideally numerical mixing should = ‘real mixing’!

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

Classification of numerical mixing on scatter plots



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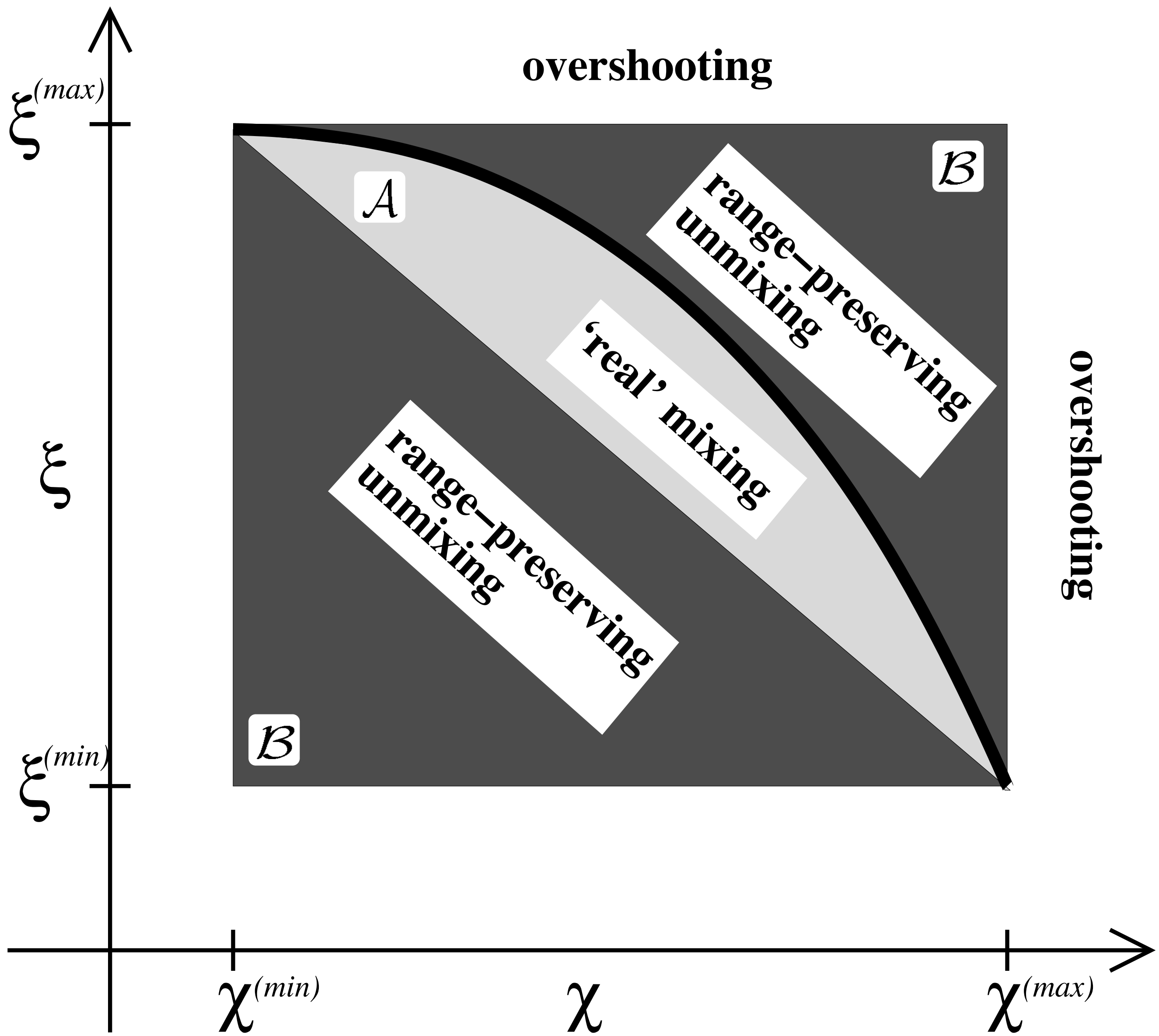
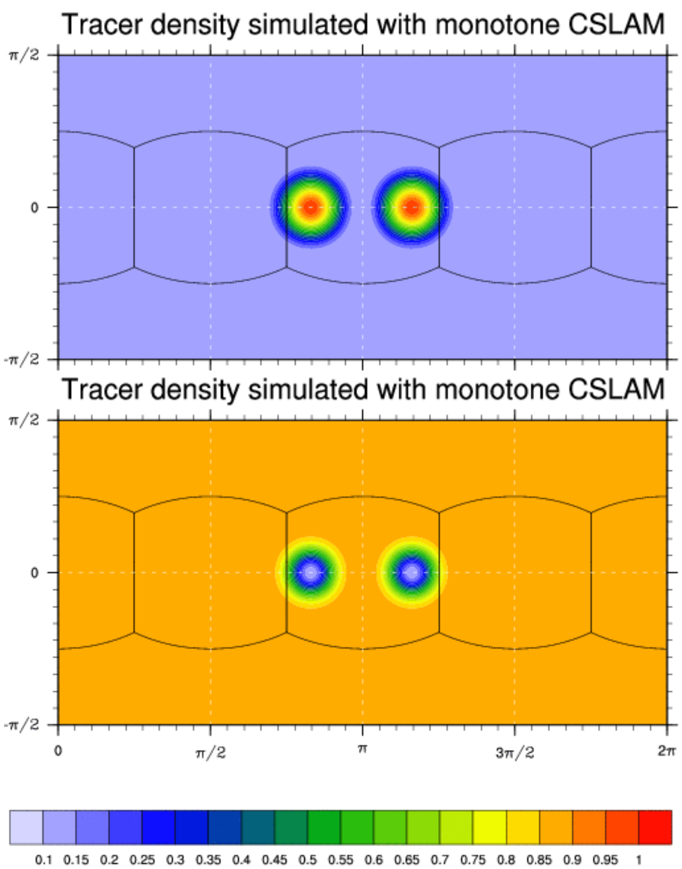
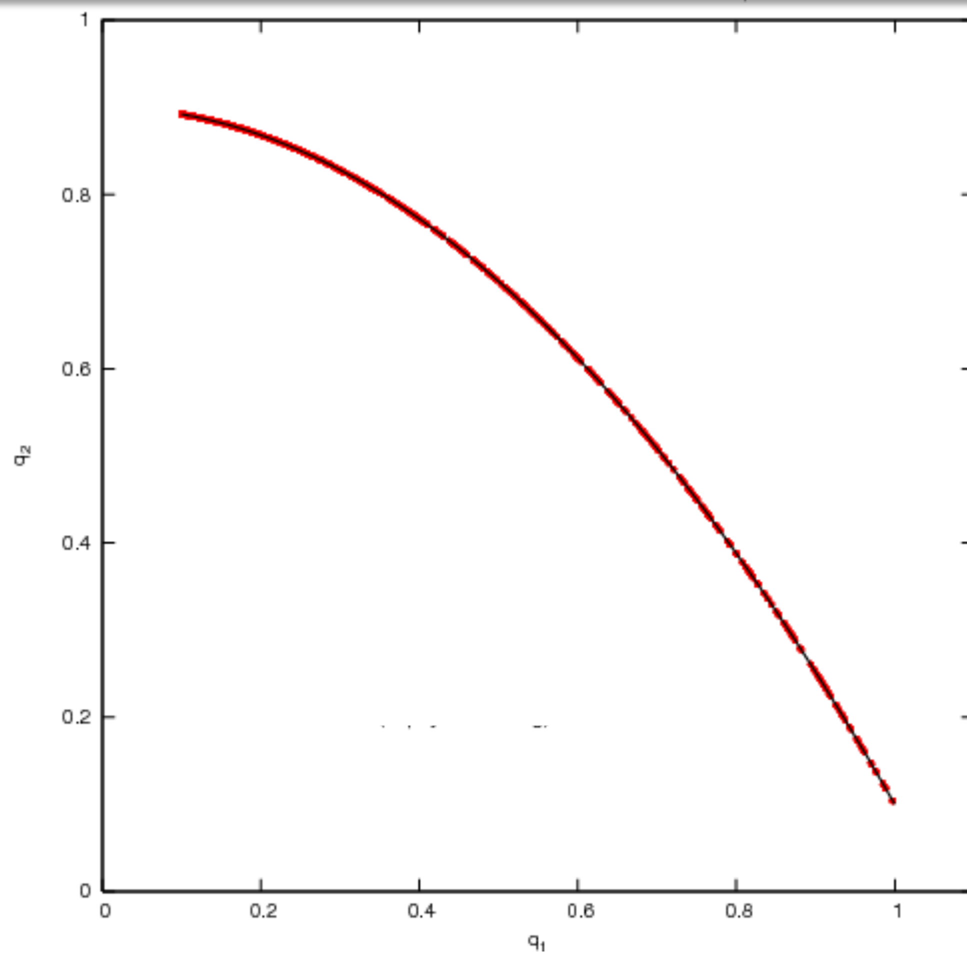


Figure from (Lauritzen and Thuburn, 2012)

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

First-order scheme: only `real mixing'

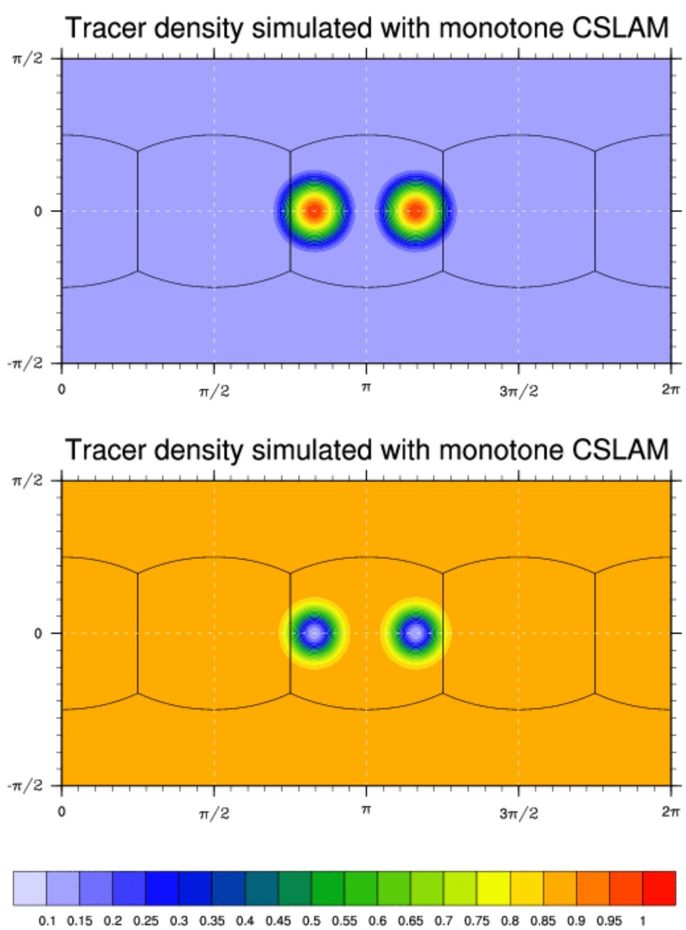


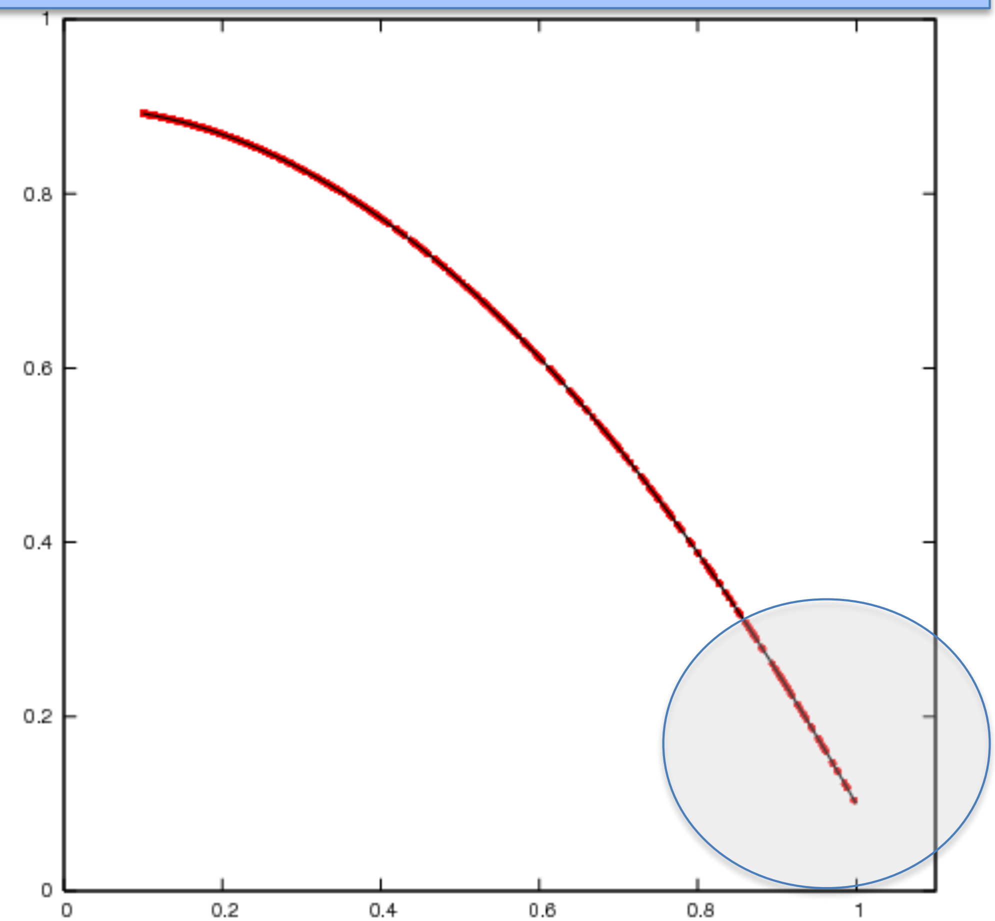


Nair and Lauritzen (2010) flow field

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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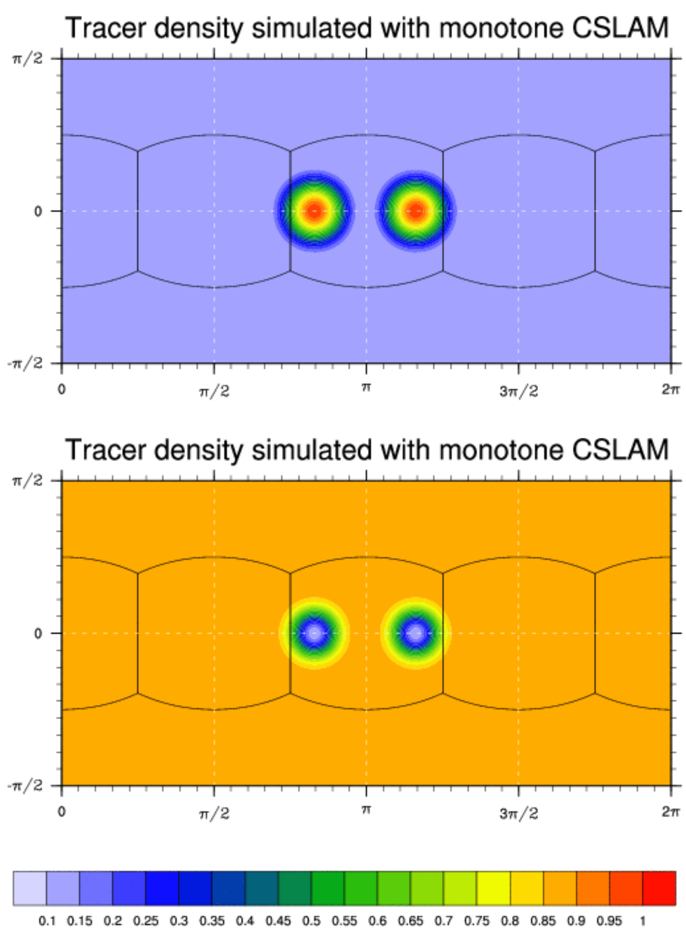

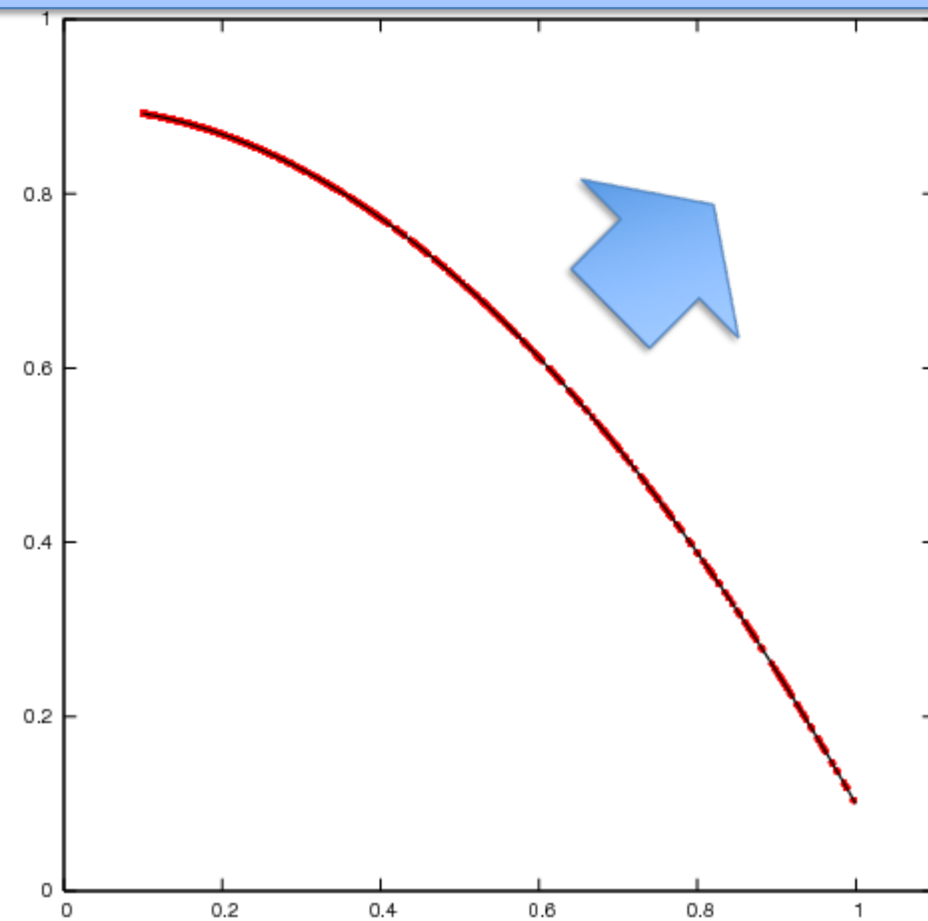

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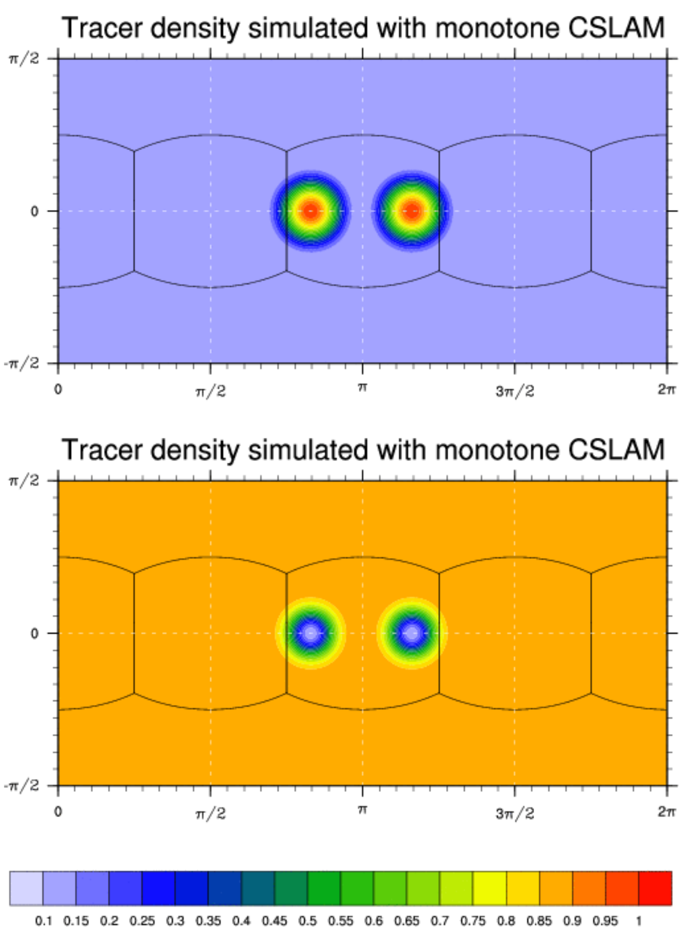

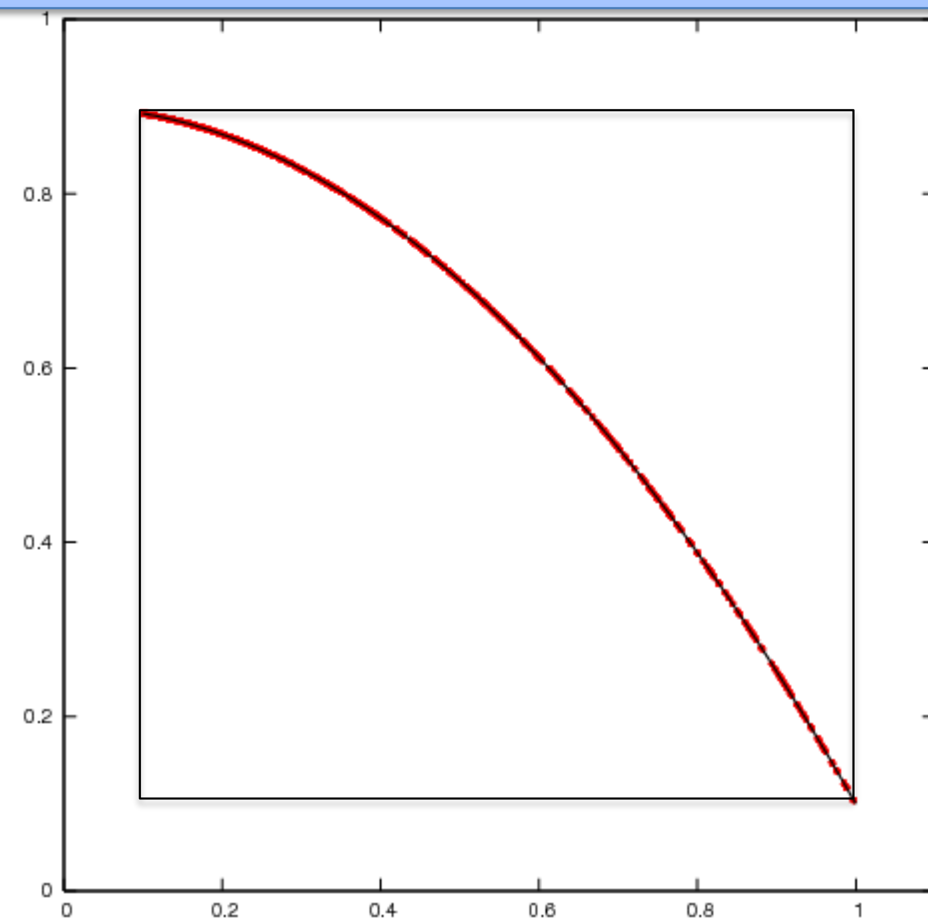

Summary

- Inherent mass-conservation is important
- Shape-preservation is important
- Filament preservation is important
- Consistency (mass-wind) is important
- Correlation preservation (linear, non-linear) is important

I have shown you several idealized test cases to assess these aspects of transport schemes

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

Email: pel@ucar.edu