Evaluating advection/transport schemes using interrelated tracers, scatter plots and numerical mixing diagnostics

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Introduction

Atmospheric tracers are often observed to be functionally related, and these relations can be physically or chemically significant.

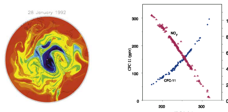


Figure (left) `Reverse domain filling' in which a tracer initially equal to latitude is advected for 10 days. (right) NO_y (triangles) and CFC-11 (dots) plotted against N_2O.

It is therefore highly desirable that the transport schemes used in chemistry and chemistry-climate models should not disrupt such functional relations in unphysical ways through numerical mixing or, indeed, unmixing.

Here, diagnostics are proposed that quantify numerical mixing by a transport scheme for a single tracer, two tracers that are nonlinearly related, and three (or more) tracers that add up to a constant.

- **1-tracer test**: It is interesting to note that single tracer mixing can be quantified using an entropy measure

$$S_\phi = -k_B \sum_{k=1}^{N} \phi_k \log \phi_k \, \rho_k \, \Delta A_k,$$

where k_B is Boltzmann's constant, ϕ_k tracer mixing ratio, ρ_k air density, and ΔA_k is the spherical area of grid cell k.

If there are no numerical errors, the entropy is conserved.

For non-Lagrangian schemes truncation errors will change the entropy. Real mixing can only increase the entropy, and S_ϕ is maximized when ϕ is uniform. See Lauritzen and Thuburn (2011) for further details.

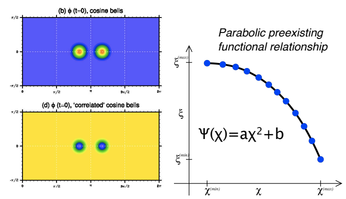
- **2-tracer test**: For the two-tracer test the question of how physically reasonable the numerical mixing is can be addressed by using scatter/correlation plots. See columns 2,3, and 4 on this poster.

- **3-tracer test**: We quantify, in terms of standard error norms, how nearly a transport scheme can preserve the sum by transporting the individual tracers. See Lauritzen and Thuburn (2011) for further details.

None of the mixing diagnostics require knowledge of the analytical solution to the continuity equation!

2-tracer test: Setup

Experiment setup (initial condition):



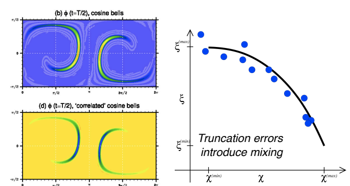
The zonal and meridional wind components are given by

$$u(\lambda,\theta,t) = \kappa \sin^2(\lambda) \sin(2\theta) \cos(\pi t/T) + 2\pi \cos(\theta)/T,$$
$$v(\lambda,\theta,t) = \kappa \sin(2\lambda) \cos(\theta) \cos(\pi t/T),$$

respectively (Nair and Lauritzen, 2010).

- Following Lagrangian parcel motion the tracer interrelationship is preserved.
- No practical Eulerian or semi-Lagrangian scheme will exactly preserve nonlinear preexisting functional relations and will therefore distort such relationships in some way.

=> **The transport scheme essentially introduces numerical mixing or numerical spreading.**



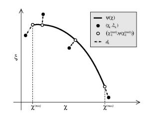
- How the scatter points deviate from the preexisiting function curve has consequences for the physical realizability of the numerically computed solution.

Note that it is key that the tracer features are collapsing to smaller scales (as is typical for atmospheric flows).

Example results using CSLAM (Conservative Semi-LAgrangian Multi-tracer, Lauritzen et al., 2010) scheme are presented.

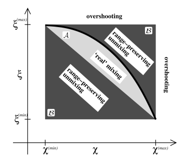
Mixing diagnostics

For the quantification of mixing define distance function d_k:



d_k is the minimum "distance" between the preexisting functional curve and the k^{th} scatter point within the range of the initial conditions

Numerical mixing is categorized into three categories:



`Real' mixing

Numerical mixing that resembles 'real' mixing in that values are only shifted to the concave side of the preexisting functional relation within the convex hull (Thuburn and McIntyre, 1997)

$$\ell_r = \frac{1}{A} \sum_{k=1}^{N} \begin{cases} d_k \, \Delta A_k, & \text{if } (\chi_k, \xi_k) \in \mathcal{A}. \\ 0, & \text{else,} \end{cases},$$

where A is the total area of the domain.

- Any other mixing is spurious *unmixing*
- Only 1st-order schemes can guarantee only 'real' mixing.

Range-preserving unmixing

Numerical unmixing within the range of the initial data

$$\ell_u = \frac{1}{A} \sum_{k=1}^{N} \begin{cases} d_k \, \Delta A_k, & \text{if } (\chi_k, \xi_k) \in \mathcal{B}, \\ 0, & \text{else.} \end{cases}$$

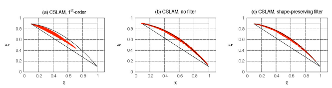
- Any higher-order scheme will produce range-preserving unmixing.

Overshooting (unmixing)

$$\ell_o = \frac{1}{A} \sum_{k=1}^{N} \begin{cases} d_k \, \Delta A_k, & \text{if } (\chi_k, \xi_k) \notin \mathcal{A} \text{ and } (\chi_k, \xi_k) \notin \mathcal{B} \\ 0, & \text{else.} \end{cases}$$

- A shape-preserving scheme will not produce overshooting

Sample results (CSLAM)



scheme	ℓ_1	ℓ_2	ℓ_∞	ℓ_r	ℓ_u	ℓ_o
1^{st}-order CSLAM	1.93×10^{-1}	3.82×10^{-1}	4.57×10^{-1}	6.02×10^{-3}	0.0	0.0
3^{rd}-order CSLAM	1.58×10^{-2}	3.28×10^{-2}	4.73×10^{-2}	7.55×10^{-4}	1.58×10^{-4}	3.79×10^{-4}
3^{rd}-order CSLAM with filter	1.58×10^{-2}	4.33×10^{-2}	8.91×10^{-2}	6.28×10^{-4}	6.73×10^{-5}	0.0

- 1st-order scheme: only 'real' mixing but excessively diffusive
- 3rd-order CSLAM without a filter:
  - some overshooting
  - 'real' mixing >> range-preserving unmixing
  - 'best' in terms of standard error norms
- 3rd-order CSLAM with filter:
  - no overshooting
  - less 'real' mixing compared to unfiltered scheme!
  - much less range-preserving unmixing than unfiltered scheme!

New test case suite

The 2-tracer test is part of a new test case suite (Lauritzen et al. 2011, *J. Comput. Phys.*, in prep.) designed to assess

- numerical order of convergence and 'minimal' resolution,
- ability of the transport scheme to preserve filaments,
- ability of the transport scheme to transport 'rough' distributions,
- ability of the transport scheme to preserve preexisting functional relations between species,
- accuracy of transport scheme under divergent flow condition,

under *challenging* flow conditions.

Test case suite was exercised by a dozen state-of-the-art transport schemes at workshop at NCAR in March 2011.

References

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