Antidiffusion techniques to refine the numerical solution of the advection equation

Case study: Smolarkiewicz' iterative approach

Gerhard Burger Jelmer Wolterink

Scientific Computing
Department of Mathematics
Utrecht University

Project presentations SOAC, 31 October 2011

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Outline

1. The advection equation in climate modelling
   - Importance
   - Diffusion
   - Antidiffusion methods
2. Case study: Smolarkiewicz
   - Analyzing the scheme
   - Implementation
   - Numerical Results
3. Current state of research
   - Possibilities
   - MPDATA
4. Conclusions

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Advection

Transport mechanism of a **substance or conserved property** by a *fluid*, due to the fluid's motion in a particular direction.

Examples in ocean, atmosphere and climate modelling

- Transport of **trace gasses** by *air* due to wind
- Transport of **warm water** by *ocean water* due to currents
- Transport of **ice** by *ocean water* due to currents
- Transport of **warm and moist air** over a colder surface by *air* due to wind: advection fog

Advection equation

Continuity equation describing the advection of a nondiffusive quantity in a flow field:

$$\frac{\partial \psi}{\partial t} + \operatorname{div}(V\psi) = 0$$

where $\psi(x, y, z, t)$ is the nondiffusive scalar quantity, $V = (u, v, w)$ is the velocity vector and x, y, z, t are the independent variables of space and time.

Advection simulation

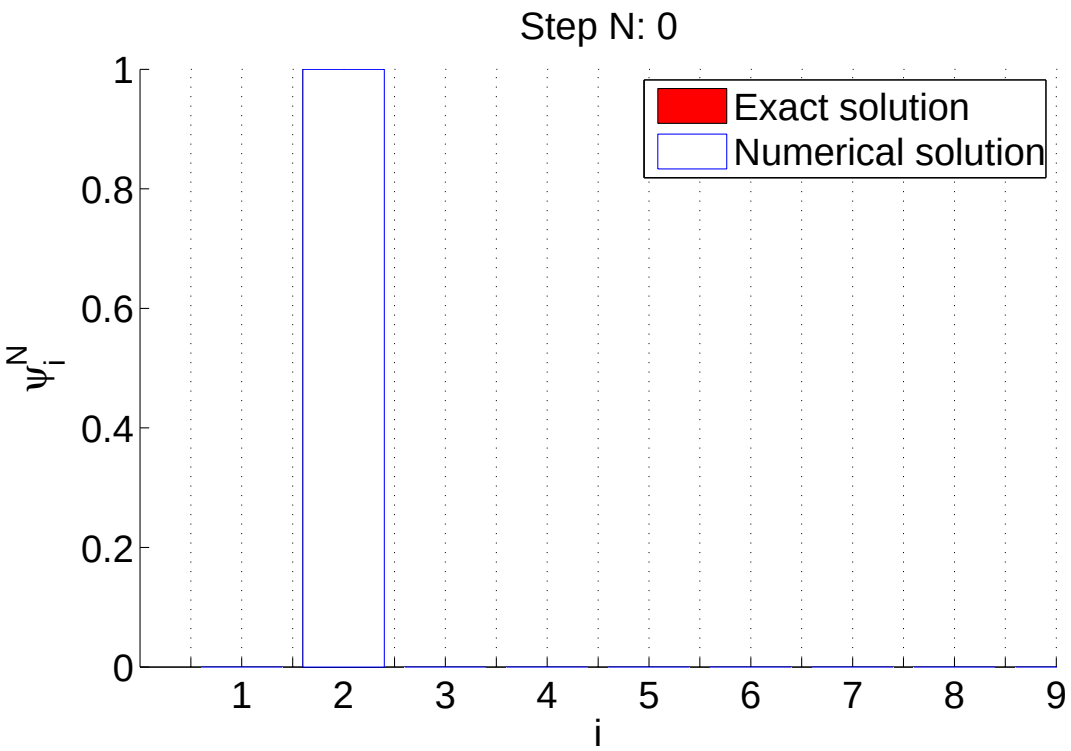
Constraints on advection simulation

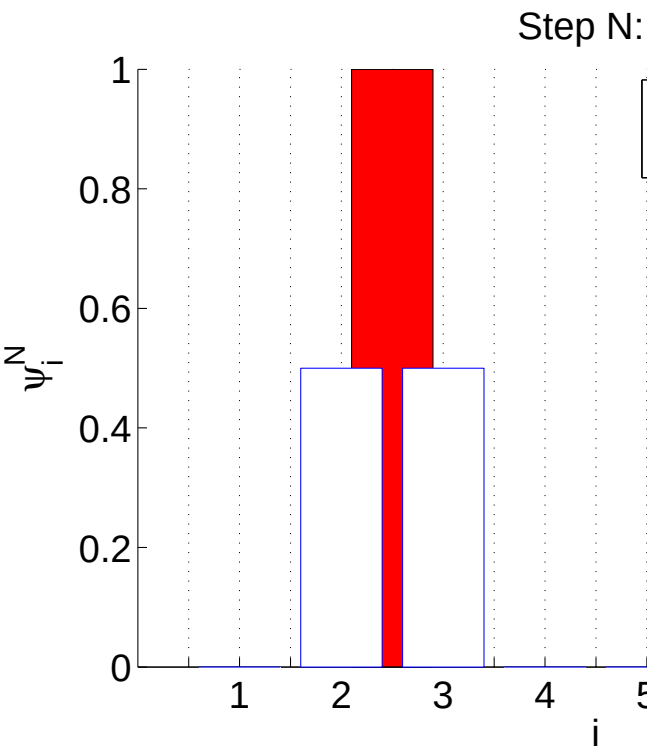
- Solutions should contain no unphysical overshoot or undershoot: positive definite schemes
- Methods should be volume preserving. No loss of matter
- The solutions should be local: the solution at any one point should not be influenced by what is going on far away from that point

Problem: diffusion

- When simulating an advective process, we need to discretize space. When doing so, we introduce numerical constraints on the calculation and we get diffusion.
- The numerical solution spreads out.
- We get interactions, our simulations become less reliable.
- $\Longrightarrow$ example

Example of diffusion with an upstream scheme





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Antidiffusion methods

- Flux-corrected transport (FCT) method (Boris and Book, 1973),
- self-adjusting hybrid scheme (SAHS) (Harten en Zwas, 1972),

Both can be very accurate but require excessive computing time, better is the

- hybrid-type scheme based on a Crowley advection scheme (Clark and Hall, 1979),

with more diffusion but half the computation time.

Antidiffusion methods

Smolarkiewicz' iterative correction, 1983

- Less time consuming while results are comparable to those of the more complex hybrid schemes
- Positive semidefinite
- Iterative method
- Does not contain strong implicit diffusion

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Basis: upstream on a staggered grid

1D case: $\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x}(u\psi) = 0$

We start with the following upstream advection equation on staggered grid:

$$\psi_i^{n+1} = \psi_i^n - \left(F\left(\psi_i^n, \psi_{i+1}^n, u_{i+1/2}^n\right) - F\left(\psi_{i-1}^n, \psi_i^n, u_{i-1/2}^n\right) \right),$$

where

$$F\left(\psi_i^n, \psi_{i+1}^n, u_{i+1/2}^n\right) = \left(\left(u_{i+1/2}^n + \left|u_{i+1/2}^n\right|\right)\psi_i^n + \left(u_{i+1/2}^n - \left|u_{i+1/2}^n\right|\right)\psi_{i+1}^n \right)\frac{\Delta t}{2\Delta x}.$$

Method of lines

Writing the scheme out and collecting terms gives

$$\begin{aligned}\psi_i^{n+1} = &\frac{\Delta t}{2\Delta x}\left(u_{i-1/2}^n + \left|u_{i-1/2}^n\right|\right)\psi_{i-1}^n \\ &+ \left(1 - \frac{\Delta t}{2\Delta x}\left(u_{i+1/2}^n + \left|u_{i+1/2}^n\right| - u_{i-1/2}^n + \left|u_{i-1/2}^n\right|\right)\right)\psi_i^n \\ &- \frac{\Delta t}{2\Delta x}\left(u_{i+1/2}^n - \left|u_{i+1/2}^n\right|\right)\psi_{i+1}^n\end{aligned}$$

Method of lines

This can be rewritten to

$$\psi_i^{n+1} = \alpha_i \psi_{i-1}^n + \beta_i \psi_i^n + \gamma_i \psi_{i+1}^n, \quad \text{for } i = 1, \ldots, M-1,$$

where we have that

$$\alpha_i = \frac{\Delta t}{2\Delta x}\left(u_{i-1/2}^n + \left|u_{i-1/2}^n\right|\right),$$
$$\beta_i = \left(1 - \frac{\Delta t}{2\Delta x}\left(u_{i+1/2}^n + \left|u_{i+1/2}^n\right| - u_{i-1/2}^n + \left|u_{i-1/2}^n\right|\right)\right),$$
$$\gamma_i = -\frac{\Delta t}{2\Delta x}\left(u_{i+1/2}^n - \left|u_{i+1/2}^n\right|\right).$$

Method of lines

We can also write this in matrix form using Dirichlet boundary conditions

- $y(0) = 0$ and $y(M) = 0$
- using periodic boundary conditions $y(0) = y(M)$

$$\begin{bmatrix} \psi_1^{n+1} \\ \psi_2^{n+1} \\ \vdots \\ \psi_{M-2}^{n+1} \\ \psi_{M-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \beta_1 & \gamma_1 & & & 0\alpha_1 \\ \alpha_2 & \beta_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{M-2} & \beta_{M-2} & \gamma_{M-2} \\ 0\gamma_{M-1} & & & \alpha_{M-1} & \beta_{M-1} \end{bmatrix} \begin{bmatrix} \psi_1^{n} \\ \psi_2^{n} \\ \vdots \\ \psi_{M-2}^{n} \\ \psi_{M-1}^{n} \end{bmatrix}$$

So the values of ψ at timestep $N+1$ can be obtained by a sparse matrix-vector multiplication

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Antidiffusion

To apply antidiffusion we need to introduce an intermediate step

$$\psi_i^* = \psi_i^n - \left(F\left(\psi_i^n, \psi_{i+1}^n, u_{i+1/2}^n\right) - F\left(\psi_{i-1}^n, \psi_i^n, u_{i-1/2}^n\right) \right),$$
$$\psi_i^{n+1} = \psi_i^* - \left(F\left(\psi_i^*, \psi_{i+1}^*, \tilde{u}_{i+1/2}^n\right) - F\left(\psi_*^n, \psi_*^n, \tilde{u}_{i-1/2}^n\right) \right),$$

were the antidiffusion velocity $\tilde{u}_{i+1/2}$ is defined as

$$\tilde{u}_{i+1/2} = \frac{\left(\left| u_{i+1/2} \right| \Delta x - \Delta t u_{i+1/2}^2 \right) \left(\psi_{i+1}^* - \psi_i^* \right)}{\left(\psi_i^* + \psi_{i+1}^* + \epsilon \right) \Delta x}$$

Since the second step is similar to the first we can also apply the method of lines to the second step.

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Stability

For stability we need that

$$\max_i \left(\frac{\left| u_{i+1/2} \right| \Delta t}{\Delta x} \right) \leq 1$$

Algorithm

input : Initial state ψ^0, velocities u, iter, tsteps, Δx, Δt
output: Final state ψ^N

```
ψ ← ψ^0;
mat1 ← ComputeMatrix(u, Δx, Δt);
for i ← 1 to tsteps do
    ψ ← MatrixMultiplication(mat1,ψ);
    for j ← 1 to iter do
        ũ ← ComputeAntidiffusionVelocity(ψ, u);
        mat2 ← ComputeMatrix(ũ, Δx, Δt);
        ψ ← MatrixMultiplication(mat2,ψ);
    end
end
ψ^N ← ψ;
```

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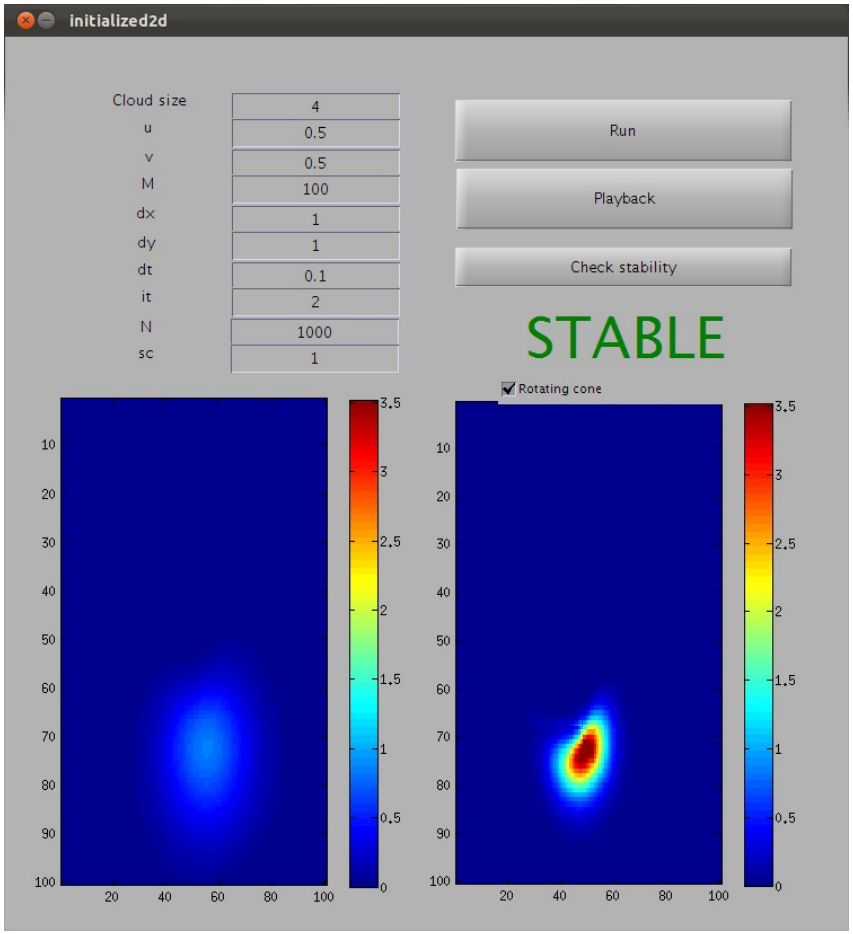
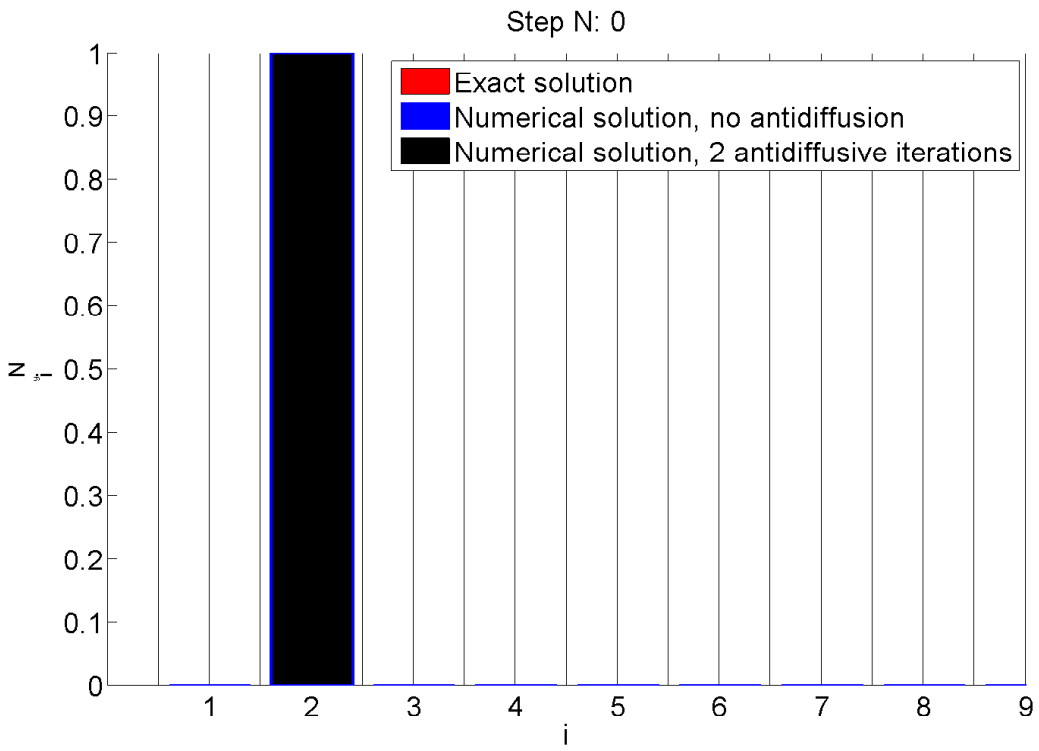
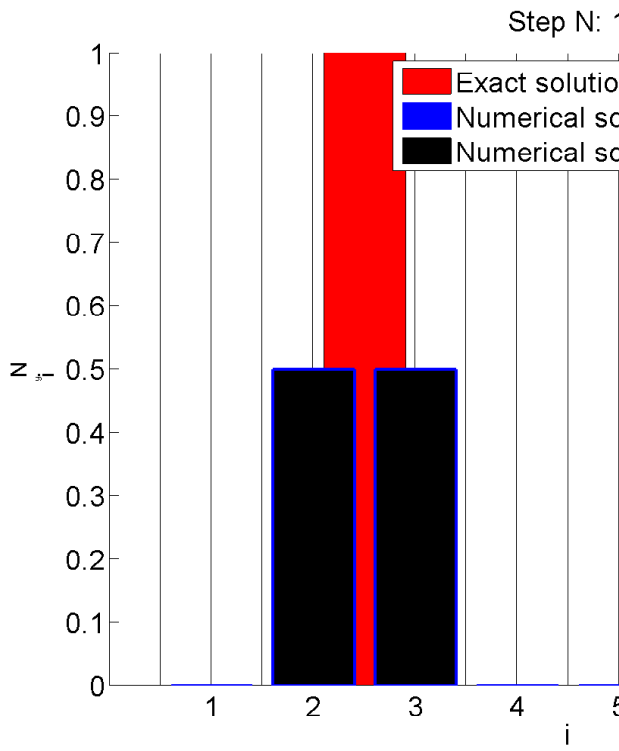
Matlab interface



Example of antidiffusion with an upstream scheme





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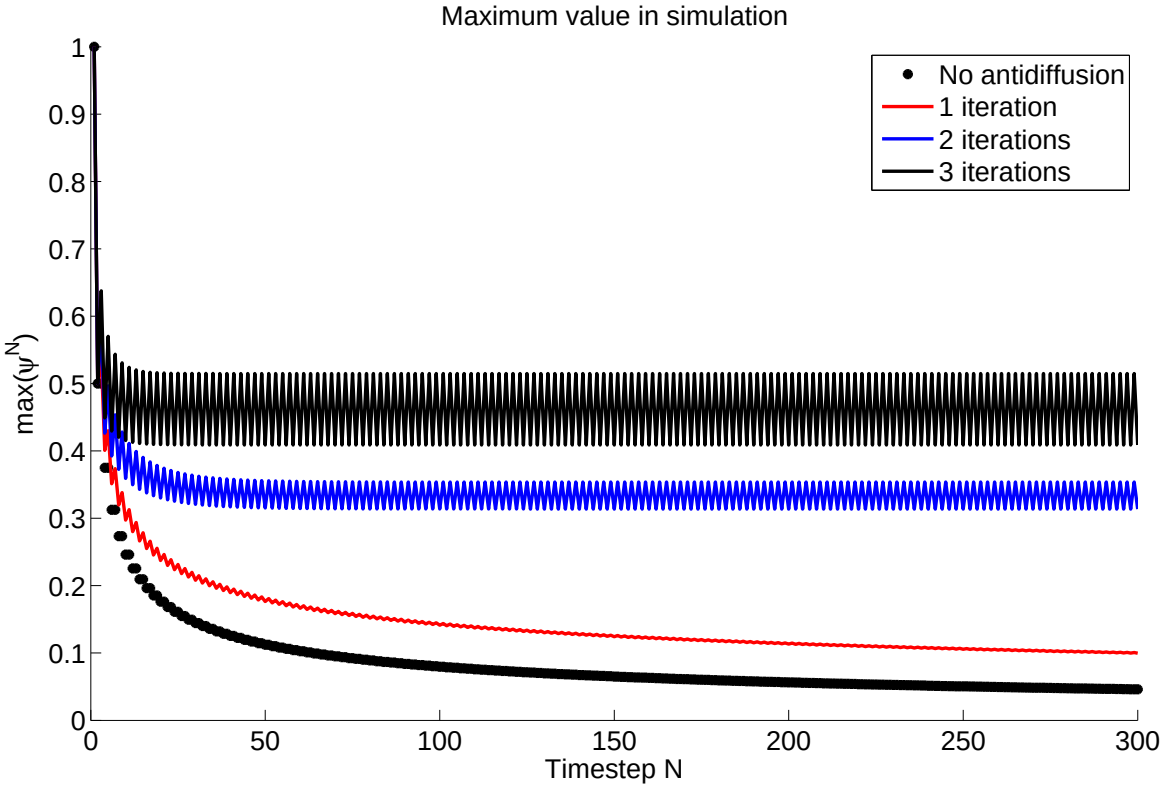
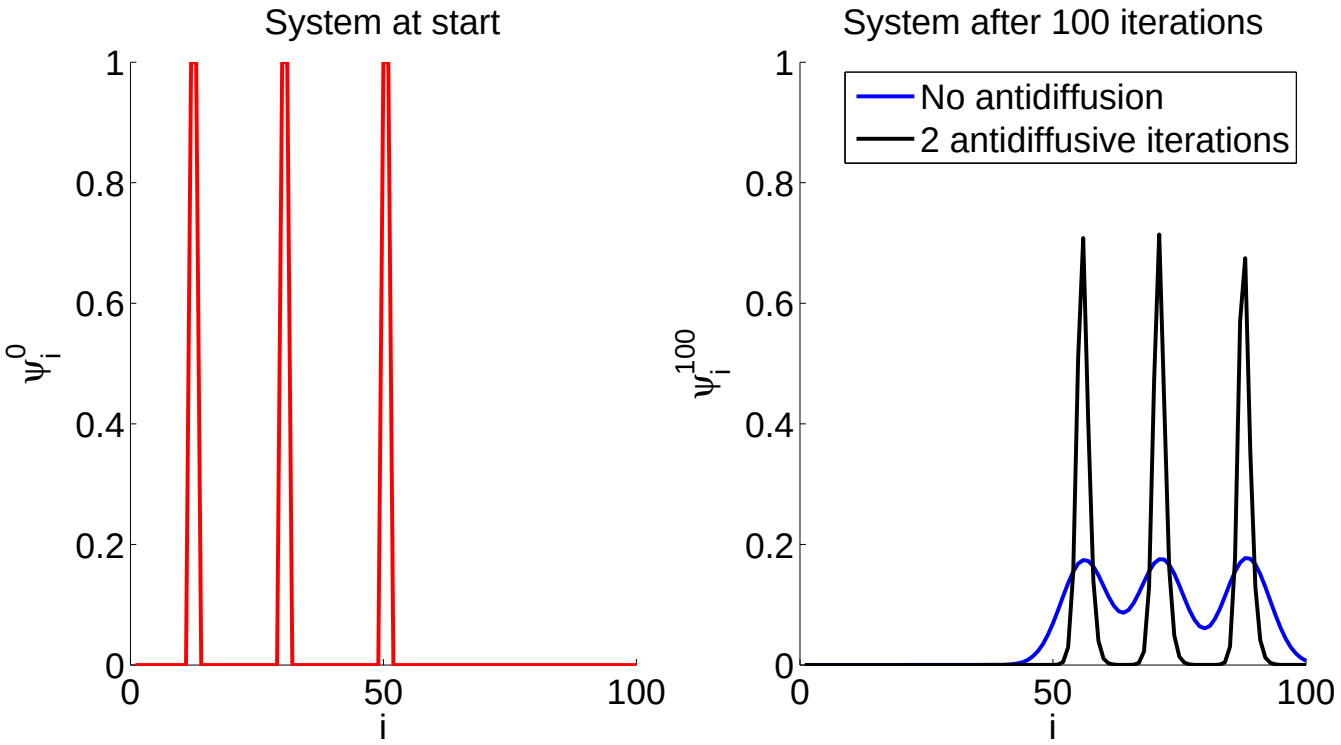
Less diffusion

Iterating with antidiffusion vector reduces diffusion.

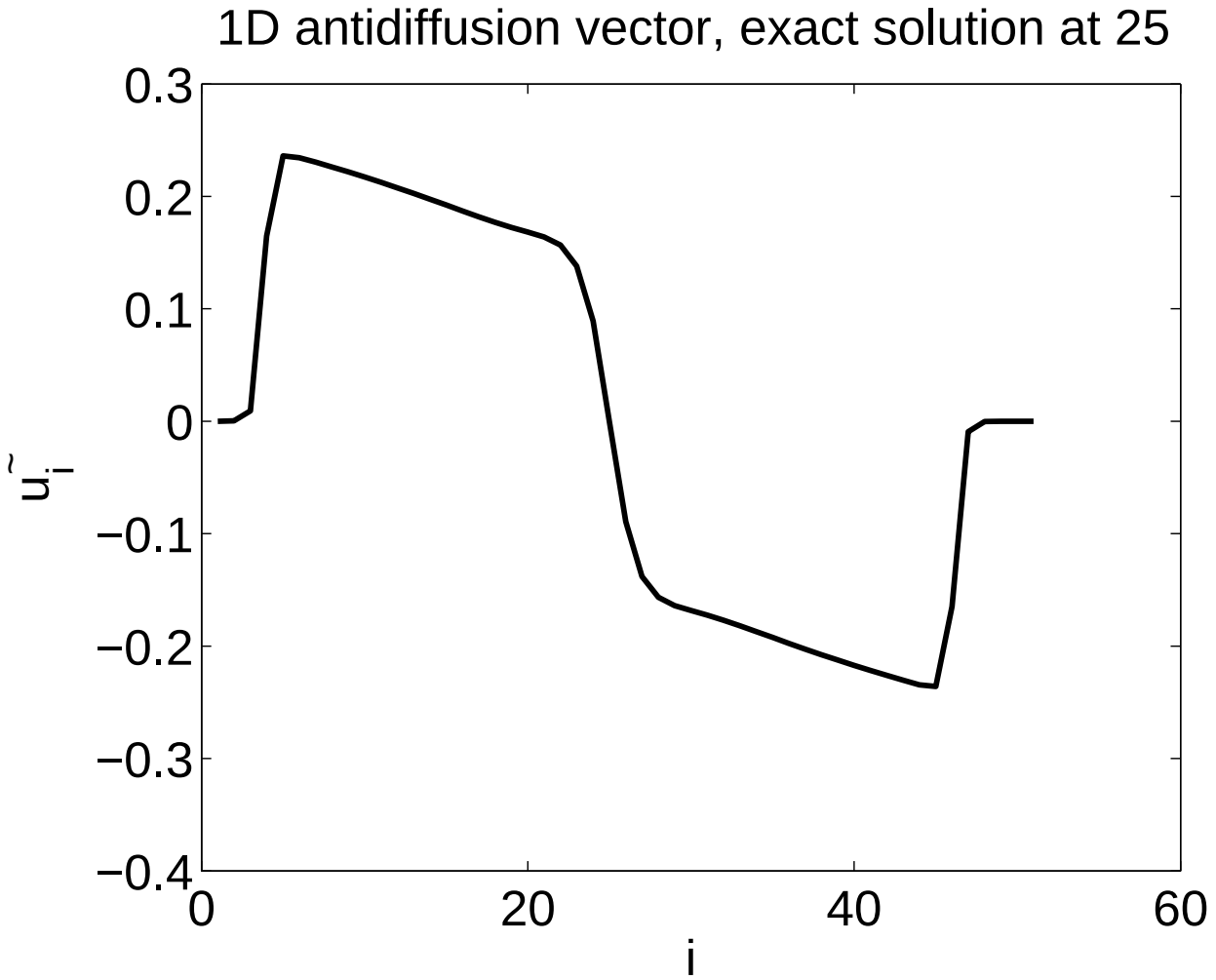


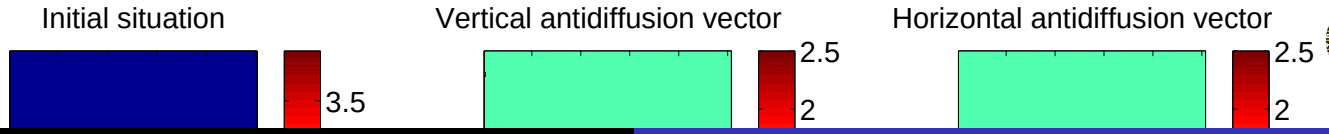
Less interaction

Simulations are more localized, less interaction between neighbouring pockets.

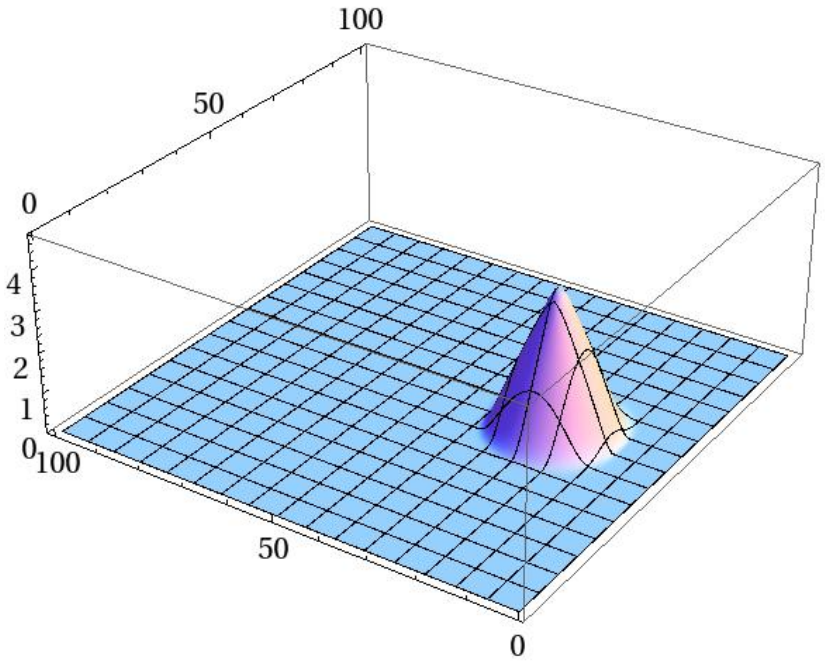


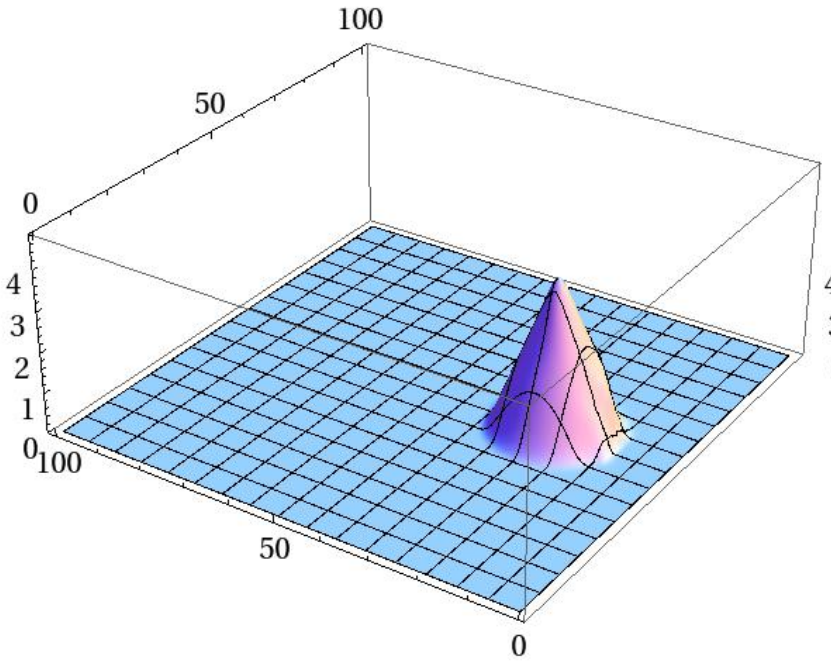
The antidiffusion vector

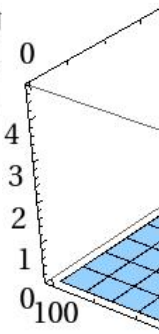




Example: solid body rotation







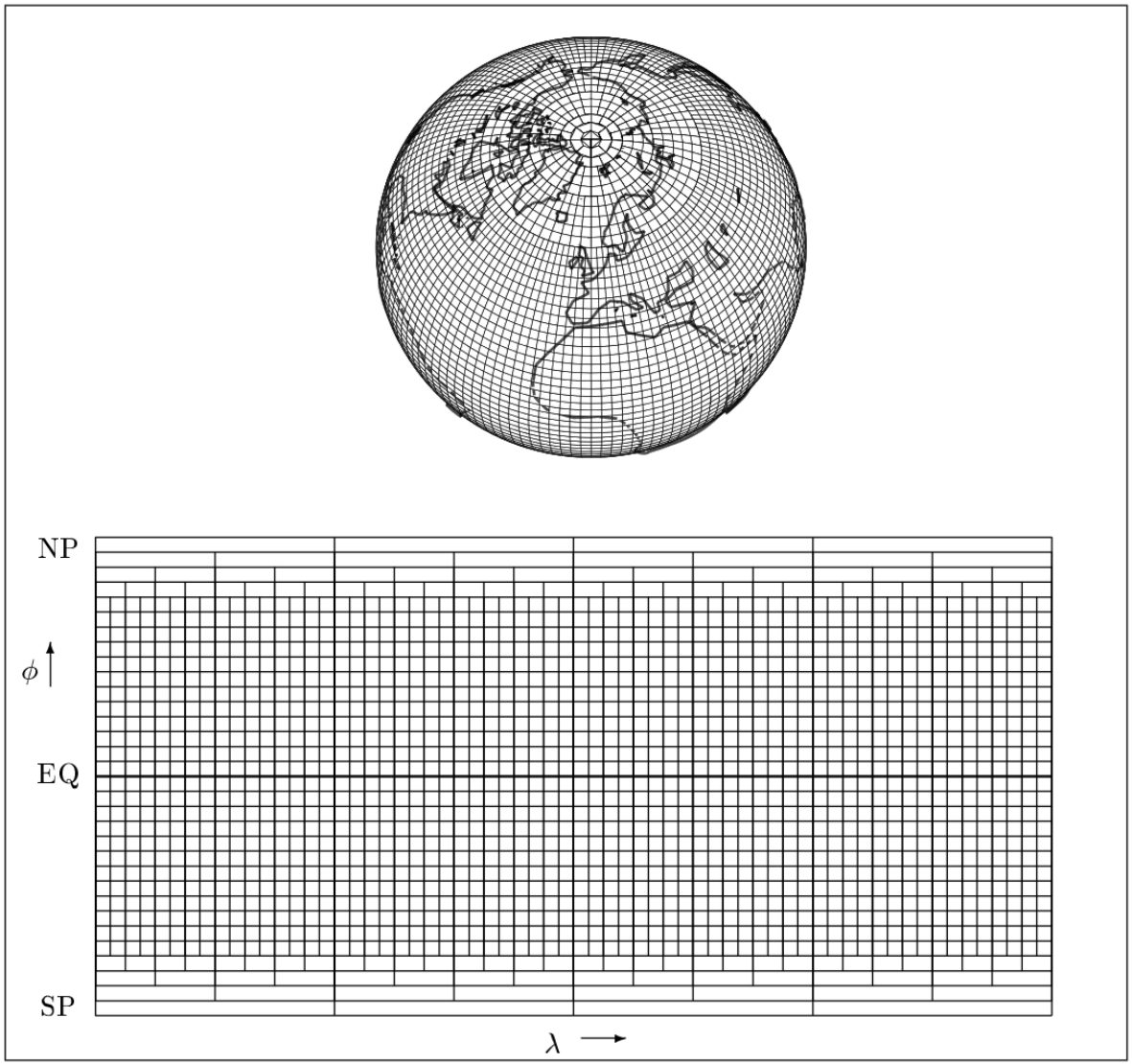
Example: solid body rotation

- Without antidiffusion, the body diffuses in one full rotation
- With antidiffusion, the body keeps its shape

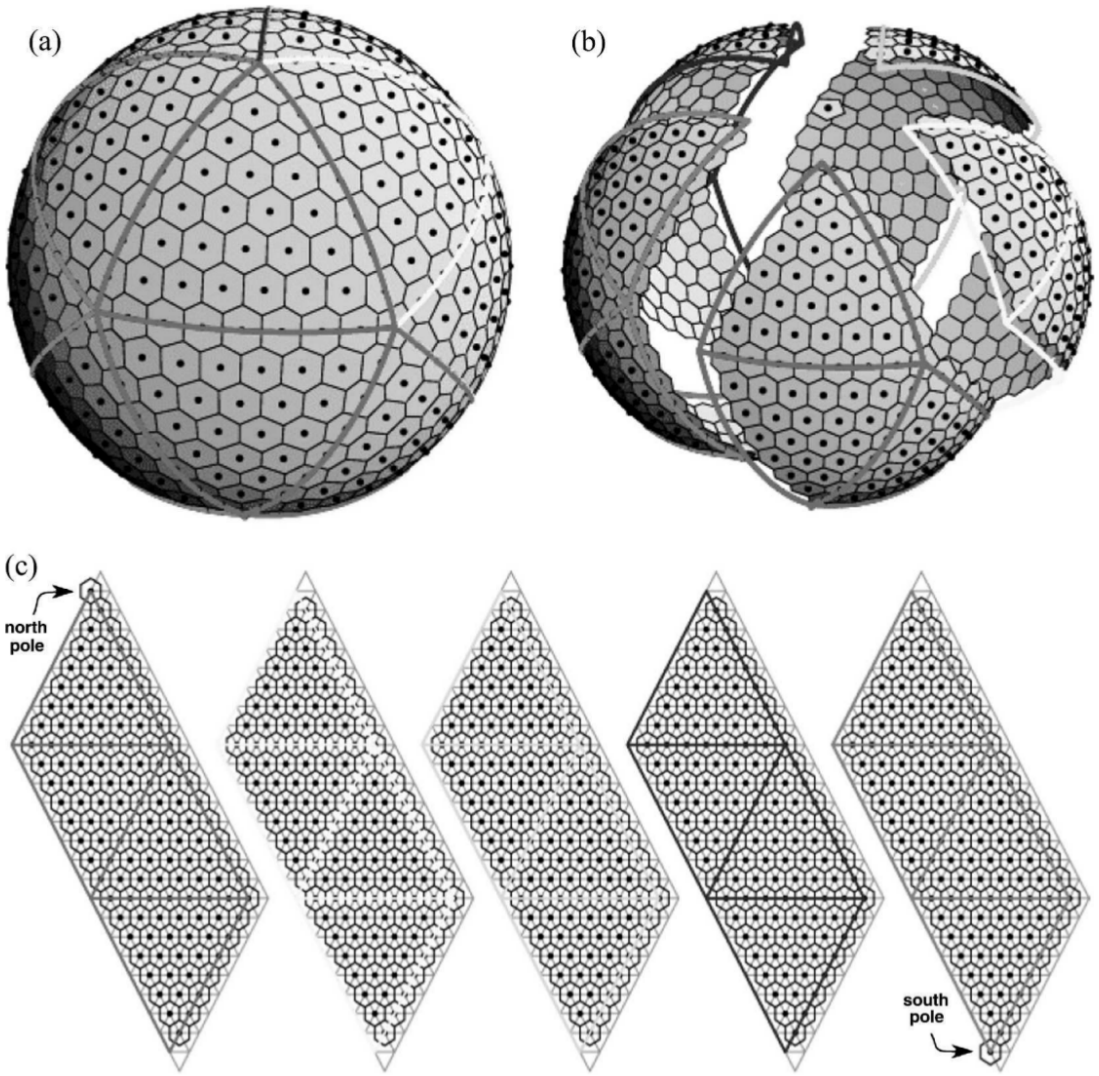
Current state of research

- Since 1983 a lot of progress has been made
- Advection calculations on the sphere pose new problems/possibilities
- Finite difference as well as finite volume methods
- Faster machines, more complex schemes
- Much higher accuracy
- Improvements by Smolarkiewicz and others

Reduced grid (Spee, 1991)



Spherical hexagonal-pentagonal grid (Lipscomb and Ringler, 2005)



MPDATA

MPDATA: Multidimensional Positive Definite Advection Transport Algorithm

- Multidimensional generalization of Smolarkiewicz' original scheme
- Widely used in finite difference form
- Recently a transition to finite volume has been made

> *Over the two decades, MPDATA evolved from an advection scheme into a class of generalized transport algorithms that expand beyond advective transport to alternate PDEs and complete fluid models with a wide range of underlying governing equations.*

Smolarkiewicz, 2005

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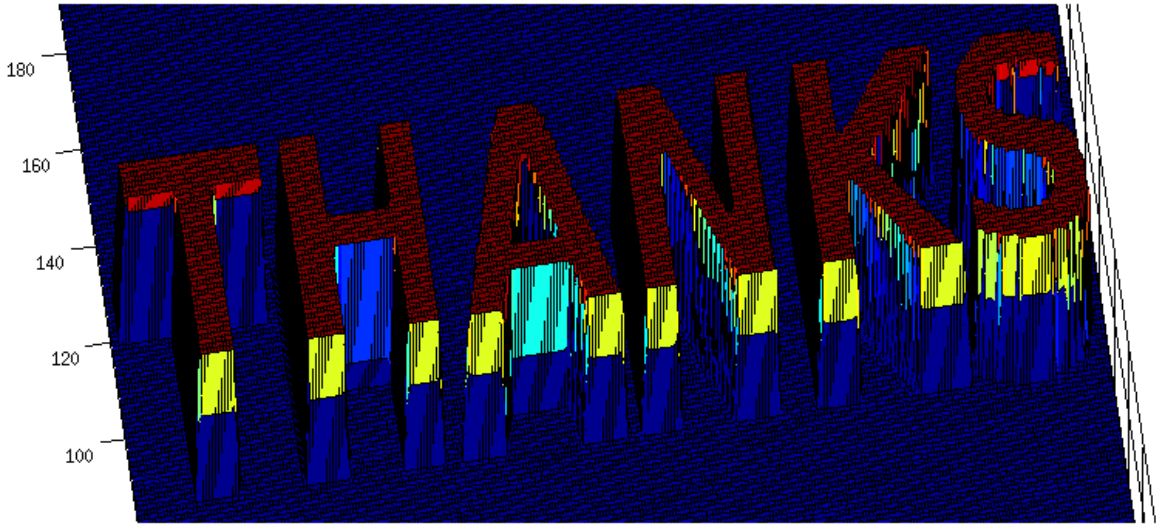
Conclusions

- Diffusion is a threat for reliable advection simulations
- Antidiffusive advection schemes reduce this threat and are thus important in SOAC
- Smolarkiewicz' relatively simple scheme already significantly improves results



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