Numerical Methods and Software for 3D-Time-Dependent Advection-Diffusion-Reaction Models

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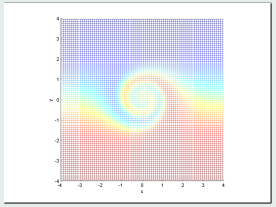

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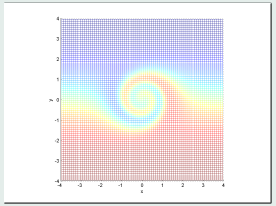
- Numerical Test: Mixing of Fronts. 
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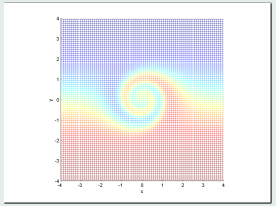
- Numerical Test: Mixing of Fronts. 

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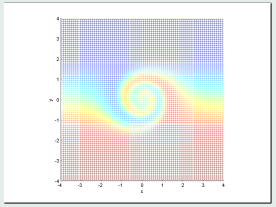
- Numerical Test: Mixing of Fronts. 
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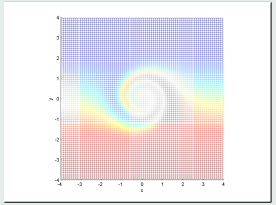
- Numerical Test: Mixing of Fronts. 
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- Conclusions.

Model Problem.

We consider the 3D time dependent ADR model

$$\frac{\partial}{\partial t}(\rho \mathbf{c}) + \nabla \cdot (\rho \mathbf{c} \mathbf{v}) - \nabla \cdot (\mathrm{D} \nabla \mathbf{c}) = \mathbf{R}(\mathbf{c}) \tag{1}$$

where $\mathbf{c} = \mathbf{c}(\mathbf{x}, t)$ with $\mathbf{c} \in \mathbb{R}^m$ and $\mathbf{x} \in \Omega \subset \mathbb{R}^3$; $\mathbf{v}(\mathbf{x}) \in \mathbb{R}^3$, and the diffusion matrix $\mathrm{D} = diag[d_{11}, d_{22}, \ldots, d_{mm}]$ are supposed to be given.

In this talk we focus on the scalar one-way wave equation

$$c_t + \sum_{s=1}^{3} (u_s c)_{x_s} = 0 \ , \tag{2}$$

with appropriate initial-boundary conditions.

Set a uniform Cartesian grid $\Omega_J \in \mathbb{R}^3$ of grid points $x_J = (j_1\Delta x_1, j_2\Delta x_2, j_3\Delta x_3)^T$, all j_s are integers. Let $c(x_J, t) \approx C_J$ and $c(x_J, t+\Delta t) \approx C_J^{\Delta t}$. We consider linear numerical schemes

$$C_J^{\Delta t} = \sum_K \gamma_K C_{J+K} \tag{3}$$

Friedrichs (1954) used the conditions:

1. $\gamma_K \geq 0$ for each coefficient;
2. $\sum_K \gamma_K = 1$;
3. $\gamma_K = 0$ except for a finite set of K in a neighbourhood of J;
4. γ_K depends Lipschitz continuously on $\mathbf{x}$.

1) and 2) imply that the solution $C_J^{\Delta t}$ is a convex combination of C_{J+K}.

3) $\Longleftarrow$ finite propagation speed.

Under the reported conditions, Friedrichs proved a bounded growth property:

$$\|C^{\Delta t}\| \leq (1 + const\Delta)\|C\| \tag{4}$$

where $\|\cdot\|$ is the discrete l^2 norm defined by

$$\|C\|^2 = \sum_J (C_J, C_J)$$

$\Delta = \min\{\Delta t, \Delta x_1, \Delta x_2, \Delta x_3\}$, and $const$ depends on the Lipschitz constant.

Example: 1D with $u > 0$, the α-scheme is

$$C_j^{\Delta t} = \gamma_{-2} C_{j-2} + \gamma_{-1} C_{j-1} + \gamma_0 C_j + \gamma_1 C_{j+1} + \gamma_2 C_{j+2} \ , \qquad (5)$$

where

$$\gamma_{-2} = -\frac{1}{2}\nu\,(1-\nu)\,\alpha \ , \qquad \gamma_{-1} = \nu\left[1 + \frac{1}{2}(1-\nu)(3\alpha - 1)\right] \ ,$$

$$\gamma_0 = 1 - \nu\left[1 + \frac{1}{2}(1-\nu)(3\alpha - 2)\right]$$

$$\gamma_1 = -\frac{1}{2}\nu(1-\nu)(1-\alpha) \ , \qquad \gamma_2 = 0 \ ,$$

and $\nu = u\Delta t/\Delta x$ is the Courant number. We get Lax-Wendroff ($\alpha = 0$), Fromm ($\alpha = 1/2$), and upwind (Warming-Beam; $\alpha = 1$). Local truncation error of α-scheme

$$\frac{1}{6}\, u\, \Delta x^2 \left[3\alpha - 1 - 3\alpha\,\nu + \nu^2\right] c_{xxx} + O\left(\Delta t^3\right) \ . \qquad (6)$$

Numerical schemes are often described as any of

- Total Variation ($\sum_{j=1}^{j_{\max}} |C_j - C_{j-1}|$) Diminishing (TVD);
- Monotone $\dfrac{\partial C_j^{\Delta t}}{\partial C_j}$ for all j;
- Monotonicity Preserving: if $C_j \geq C_{j+1}$ for all j, then $C_j^{\Delta t} \geq C_{j+1}^{\Delta t}$ for all j;
- Positive $\gamma_k \geq 0$ for all k;
- Positivity Preserving: $0 \leq \dfrac{C_j^{\Delta t} - C_j}{C_{j+1} - C_j} \leq 1$ for all j;
- Non-Oscillatory (free of spurious oscillations);
- satisfying a Maximum Principle;

though each has a slightly different meaning.

Nonlinear Schemes: Limiter Functions.

In 1959, Godunov showed that it is not possible for a linear scheme to be both higher than first order accurate and free of spurious oscillations. Early attempts to address this include:

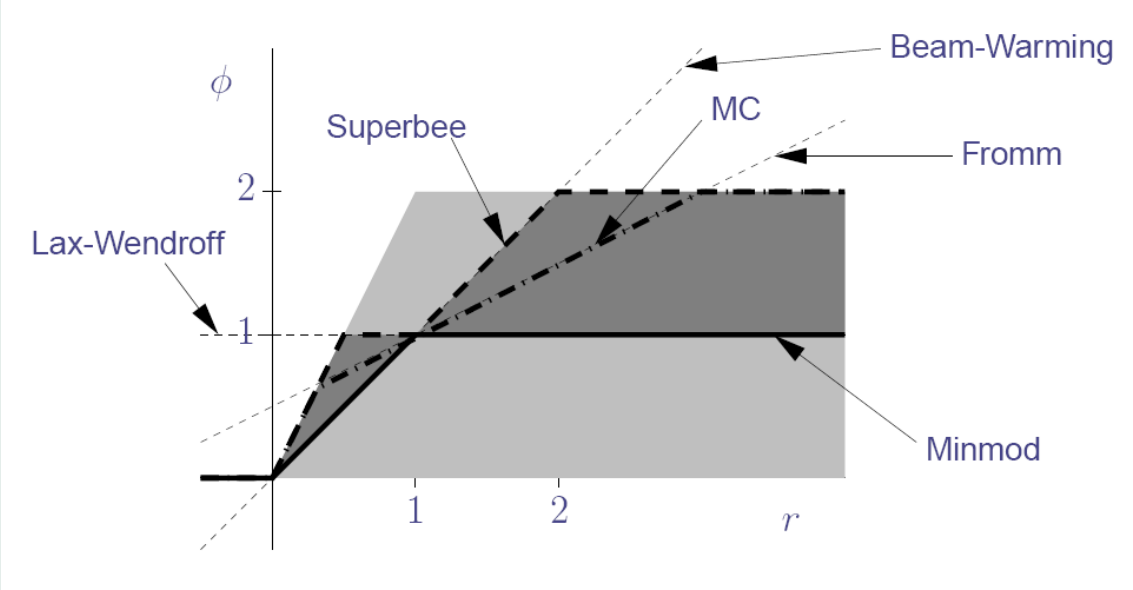
- adding artificial diffusion/viscosity;
- Flux-Corrected Transport (Boris and Book, 1973);

but the most successful (e. i. in Harten and Zwas, 1972):

- choose one low order, non-oscillatory flux and one higher order oscillatory flux,
- and weight them to get the ideal combination.

A limiter function $\phi(r)$ (r is the ratio of successive solution differences) verifies:

$$0 \leq \phi(r) \leq 2 \ , \quad \phi(r)/r = \phi\left(\frac{1}{r}\right) \ , \quad \phi(1) = 1 \ ,$$

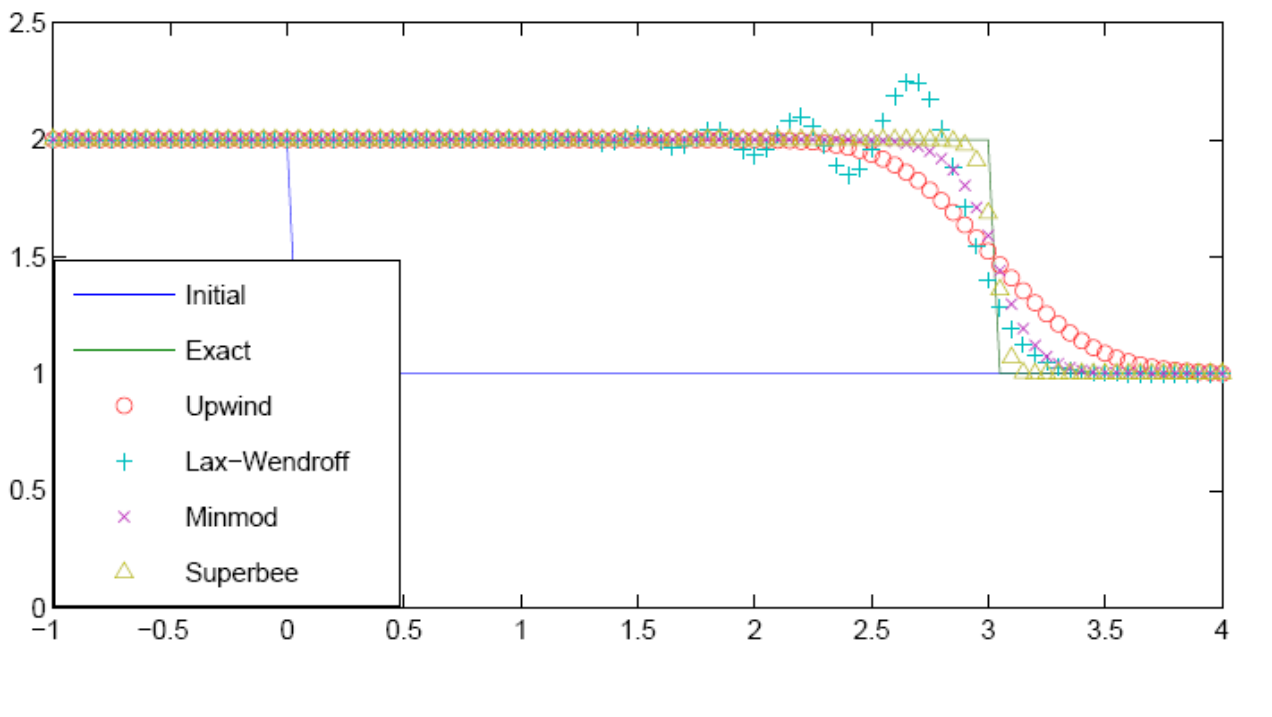


The second order TVD region of Sweby (1984) is dark-grey.

- Indeed, it's just parameter-free artificial diffusion;
- it can also be described as upwinding with additional "antidiffusion";
- For full second order accuracy the limiter should be smooth near $r = 1$;
- note that in any case we must use an appropriately small time-step ($CFL \leq 1$ usually).

The figure below contains a series of results obtained for the 1D advection equation

$$c_t + c_x = 0$$



Multi-D and Transverse Propagation.

For the sake of simplicity we consider the 2D case

$$c_t + \sum_{s=1}^{2} (u_s c)_{x_s} = 0 \ . \tag{7}$$

To grasp the multi-D context we use the Taylor formula:

$$\begin{aligned} c\left(x_1, x_2, t + \Delta t\right) &= c\left(x_1, x_2, t\right) + \Delta t c_t + \tfrac{1}{2}(\Delta t)^2 c_{tt} + \ldots \\ &= c\left(x_1, x_2, t\right) - u_1 \Delta t c_{x_1} - u_2 \Delta t c_{x_2} + \\ &+ \frac{1}{2}(\Delta t)^2 \left[u_1^2 c_{x_1 x_1} + u_1 u_2 c_{x_2 x_1} + u_2 u_1 c_{x_1 x_2} + u_2^2 c_{x_2 x_2}\right] + \ldots \end{aligned}$$

where all derivatives are evaluated at (x_1, x_2, t).

A naive multi-D scheme.

Consider the simple case $u_1 > 0$ and $u_2 > 0$

$$C_J^{\Delta t} = C_J - \nu_1 \ (C_J - C_{j_1-1}) - \nu_2 \ (C_J - C_{j_2-1})$$

where $\nu_1 = u_1 \ \frac{\Delta t}{\Delta x_1}$ and $\nu_2 = u_2 \ \frac{\Delta t}{\Delta x_2}$. Note that $C_{j_1-1 j_2-1}$ does not contribute to define the value of $C^{\Delta t}$, this is wrong for sure.

Corner-transport scheme. (Colella, 1990)

$$\begin{aligned} C_J^{\Delta t} &= C_J - \nu_1 \ (C_J - C_{j_1-1}) - \nu_2 \ (C_J - C_{j_2-1}) \\ &+ \frac{1}{2}\Delta t^2 \left\{ \frac{u_1}{\Delta x_1} \left[\frac{u_2}{\Delta x_2} (C_J - C_{j_2-1}) - \frac{u_2}{\Delta x_2} (C_{j_1-1} - C_{j_1-1 j_2-1}) \right] \right. \\ &+ \left. \frac{u_2}{\Delta x_2} \left[\frac{u_1}{\Delta x_1} (C_J - C_{j_1-1}) - \frac{u_1}{\Delta x_1} (C_{j_2-1} - C_{j_1-1 j_2-1}) \right] \right\} \end{aligned}$$

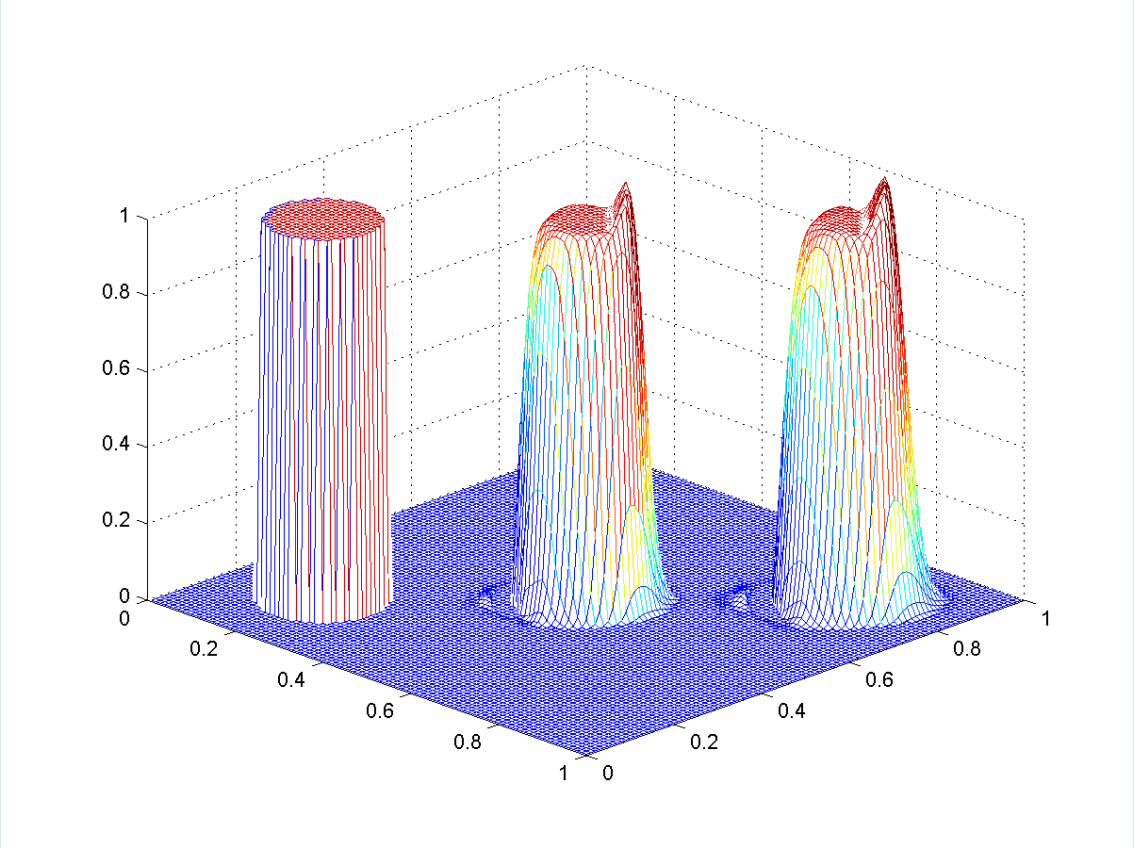


Figure 1: Naive scheme.

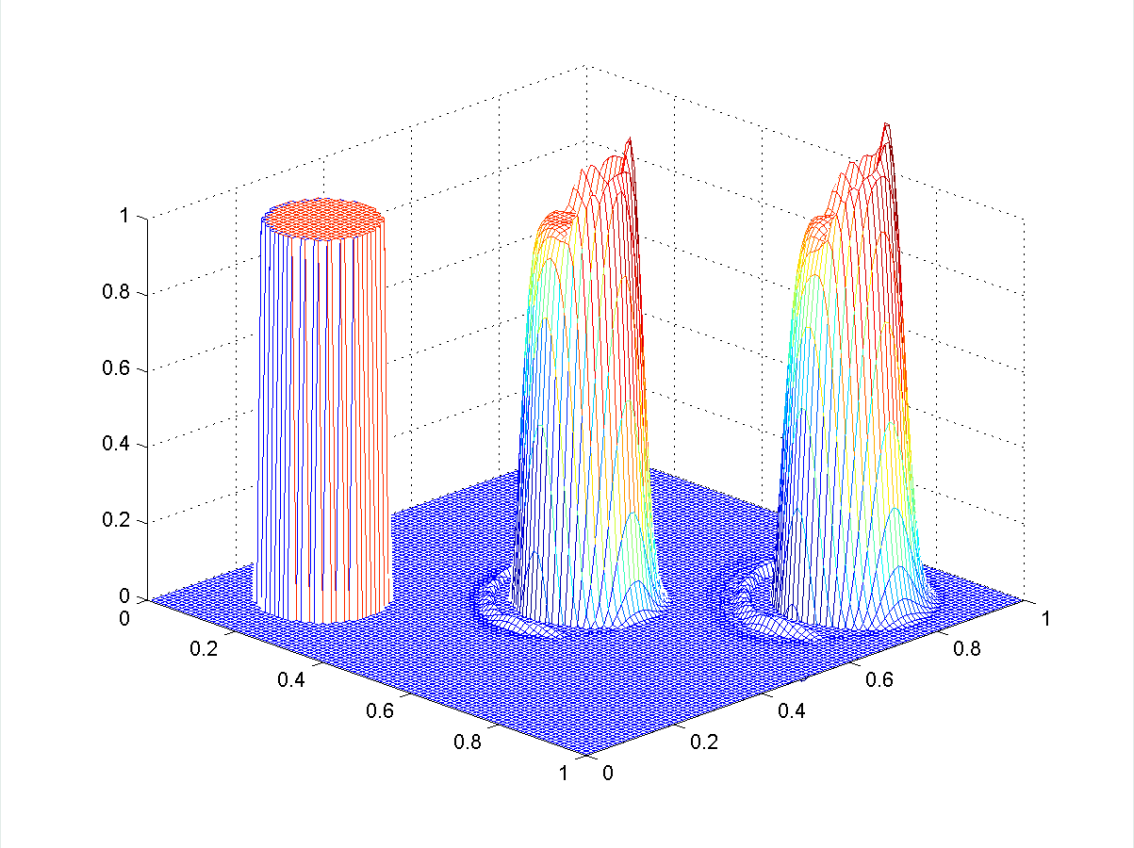


Figure 2: Corner-transport scheme without limiter.

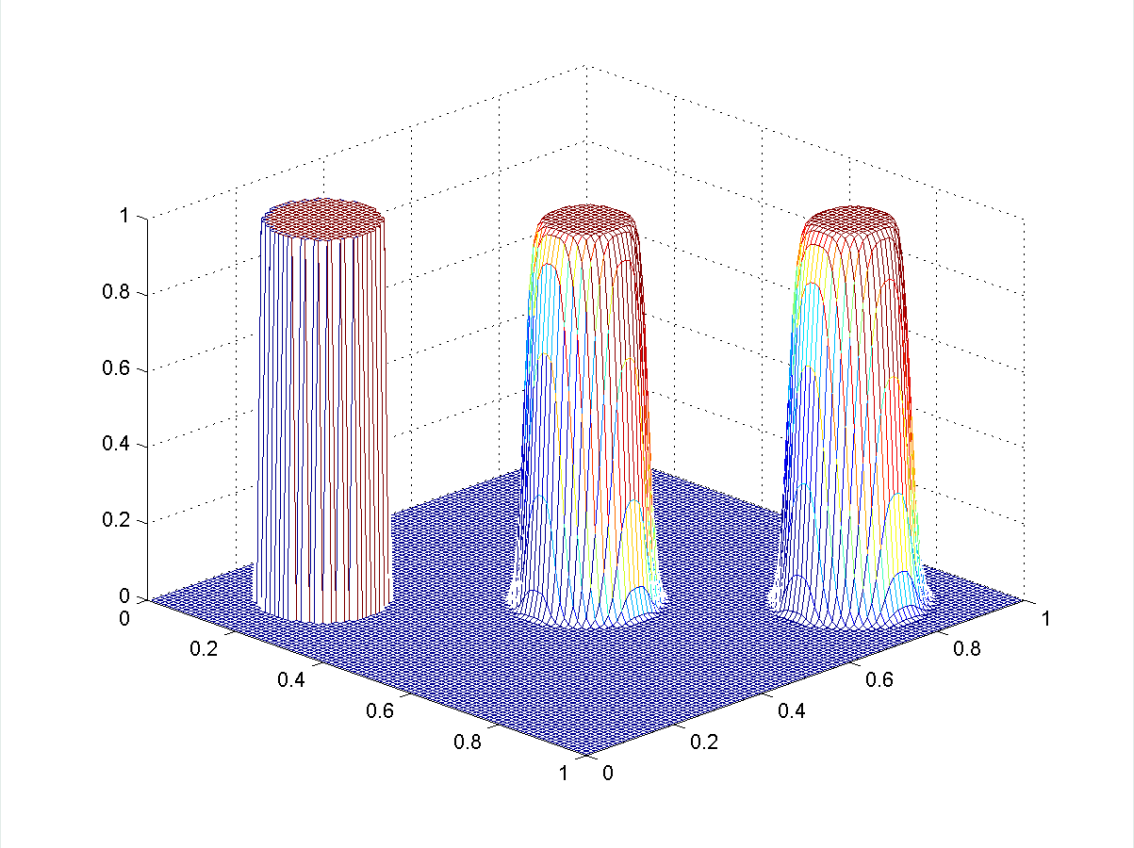


Figure 3: Corner-transport scheme with a limiter.

Stability Analysis.

von Neumann analysis use Fourier decomposition and a single arbitrary component

$$C_J = e^{i(\omega_1 j_1 \Delta x_1 + \omega_2 j_2 \Delta x_2)} \ ,$$

where i is the imaginary unit, and ω_2 and ω_2 are the x_1 and x_2 wave-numbers, respectively. Defining

$$C_J^{\Delta t} = \lambda(\Delta x_1, \Delta x_2, \Delta t) C_J$$

where $\lambda(\cdot)$ is an amplification factor. A given method is stable if

$$|\lambda| \leq 1$$

for all ω_1 and ω_2.

A naive multi-D scheme based on the 1D case have an amplification factor

$$\lambda = 1 - \nu_1 \left(1 - e^{-i\omega_1 \Delta x_1}\right) - \nu_2 \left(1 - e^{-i\omega_2 \Delta x_2}\right)$$

where $\nu_1 = u_1 \frac{\Delta t}{\Delta x_1}$ and $\nu_2 = u_2 \frac{\Delta t}{\Delta x_2}$ are 1D Courant numbers. We end up with the stability condition

$$\frac{\Delta t}{\Delta x_1} |u_1| + \frac{\Delta t}{\Delta x_2} |u_2| \leq 1 \ .$$

By taking into account the transverse propagation we have

$$\lambda = \left[1 - \nu_1 \left(1 - e^{-i\omega_1 \Delta x_1}\right)\right] \cdot \left[1 - \nu_2 \left(1 - e^{-i\omega_2 \Delta x_2}\right)\right]$$

so that for the stability

$$\max \left(\frac{\Delta t}{\Delta x_1} |u_1| \, , \frac{\Delta t}{\Delta x_2} |u_2| \right) \leq 1 \ .$$

Numerical Test: Mixing of Fronts.

Let us consider the test problem

$$c_t + (u_1\, c)_{x_1} + (u_2\, c)_{x_2} = 0$$
$$c(x_1, x_2) = \tanh\left(-0.5\, x_2\right) \ , \quad -4 \le x_1, x_2 \le 4 \qquad (8)$$
$$c(-4, x_2, t) = c(4, x_2, t) \ , \quad c(x_1, -4, t) = c(x_1, 4, t) \ ,$$

where the velocity field is given by

$$u_1(x_1, x_2) = -\omega(r)\, x_2 \ , \quad u_2(x_1, x_2) = \omega(r)\, x_1 \ , \quad r = \sqrt{x_1^2 + x_2^2}$$

and

$$\omega(r) = \frac{U(r)}{r\, U_{\max}} \ , \quad U(r) = \frac{\tanh(r)}{\cosh^2(r)} \ .$$

This problem was used by several authors to evaluate the performance of different numerical methods.

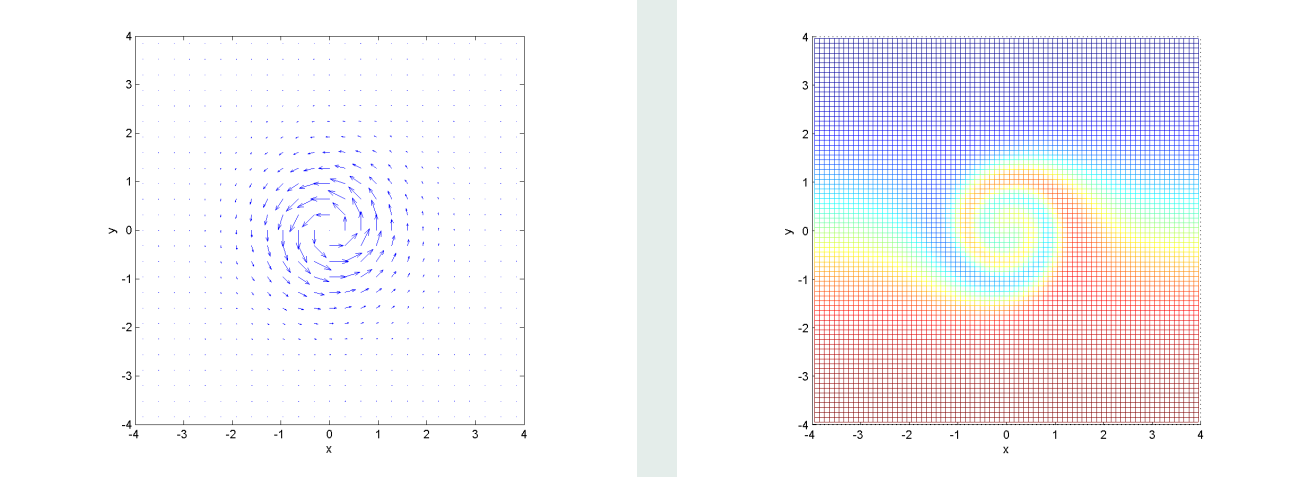
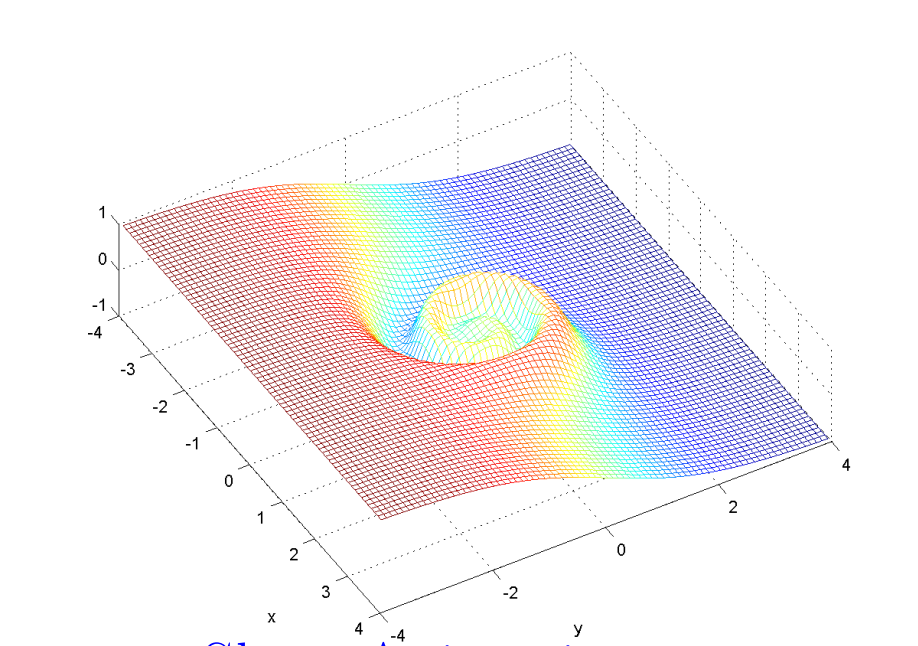


Figure 4 Left: velocity field on a 25×25 grid. Right: counter plot on a 80×80 grid.

This provides a simple model describing the mixing of cold and hot air due to the rotational velocity field which is similar to the cyclonic air motion at low pressure systems observed on the weather maps.



Show Animation.

Figure 5 Numerical solution at final time $t_{\max} = 4$ with a Courant number 0.9. We used $U_{\max} = 0.385$.

Model Problem: Diffusion Step.

Solve

$$\frac{\partial}{\partial t}(\rho c) - \nabla \cdot (D \nabla c) = 0 \ ,$$

subject to Neumann boundary conditions.

Basic idea, use the implicit Cranck-Nicolson scheme:

$$\Delta\left(c_J\right) \approx \frac{C_{j_1+1} - 2C_J + C_{j_1-1}}{\Delta x_1^2} + \frac{C_{j_2+1} - 2C_J + C_{j_2-1}}{\Delta x_2^2} + \\ + \frac{C_{j_3+1} - 2C_J + C_{j_3-1}}{\Delta x_3^2} + O[\Delta x_1^2 + \Delta x_2^2 + \Delta x_3^2]$$

Write all terms in conservation form

$$C_J^{\Delta t} - \frac{\Delta t}{2\Delta x_1 \Delta x_2 \Delta x_3} w_J^{\Delta t} = C_J - \frac{\Delta t}{2\Delta x_1 \Delta x_2 \Delta x_3} w_J$$

where

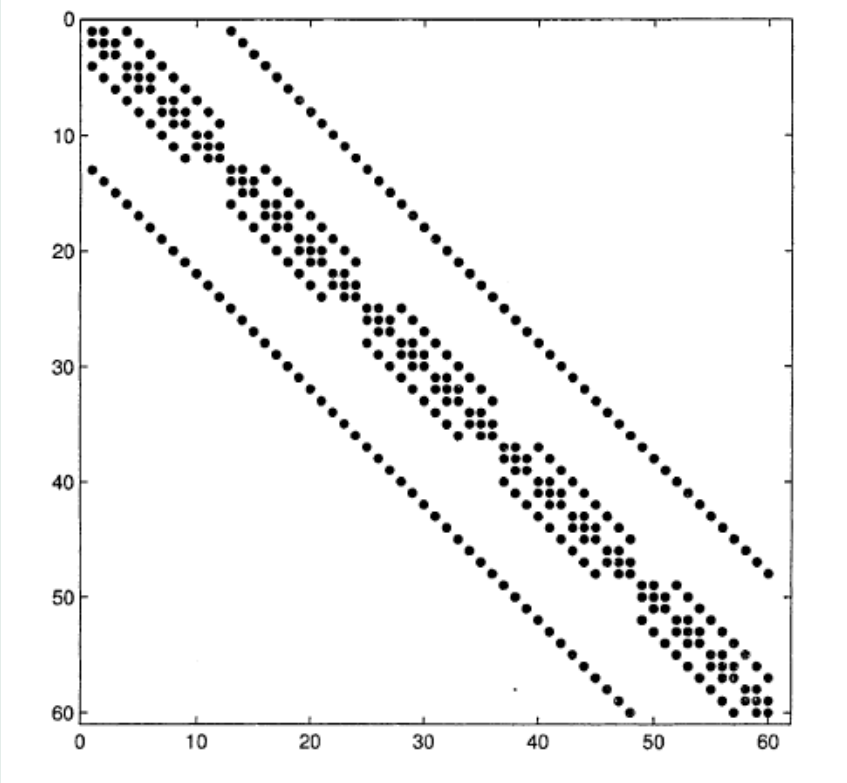
$$w_J = -\left\{\Delta x_2 \Delta x_3 \left(F_{j_1+\frac{1}{2}} - F^n_{j_1-\frac{1}{2}}\right)\right.$$
$$\left. + \Delta x_1 \Delta x_3 \left(G_{j_2+\frac{1}{2}} - G_{j_2-\frac{1}{2}}\right) + \Delta x_1 \Delta x_2 \left(H_{j_3+\frac{1}{2}} - H^n_{j_3-\frac{1}{2}}\right)\right\}$$

and

$$F_{j_1+\frac{1}{2}} = -D_{j_1+\frac{1}{2}} \frac{C_{j_1+1} - C_J}{\Delta x_1}$$

$$G_{j_2+\frac{1}{2}} = -D_{j_2+\frac{1}{2}} \frac{C_{j_2+1} - C_J}{\Delta x_2}$$

$$H_{j_3+\frac{1}{2}} = -D_{j_3+\frac{1}{2}} \frac{C_{j_3+1} - C_J}{\Delta x_3}.$$



Mass matrix for Crank-Nicolson with $3 \times 4 \times 5$ mesh points.[1]

[1] H. Van Der Vorst. SIAM J. Sci. Stat. Comput., 13:631-644,1992.

Model Problem: Reaction Step.

Solve

$$\frac{d}{dt}(\rho \mathbf{c}) = \mathbf{R}(\mathbf{c})$$

with suitable initial conditions.

Numerical methods are able to deal with stiff problems such as the following second order one-leg method, known as the implicit midpoint rule,

$$\mathbf{C}^{\Delta t} = \mathbf{C} + \Delta t \mathbf{R}\left(\frac{\mathbf{C} + \mathbf{C}^{\Delta t}}{2}\right),$$

which is A-stable.

Or in the case of stiff oscillatory phenomena the BDF2 method

$$\mathbf{C}^{\Delta t} = \frac{1}{3}\left(4\mathbf{C} - \mathbf{C}^{-\Delta t} + 2\Delta t\mathbf{R}(\mathbf{C}^{\Delta t})\right) \ ,$$

which is L-stable and G-stable.

Another method is TR-BDF2 (Tyson et al., 2000)

$$\mathbf{C}^{\frac{\Delta t}{2}} = \mathbf{C} + \frac{\Delta t}{4}\left(\mathbf{R}(\mathbf{C}) + \mathbf{R}(\mathbf{C}^{\frac{\Delta t}{2}})\right)$$

$$\mathbf{C}^{\Delta t} = \frac{1}{3}\left(4\mathbf{C}^{\frac{\Delta t}{2}} - \mathbf{C} + 2\Delta t\mathbf{R}(\mathbf{C}^{\Delta t})\right)$$

which is A-stable and L-stable, and second order accurate.

Available Software

Adaptive solver has been proposed by Blom and co-workers both for 2D (in ACM Trans. Math. Softw., 22:302-328, 1996) and 3D (in ACM Trans. Math. Softw., 22:329-347, 1996) problems.

If a Strang splitting approach has been adopted, then the software availability will be greatly increased. We can quote the CLAWPACK software developed and documented by Randy LeVeque and his collaborators. This software is freely available from the web site `www.amath.washingthon.edu/~claw/`. The interested reader may find useful to refer to the recent book by LeVeque (Cambridge University Press, 2002).

Conclusions.

1) we have presented a survey on robust, efficient, flexible and reliable schemes for the multi-D one way wave equation;

2) the *epitome* of this story is that to solve a linear problem we may need a nonlinear scheme;

3) we have not the answer to everything.