Numerical analysis of transport phenomena and hyperbolic equations using flux correction techniques.

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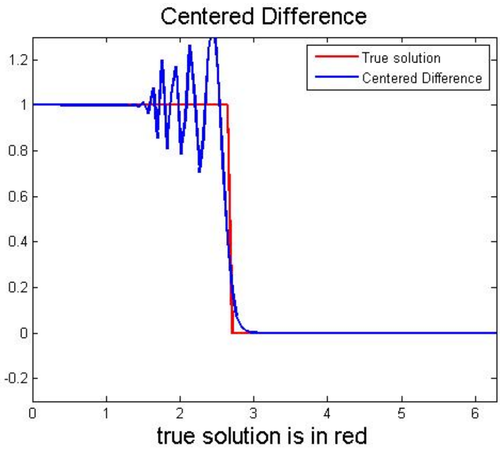
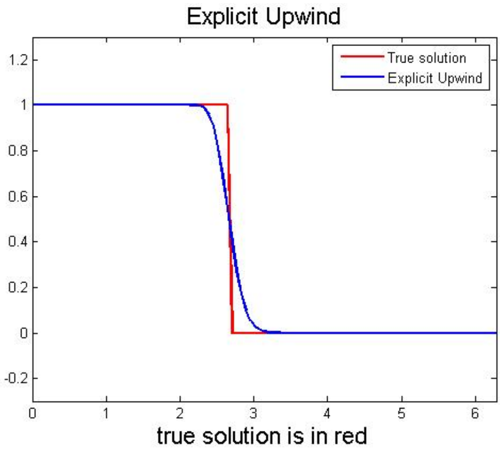
October 30, 2012

Outline

1. Transport Phenomena and Convection-Diffusion Equations.
2. Finite Difference and Finite Element Approximations in 1D.
3. Modified Equation Analysis for Explicit Time Discretizations.
4. Taylor Series Approach to Stabilization of Convective Terms.
5. Nonlinear High-Resolution Schemes Based on Flux Limiting.


Centered Difference
True solution
Centered Difference
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
1
2
3
4
5
6
true solution is in red


Explicit Upwind
True solution
Explicit Upwind
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
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1
2
3
4
5
6
true solution is in red

Introduction

- A major bottleneck in finite element simulation of transport phenomena is the instability of the standart Galerkin discretization to satisfy the relevant **maximum principles** and/or maintain positivity on general meshes.
- **Maximum principle** for transport equations yields a set of sufficient conditions that guarantee: **positivity, monotonicity and/or nonincreasing total variation**
- According to the **Godunov theorem**, a linear scheme, satisfying these constraits can be at most 1st order accurate.
- To overcome this order barrier, numerical methods for convection-dominated transport are frequently equipped with **flux or slope limiters**.

Historical background

- A variety of **stabilization techniques** have been presented in the literature so as to combat the formation of non-physical oscillations which would be generated otherwise
- The advent of nonlinear high-resolution schemes traces its origins to the **flux-corrected transport** (FCT) methodology introduced in early 1970s by *Boris and Book*
- The fully multidimensional **generalization** proposed by *Zalesak* has formed a framework for the design of FCT algorithms as a blend of high and low order approximations.

Conservation Laws

Convection and diffusion change the distribution but not the total amount of the transported material property.

Physical principles		Mathematical models
Conservation of mass	$\Longrightarrow$	Continuity equation
Newton's second law		Momentum equation
Conservation of energy		Energy equation

Scalar conservation law:

$$\frac{\partial u(x,t)}{\partial t} + \nabla f(x,t,u,\nabla u) = g(x,t,u),$$

where f is the flux function, g is the source, $\nabla = (\partial_x, \partial_y, \partial_z)$.

Generic transport equation

Flux function:

$$f = vu - d\nabla u, \Rightarrow \frac{\partial u}{\partial t} + \nabla(vu - d\nabla u) = g,$$

where $v(x,t)$ is the velocity, d is a constant diffusion coefficient.

Convective transport:

$\nabla(vu) = v\nabla u + u\nabla v$

Diffusive transport

$d\nabla^2 u$

Interplay of convection and diffusion depends on the Peclet number.

$Pe = \frac{v_0 l_0}{d}$, where v_0 is a reference velocity and l_0 is a length scale.

Useful model problems

1. Convection-diffusion:

$$\frac{\partial u}{\partial t} + \nabla v u = d\nabla^2 u \text{ in } \Omega$$

$$u(x,0) = u_0(x) \text{ in } \Omega; u = \bar{u} \text{ on } \Gamma_D; n\nabla u = 0 \text{ on } \Gamma_N;$$

2. Pure diffusion:

$$v = 0 \Rightarrow \frac{\partial u}{\partial t} = d\nabla^2 u \text{ in } \Omega$$

$$u(x,0) = u_0(x) \text{ in } \Omega; u = \bar{u} \text{ on } \Gamma_D; n\nabla u = 0 \text{ on } \Gamma_N;$$

3. Pure convection:

$$d = 0 \Rightarrow \frac{\partial u}{\partial t} + \nabla v u = 0 \text{ in } \Omega$$

$$u(x,0) = u_0(x) \text{ in } \Omega; u = \bar{u} \text{ on } \Gamma_{in} = \{x \in \Gamma : vn < 0\}$$

Numerical methods: finite differences, finite volumes, **finite elements**.

Numerical solutions

- The numerical solution of such problems is a highly challenging task since the computation may cause significant **conservation errors** and/or numerical instabilities.
- This deficiency manifests itself in spurious undershoots and overshoots.
- As a consequence, the transported quantities (temperature, concentration) may assume nonphysical values.

Key idea:

to use high-order approximation in regions where the solution varies smoothly and a **nonoscillatory** low-order scheme elsewhere.

Ingredients

- A **high-order approximation** which may fail to possess the desired properties;
- A **low-order** approximation which does enjoy these properties but is less accurate;
- A way to **decompose the difference** between the above into a sum of skew-symmetric internodal fluxes which can be manipulated without violating mass conservation;
- A cost-effective **mechanism for adjusting** these antidiffusive fluxes in an adaptive fashion so that the imposed constraints are satisfied for a given solution.

Numerical diffusion

Pure convection:

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0; \quad u(x,t) = u_0(x - vt)$$

Backward difference scheme: $\frac{u_i^{n+1} - u_i^n}{\Delta t} + v\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 \Leftrightarrow$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + v\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \frac{v\Delta x}{2}\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

Is equivalent to the central difference approximation of the convection-diffusion equation:

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \left(\frac{v\Delta x}{2}\right)\frac{\partial^2 u}{\partial x^2}, \quad \epsilon = \frac{v\Delta x}{2} \text{ vanishes as } \Delta x \to 0$$

Modified equations

The **modified equation** is the PDE that is actually solved when a given numerical scheme is applied. (Warming and Hyett, 1974).

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \sum_{p=1}^{\infty} \mu_{2p} \frac{\partial^{2p} u}{\partial x^{2p}} + \sum_{p=1}^{\infty} \mu_{2p+1} \frac{\partial^{2p+1} u}{\partial x^{2p+1}}$$

- The right hand side of ME represents the truncation error
- Even derivatives⇒ amplitude errors (numerical diffusion)
- Odd derivatives⇒ phase errors (numerical dispersion)

Stability condition:

$$\mu_2 > 0, \text{ sign } \mu_{2p} = - \text{ sign } \mu_{2p-2}$$

Stabilization techniques

Interim summary

- central difference/Galerkin approximation works well for small Pe
- numerical instabilities/spurious wiggles to be expected at large Pe
- numerical diffusion makes the scheme more robust but less accurate
- explicit schemes must satisfy the CFL stability condition $\Delta t < \frac{\Delta x}{\Delta v}$

Stabilized high-order schemes

- add some artificial diffusion **in the streamline direction**
- use an **upwind-biased discretization** of the convective term
- use **modified test functions** in the variational formulation
- use a time-stepping scheme that provides extra stability

Lax - Wendroff method

Taylor series expansion: $u^{n+1} = u^n + \Delta t u_t^n + \frac{(\Delta t)^2}{2} u_{tt}^n + O(\Delta t)^3$

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0 \quad \Rightarrow u_t = -vu_x, \quad u_{tt} = -v(u_t)_x = v^2 u_{xx}$$

Time discretization: $u^{n+1} = u^n - v\Delta t u_x^n + \frac{(v\Delta t)^2}{2} u_{xx}^n + O(\Delta t)^3$

Lax-Wendroff/central difference scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + v\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \frac{(v\Delta t)^2}{2}\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

- second-order term in the Taylor series makes scheme stable
- numerical diffusion coefficient $\epsilon = \frac{(v\Delta t)^2}{2}$ vanishes as $\Delta t \to 0$

Classical FCT methodology

The basic idea behind:

1. Advance the solution in time by a low-order scheme that incorporates enough **numerical diffusion** to suppress undershoots and overshoots.
2. Correct the solution using **antidiffusive fluxes** limited in such a way that no new maxima or minima can form and existing extrema cannot grow.

- **Numerical diffusion** $\Rightarrow$ enforces **the positivity constraint**, provides **phase accuracy**.
- Limited **antidiffusive correction** $\Rightarrow$ reduces **amplitude errors** in a local extrema diminishing manner.

Modern high-resolution schemes

Hyperbolic conservation law

$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$, where $f = vu$, - convective flux

Conservative difference scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{f_{i+1/2}^n - f_{i-1/2}^n}{\Delta x} = 0, \quad f_{i+1/2} \approx vu(x_{i+1/2})$$

- $f_{i+1/2}^L = v\frac{u_{i+1}+u_i}{2} - |v|\frac{u_{i+1}-u_i}{2}$, – upwind difference scheme
- $f_{i+1/2}^H = v\frac{u_{i+1}+u_i}{2} - \left(\frac{v^2 \Delta t}{2}\right)\frac{u_{i+1}-u_i}{\Delta x}$, – Lax-Wendroff method

Combination of high and low order fluxes

$$f_{i+1/2} = f_{i+1/2}^L + \alpha_{i+1/2}[f_{i+1/2}^H - f_{i+1/2}^L], \quad 0 \le \alpha_{i+1/2} \le 1$$

Flux Corrected Transport (FCT)

Classical FCT algorithm: (Boris and Book, 1972)

1. Compute the transported and diffused solution:

$$u_i^L = u_i^n - \frac{\Delta t}{\Delta x}[f_{i+1/2}^L - f_{i-1/2}^L]$$

2. Evaluate the raw antidiffusive fluxes given by:

$$f_{i+1/2}^{AD} := f_{i+1/2}^H - f_{i+1/2}^L$$

3. Apply the solution dependent correction factors:

$$\bar{f}_{i+1/2}^{AD} = \alpha_{i+1/2} f_{i+1/2}^{AD}$$

4. Compute the flux-corrected end-of-step solution:

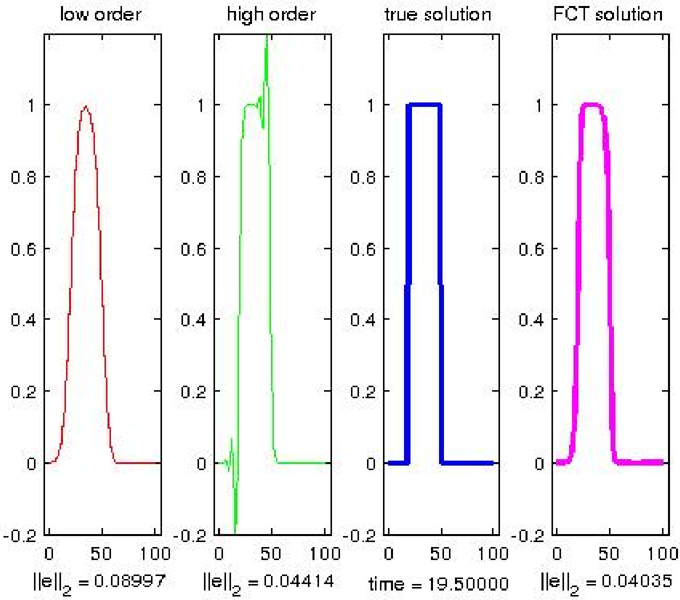
$$u_i^{n+1} = u_i^L - \frac{\Delta t}{\Delta x}[\bar{f}_{i+1/2}^{AD} - \bar{f}_{i-1/2}^{AD}]$$

Criterion: no new extrema, no enhancement of already existing ones.

$$u_i^{max} = \max\{u_{i-1}^L, u_i^L, u_{i+1}^L\}, \qquad u_i^{min} = \min\{u_{i-1}^L, u_i^L, u_{i+1}^L\}$$

- maximum increment: $P_i^+ = \max\{0, f_{i-1/2}^{AD}\} - \min\{0, f_{i+1/2}^{AD}\}$
- upper bound: $Q_i^+ = \frac{\Delta x}{\Delta t}(u_i^{max} - u_i^L), \quad R_i^+ = \min\{1, \frac{Q_i^+}{P_i^+}\}$
- minimum increment: $P_i^- = \min\{0, f_{i-1/2}^{AD}\} - \max\{0, f_{i+1/2}^{AD}\}$
- lower bound: $Q_i^- = \frac{\Delta x}{\Delta t}(u_i^{min} - u_i^L), \quad R_i^- = \min\{1, \frac{Q_i^-}{P_i^-}\}$

Correction factors: $\alpha_{i+1/2} = \begin{cases} \min\{R_{i+1}^+, R_i^-\} & \text{if } f_{i+1/2}^{AD} \geq 0 \\ \min\{R_{i+1}^-, R_i^+\} & \text{if } f_{i+1/2}^{AD} < 0 \end{cases}$


low order
high order
true solution
FCT solution
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
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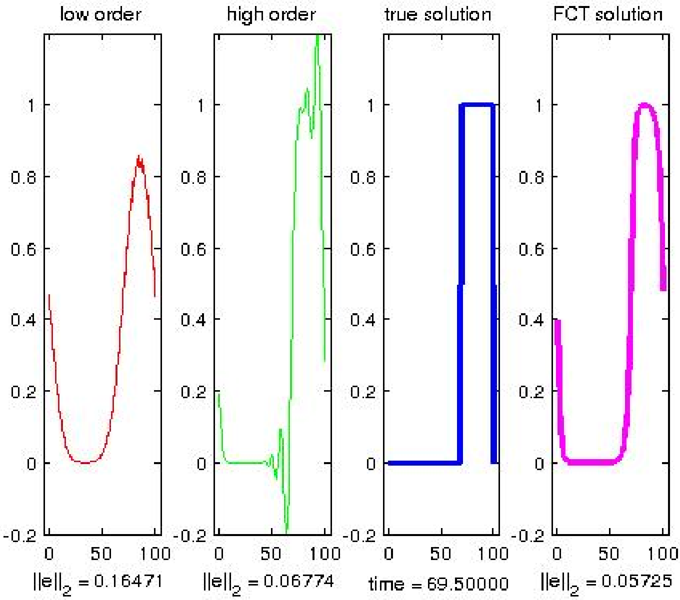
||e||2 = 0.04414
time = 19.50000
||e||2 = 0.04035


low order
high order
true solution
FCT solution
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
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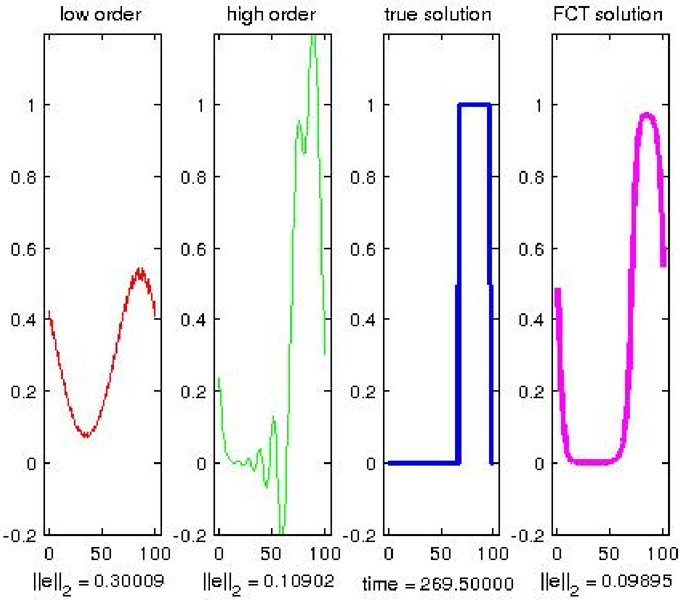
low order
high order
true solution
FCT solution
1
0.8
0.6
0.4
0.2
0
-0.2
0
50
100
||e||2 = 0.30009
||e||2 = 0.10902
time = 269.50000
||e||2 = 0.09895

Summary and Outlook

Topics covered

- Explicit finite differences and finite elements approximations in 1D
- Modified equation approach to evaluation of numerical scheme
- High resolution schemes based on classical FCT algorithm

Results obtained

- MatLab implementation of algorithms
- Verification of the state-of art results for high-resolution schemes
- Comparative study of various numerical approaches
- Multidimensional numerical solutions for standard schemes

Literature

1. Boris, J. P., Book, D. L., Flux Corrected Transport I, 1973, SHASTA, a fluid transport algorithm that works, J. Comput. Phys., 11, pp.38-69.
2. Kuzmin, D. A guide to numerical methods for transport equations.
3. LeVeque, R. J, Numerical methods for conservation laws, Lectures in mathematics, ETH, Zurich.