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Implicit flux-corrected transport algorithm for finite element simulation of the compressible Euler equations

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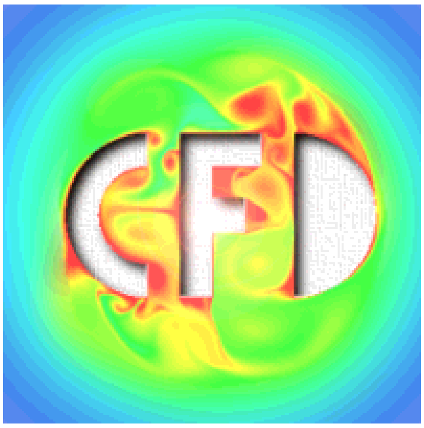


- State of the art
- Discrete approach to 'upwinding'
- Nonlinear FEM-FCT formulation
- Unified limiting strategy
- Numerical examples in 2D

Compressible Euler equations

Governing equation

$$\frac{\partial U}{\partial t} + \frac{\partial F^x}{\partial x} + \frac{\partial F^y}{\partial y} + \frac{\partial F^z}{\partial z} = 0$$

Conservative variables and fluxes

$$U = \begin{bmatrix} \rho \\ \rho v^x \\ \rho v^y \\ \rho v^z \\ E \end{bmatrix}, \quad F^d = \begin{bmatrix} \rho v^d \\ \rho v^x v^d + p\delta_{xd} \\ \rho v^y v^d + p\delta_{yd} \\ \rho v^z v^d + p\delta_{zd} \\ v^d(E+p) \end{bmatrix}$$

Equation of state (for a polytropic gas)

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho||\mathbf{v}||_2^2$$

Quasi-linear formulation

$$\frac{\partial U}{\partial t} + A^x \frac{\partial U}{\partial x} + A^y \frac{\partial U}{\partial y} + A^z \frac{\partial U}{\partial z} = 0, \quad A^d = \frac{\partial F^d}{\partial U}$$

Mathematical challenges:
hyperbolicity, nonlinearity, strong coupling

State of the art: scalar convection

Godunov Theorem (1959)

No linear discretization scheme of order higher than first is monotonicity preserving :-(

- High-order methods: oscillatory
- Low-order methods: overdiffusive
- High-resolution methods: nonlinear

Flux-Corrected Transport algorithm

Boris and Book (1973), Zalesak (1979)

1. Compute a *transported and diffused* solution by a linear monotonicity-preserving scheme
2. Invoke *flux limiter* to determine the percentage of artificial diffusion which can be removed without generating oscillations
3. Add (limited) compensating *antidiffusion* to recover the high accuracy in smooth regions

Finite element FCT procedure

Löhner *et al.* (1987)

Given u^n at time t^n:

step 1: High-order finite element scheme

$$M_C u^H = M_C u^n + R$$

step 2: Low-order finite element scheme

$$M_L u^L = [(1 - c_d) M_L + c_d M_C]\, u^n + R$$

step 3: Antidiffusive Element Contributions

$$F_e = M_L^{-1}\Big|_e \left[\hat{M}_L - \hat{M}_C\right] ((c_d - 1)\hat{u}^n + \hat{u}^H)$$

step 4: Zalesak's limiter

$$F_e^* = \alpha_e F_e, \quad 0 \le \alpha_e \le 1$$

step 5: Element-by-element correction

$$u_i^{n+1} = u_i^L + \sum_e F_{e,i}^*$$

Remarks:

– CFL restriction due to explicit time stepping
– formulation in terms of AEC rather than fluxes
– arbitrarily chosen constant artificial diffusion

Discrete positivity criteria

Lemma

A discrete scheme of the form

$$Lu^{n+1} = Ru^n, \quad u^n \geq 0$$

is positivity-preserving if L is an **M-matrix** and all entries of R are non-negative.

Galerkin discretization	Low-order counterpart
$M_C \frac{du}{dt} = K^H u$	$M_L \frac{du}{dt} = K^L u$

Discrete diffusion operators

$$d_{ij} = d_{ji}, \quad \sum_j d_{ij} = \sum_i d_{ij} = 0$$

$$(Du)_i = \sum_j d_{ij} u_j = \sum_{j \neq i} d_{ij}(u_j - u_i) = \sum_{j \neq i} f_{ij}$$

$$f_{ij} = d_{ij}(u_j - u_i), \quad f_{ji} = -f_{ij}$$

Adaptive artificial diffusion $\qquad K^L = K^H + D$

$$d_{ij} = d_{ji} = \max\left\{0, -k_{ij}^H, -k_{ji}^H\right\}, \quad d_{ii} = -\sum_{k \neq i} d_{ik}$$

Admissible time steps

$$\Delta t \leq \frac{1}{1-\theta} \min_i \left\{-m_i/k_{ii}^L \mid k_{ii}^L < 0\right\}$$

Example: 'upwind'

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0, \qquad v > 0$$

Element matrices

$$\hat{M}_L = \frac{\Delta x}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \hat{K}^H = \frac{v}{2}\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$$

$$\boxed{\frac{du_i}{dt} = -v\frac{u_{i+1}-u_{i-1}}{2\Delta x} \qquad \textit{(central difference)}}$$

Low-order operator

$$\hat{D} = \frac{v}{2}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \Rightarrow \hat{K}^L = v\begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}$$

$$\boxed{\frac{du_i}{dt} = -v\frac{u_i-u_{i-1}}{\Delta x} \qquad \textit{(upwind difference)}}$$

Positivity condition

$$v\frac{\Delta t}{\Delta x} \leq \frac{1}{1-\theta}$$

Flux-based FEM-FCT formulation

Kuzmin, Turek (2002)

Galerkin θ-scheme

$$\left[M_L - \theta\Delta t K^L\right] u^H = \left[M_L + (1-\theta)\Delta t K^L\right] u^n + F(u^H, u^n)$$

Flux decomposition for antidiffusive terms

$$\begin{aligned} F(u^H, u^n) &= -\left[(M_C - M_L) + \theta\Delta t \left(K^L - K^H\right)\right] u^H \\ &+ \left[(M_C - M_L) - (1-\theta)\Delta t \left(K^L - K^H\right)\right] u^n \end{aligned}$$

$$F(u^H, u^n) = \sum_{j\neq i} f_{ij}, \qquad F^*(u^H, u^n) = \sum_{j\neq i} \alpha_{ij} f_{ij}$$

$$\begin{aligned} f_{ij} &= -(m_{ij} + \theta\Delta t d_{ij})(u_j^H - u_i^H) \\ &+ (m_{ij} - (1-\theta)\Delta t d_{ij})(u_j^n - u_i^n) \end{aligned} \qquad \begin{aligned} f_{ji} &= -f_{ij} \\ i &\neq j \end{aligned}$$

Implicit FEM-FCT algorithm

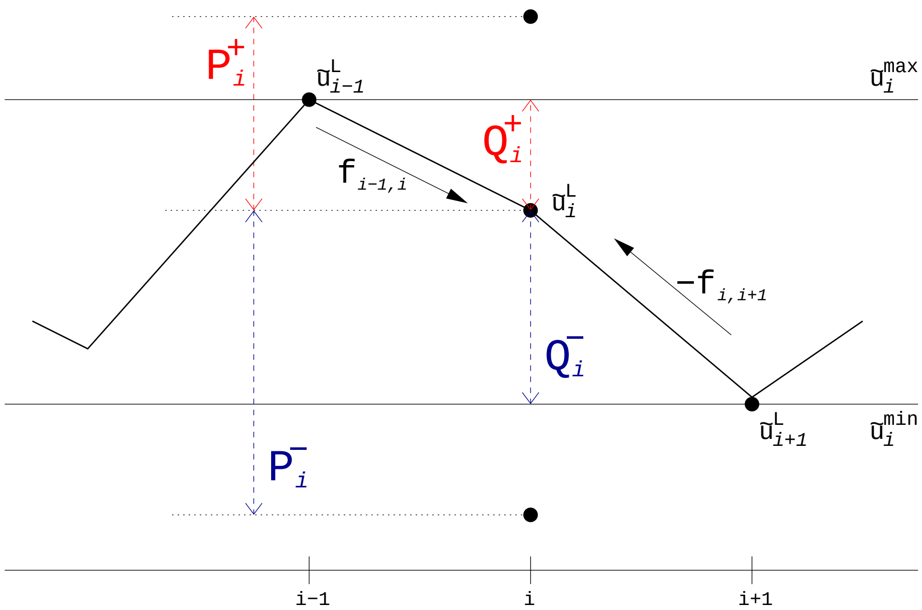
$$[M_L - \theta\Delta t K^L] u^{n+1} = M_L \tilde{u} + F^*(u^H, u^n)$$

Intermediate solution $\quad \tilde{u} = u^L(t^{n+1-\theta})$

$$M_L \tilde{u} = [M_L + (1-\theta)\Delta t K^L] u^n$$

Zalesak's limiter

Prelimiting: $f_{ij} := 0, \quad \text{if} \quad f_{ij}(\tilde u_i - \tilde u_j) < 0$



Auxiliary quantities

$$P_i^\pm = \frac{1}{m_i} \sum_{j \neq i} \max_{\min} \{0, f_{ij}\}, \qquad Q_i^\pm = \tilde u_i^{\max/\min} - \tilde u_i$$

$$R_i^\pm = \begin{cases} \min\{1, Q_i^\pm / P_i^\pm\}, & \text{if } P^+ > 0 > P^- \\ 0, & \text{if } P_i^\pm = 0 \end{cases}$$

Correction factors

$$\alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\}, & \text{if } f_{ij} \geq 0 \\ \min\{R_j^+, R_i^-\}, & \text{if } f_{ij} < 0 \end{cases}, \quad \alpha_{ji} = \alpha_{ij}$$

Euler equations: matrix assembly

Galerkin flux decomposition

$$M\frac{dU}{dt} = \sum_{j\neq i} \mathbf{k}_{ij}\cdot(\mathbf{F}_j - \mathbf{F}_i) = \sum_{j\neq i} |\mathbf{k}_{ij}|\hat{A}_{ij}(U_j - U_i)$$

Coefficients for the ‘numerical edge’ $\mathbf{e}_{ij} = \mathbf{k}_{ij}/|\mathbf{k}_{ij}|$

$$\mathbf{k}_{ij} = \left(k_{ij}^x, k_{ij}^y, k_{ij}^z\right), \quad |\mathbf{k}_{ij}| = \sqrt{(k_{ij}^x)^2 + (k_{ij}^y)^2 + (k_{ij}^z)^2}$$

Cumulative Jacobian matrix

$$A_{ij} = e_{ij}^x A^x + e_{ij}^y A^y + e_{ij}^z A^z \quad \in \mathbb{R}^{5\times 5}$$

Roe mean values

$$\hat{A}_{ij} = A_{ij}(\hat{\rho}_{ij}, \hat{\mathbf{v}}_{ij}, \hat{h}_{ij}), \qquad \hat{\rho}_{ij} = \sqrt{\rho_i\rho_j}$$

$$\hat{\mathbf{v}}_{ij} = \frac{\sqrt{\rho_i}\mathbf{v}_i + \sqrt{\rho_j}\mathbf{v}_j}{\sqrt{\rho_i} + \sqrt{\rho_j}}, \quad \hat{h}_{ij} = \frac{\sqrt{\rho_i}h_i + \sqrt{\rho_j}h_j}{\sqrt{\rho_i} + \sqrt{\rho_j}}$$

Edge-by-edge assembly

$$\hat{A}_{ij} \in \mathbb{R}^{5\times 5} \longrightarrow K_{kl} \in \mathbb{R}^{N\times N}, \quad k, l = 1, \ldots, 5$$

High-order scheme $\quad S^H U^H = G^H$

$$S_{kl}^H = \delta_{kl} M_C - \theta\Delta t K_{kl}$$
$$G_k^H = M_C U_k^n + (1-\theta)\Delta t \sum_l K_{kl} U_l^n$$

Euler equations: discrete diffusion

Characteristic decomposition

$$\hat{A}_{ij} = R_{ij}\Lambda_{ij}R_{ij}^{-1}$$

Eigenvalues of the Jacobian

$$\Lambda = \mathrm{diag}\,\{\hat{v}_{ij} - \hat{c}_{ij}, \hat{v}_{ij}, \hat{v}_{ij}, \hat{v}_{ij}, \hat{v}_{ij} + \hat{c}_{ij}\}$$

$$\hat{v}_{ij} = \mathbf{e}_{ij} \cdot \hat{\mathbf{v}}_{ij} \qquad \text{velocity projected onto the edge}$$

$$\hat{c}_{ij} = \sqrt{(\gamma - 1)(\hat{h}_{ij} - \frac{1}{2}||\hat{\mathbf{v}}_{ij}||_2^2)} \qquad \text{speed of sound}$$

Discrete 'upwinding' for hyperbolic systems

$$\hat{A}_{ij}, T_{ij} \in \mathbb{R}^{5\times 5} \longrightarrow K_{kl} + D_{kl} \in \mathbb{R}^{N\times N}$$

Roe's approximate Riemann solver

$$T_{ij} = \frac{1}{2}|\hat{A}_{ij}| = \frac{1}{2}R_{ij}|\Lambda_{ij}|R_{ij}^{-1}$$

Scalar artificial diffusion

$$T_{ij} = d_{ij}I, \qquad d_{ij} = \frac{|\hat{v}_{ij}| + \hat{c}_{ij}}{2}$$

Low-order scheme $\quad S^L U^L = G^L$

$$S_{kl}^L = \delta_{kl}[M_L - \theta\Delta t D] - \theta\Delta t K_{kl}$$

$$G_k^L = [M_L + (1-\theta)\Delta t D]U_k^n + (1-\theta)\Delta t \sum_l K_{kl}U_l^n$$

Euler equations: FEM-FCT algorithm

Fully discretized Euler equations

$$\begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix} = \begin{bmatrix} G_1 \\ G_2 \\ G_3 \\ G_4 \\ G_5 \end{bmatrix}$$

Defect correction loop

$$U^{(l+1)} = U^{(l)} + \omega^{(l)}[C(U^{(l)})]^{-1}(S(U^{(l)})U^{(l)} - G)$$

$$C(U^{(l)}) = \mathrm{diag}\{C_1^{(l)}, \ldots, C_5^{(l)}\} \qquad l = 0, 1, 2, \ldots$$

Scalar subproblems

$$\underbrace{[M_L - \theta\Delta t(K_{ii}^{(l)} + D^{(l)})]}_{C_i^{(l)}} \delta U_i = R_i$$

$$R_i = [M_L + (1-\theta)\Delta t D^n]U^n + (1-\theta)\Delta t \sum_j K_{ij}^n U_j^n$$
$$- [M_L - \theta\Delta t D^{(l)}]U^{(l)} - \theta\Delta t \sum_j K_{ij}^{(l)} U_j^{(l)} + F^*(U_i^{(l)}, U_i^n)$$

Antidiffusive terms

$$\begin{aligned} F(U_i^{(l)}, U_i^n) &= -[M_C - M_L](U_i^{(l)} - U_i^n) \\ &- \theta\Delta t D^{(l)} U_i^{(l)} - (1-\theta)\Delta t D^n U_i^n \end{aligned}$$

synchronized limiter: $\alpha = \min\{\alpha_\rho, \alpha_E\}$

Solution update

$$U_i^{(l+1)} = U_i^{(l)} + \omega_i^{(l)} \delta U_i, \qquad U_i^{(0)} = U_i^n$$

Summary of the algorithm

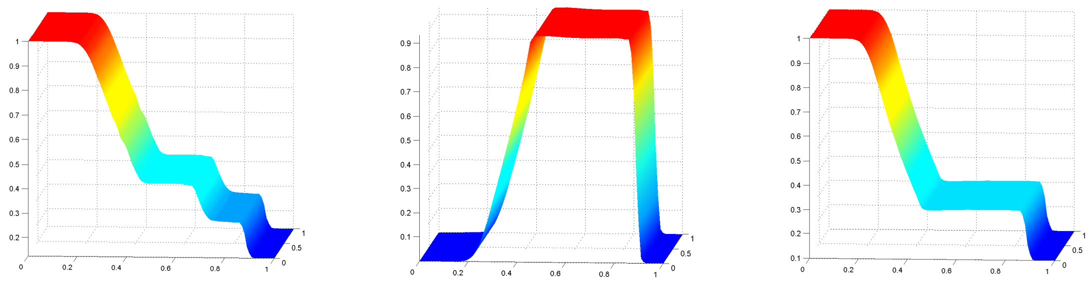
1. Perform edge-by-edge assembly of the diagonal preconditioner blocks and of the defect vector corresponding to the low-order discretization
2. Compute correction factors for the indicator variables and apply the synchronized limiter to the raw antidiffusive fluxes
3. Add the limited antidiffusive terms to the defect vector and solve the resulting linear systems for the scalar subproblems
4. Update all variables and proceed to the next nonlinear iteration / time step

Iterative solver

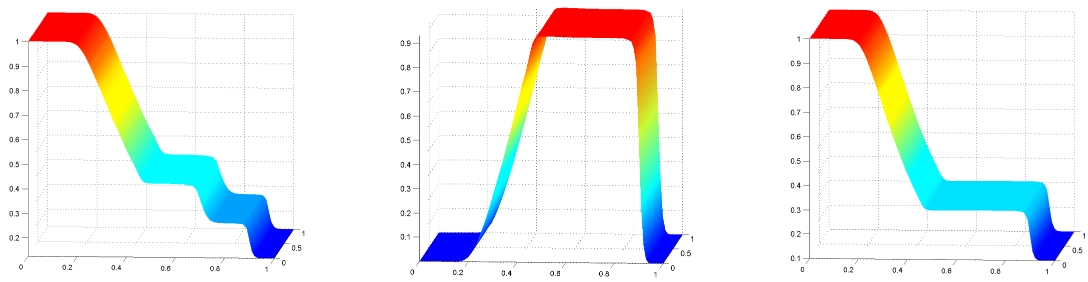
Δt (small)	*Jacobi-like iteration* lumped mass matrix
Δt	*BiCGSTAB / multigrid* Jacobi Gauß–Seidel / SOR
Δt (large)	ILU + renumbering

Sod's shock tube

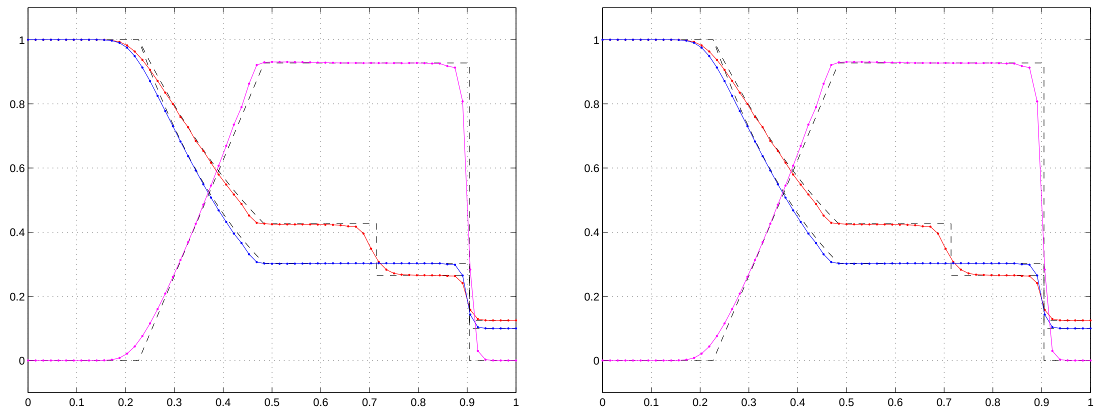
geometry:	$D = [0,1] \times [0,1]$
grid:	65×65
initial cond.:	$U(x,0) = \begin{cases} U_l & \text{for } \lvert x \rvert < 0.5 \\ U_r & \text{for } \lvert x \rvert \geq 0.5 \end{cases}$
	$U_l = (1,0,0,1)^T$ and $U_r = (0.125,0,0,0.1)^T$
boundary cond.:	solid wall



CN, $\Delta t = 1 \cdot 10^{-3}$, $t = 0.231$



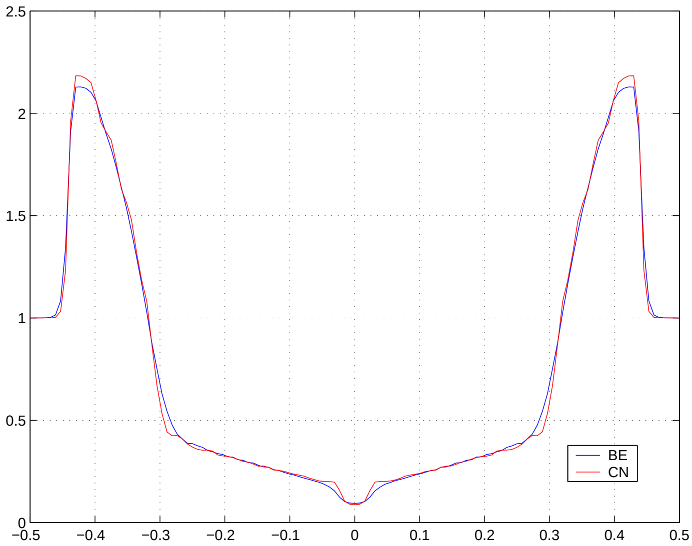
BE, $\Delta t = 1 \cdot 10^{-3}$, $t = 0.231$



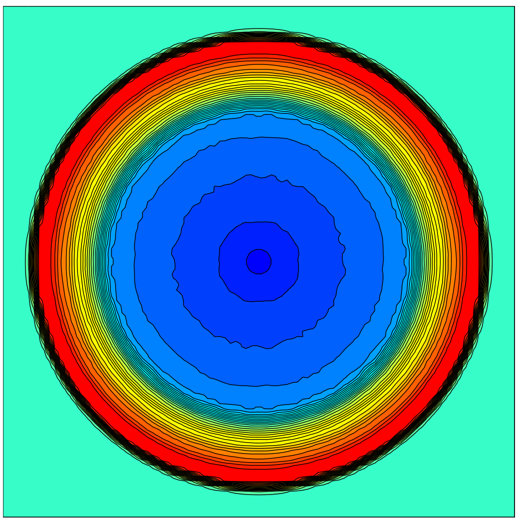
Sod, 1978

Radially Symmetric Riemann-Problem

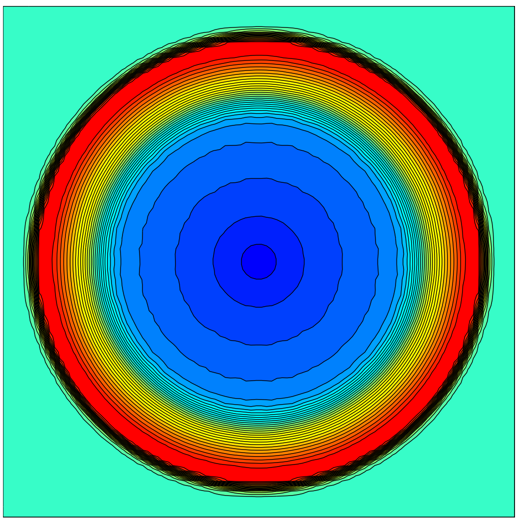
geometry:	$D = [-0.5, 0.5] \times [-0.5, 0.5]$
grid:	129×129
initial cond.:	$U(x,0) = \begin{cases} U_{int} \text{ for } \|\|x\|\|_2 < 0.13 \\ U_{ext} \text{ for } \|\|x\|\|_2 \geq 0.13 \end{cases}$
	$U_{int} = (2,0,0,15)^T$ and $U_{ext} = (1,0,0,1)^T$
boundary cond.:	$U(x,t) = U_{ext}$ for $x \in \partial D, t \in \mathbb{R}_0^+$



Density distribution along the x_1-axis



CN, $\Delta t = 1 \cdot 10^{-3}$, $t = 0.13$

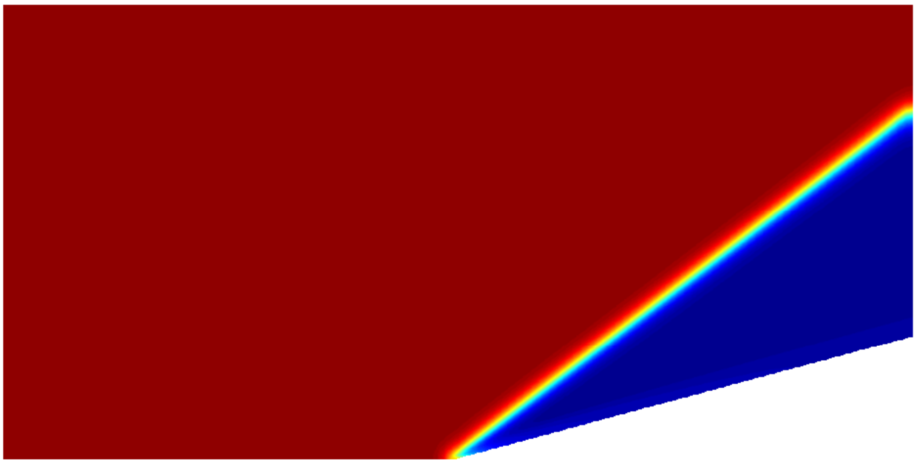


BE, $\Delta t = 1 \cdot 10^{-3}$, $t = 0.13$

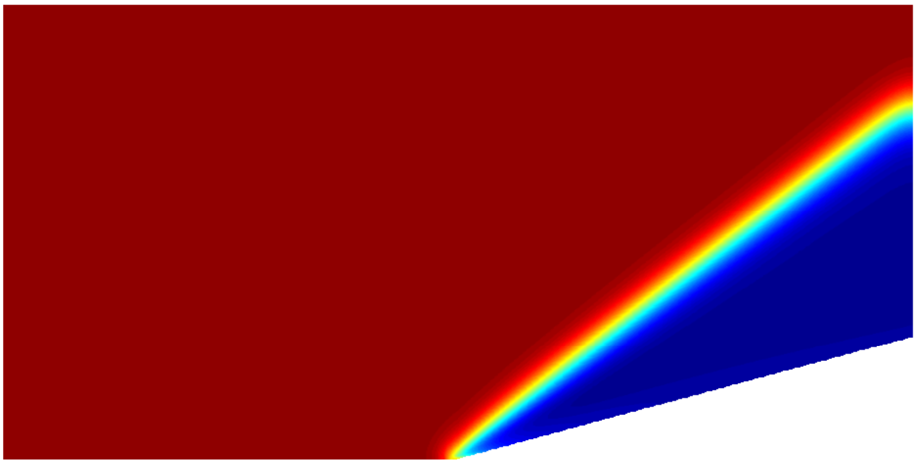
LeVeque, 1993

Compression corner at Mach 2.5

geometry:	wegde with half-angle of 15°
grid:	129×129
initial cond.:	$U(x, y, 0) = U_0(x, y)$
	$U_0(x, y) = (1.4, 2.5, 0, 1)^T$
boundary cond.:	$U(0, y, t) = U_0(0, y)$



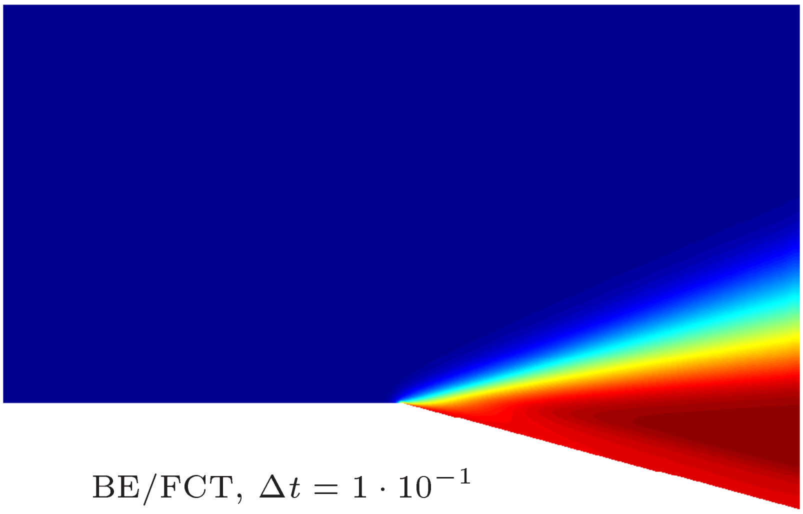
BE/FCT, $\Delta t = 1 \cdot 10^{-1}$



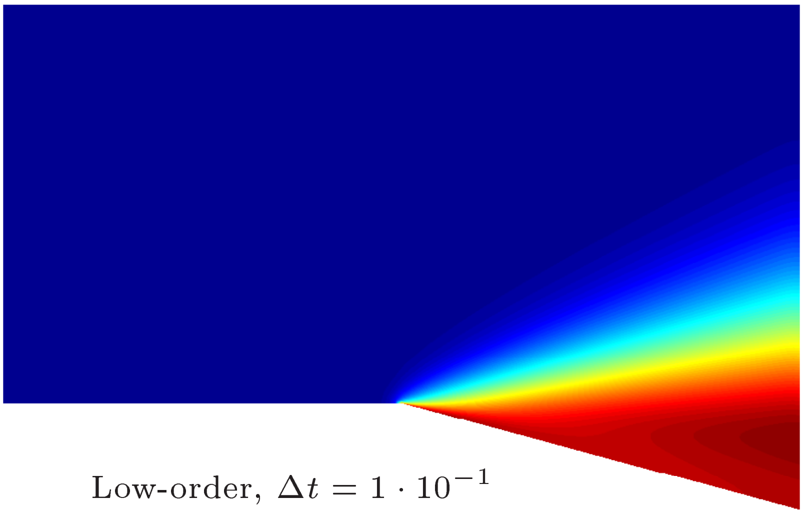
Low-order, $\Delta t = 1 \cdot 10^{-1}$

Prandtl-Meyer expansion at Mach 2.5

geometry:	wegde with half-angle of 15°
grid:	129×129
initial cond.:	$U(x, y, 0) = U_0(x, y)$
	$U_0(x, y) = (1.4, 2.5, 0, 1)^T$
boundary cond.:	$U(0, y, t) = U_0(0, y)$



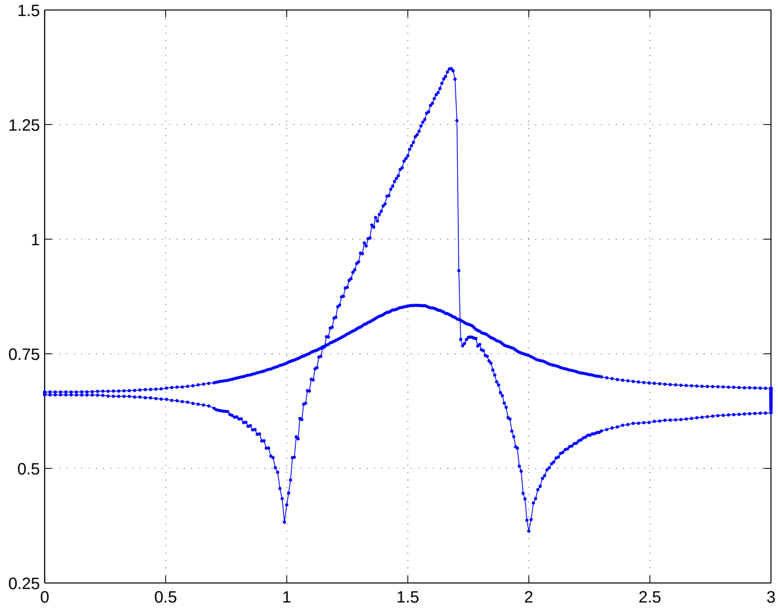
BE/FCT, $\Delta t = 1 \cdot 10^{-1}$

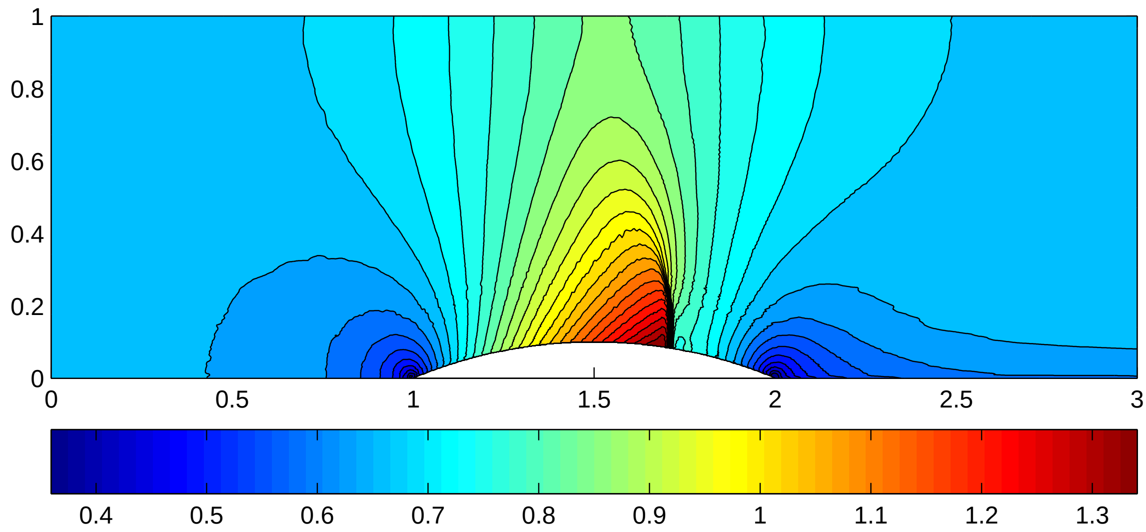


Low-order, $\Delta t = 1 \cdot 10^{-1}$

Transonic flow in the GAMM channel

geometry:	parallel channel with a 10.0% thick circular bump
grid:	40960 Q_1 elements, 41377 nodes
boundary cond.:	inlet: $v = 0$, $p = 73340\,\rho^\gamma \frac{N}{m^2}$, $h = 278850\ \frac{m^2}{s^2}$
	outlet: $p = 72218\ \frac{N}{m^2}$





Isolines of the Mach number (M_{max}=1.38, M_{out}=0.675)

Conclusions

- Implicit FEM-FCT schemes can be derived on the basis of rigorous positivity criteria.
- Low-order method can be constructed by adding discrete diffusion so as to eliminate negative off-diagonal entries of the high-order operator.
- Antidiffusive terms can be decomposed into a sum of internodal fluxes, which can be limited in an essentially one-dimensional fashion.
- A generalization to hyperbolic systems involves scalar artificial diffusion proportional to the spectral radius of the Roe matrix.
- Flux correction is to be carried out in each nonlinear iteration using a synchronized limiter.
- Robust iterative solvers are required to take advantage of the fully implicit time-stepping.