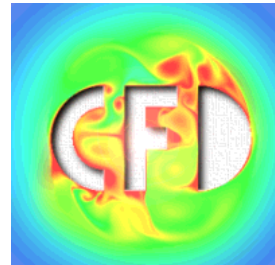




Implicit FEM-FCT algorithm for compressible flows

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- State of the art: discretisation techniques
- Discrete upwinding for scalar equations
- Iterative defect correction scheme
- Generalised FEM-FCT formulation
- Matrix assembly for the Euler equations
- Artificial viscosity, scalar dissipation
- Synchronised flux limiter for systems

Convection dominated flows

Generic conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) - \nabla \cdot (\epsilon \nabla u) = 0$$

Compressible Euler equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla p = 0$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho H \mathbf{v}) = 0$$

Godunov's Theorem (1959)

No linear discretisation scheme of order higher than first is monotonicity preserving

- ⊖ High-order methods: oscillatory
- ⊖ Convergence to nonphysical weak solution
- ⊖ Low-order methods: overdiffusive
- ⊖ Non-symmetric, ill-conditioned matrices
- ⊕ High-resolution methods: **nonlinear**

High-resolution methods

Flux-Corrected Transport (FCT) algorithm

Boris & 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

State of the art

- ⊖ finite differences/volumes
- ⊖ explicit FEM-FCT formulation Löhner (1987)
- ⊖ 1D nature, cartesian/simplex meshes

Objective: a *methodology* which is

- ⊕ based on mathematical theory, parameter-free
- ⊕ applicable to arbitrary time/space discretisations
- ⊕ multidimensional, independent of underlying mesh

FEM-FCT

or

FEM-TVD

Discrete positivity criteria

LED: $\frac{du_i}{dt} = \sum_{j \neq i} c_{ij}(u_j - u_i), \quad c_{ij} \geq 0$

Jameson
(1993)

e.g. $u_i = \max_{j \in S_i} u_j \Rightarrow u_j - u_i \leq 0 \Rightarrow \frac{du_i}{dt} \leq 0$

Lemma. A discrete scheme of the form

$$Au^{n+1} = Bu^n, \quad u^n \geq 0$$

is positivity-preserving if A is an M -matrix and all entries of B are non-negative.

Discrete diffusion operators $D = \{d_{ij}\}$

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

Flux decomposition of diffusive terms

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

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

Discrete upwinding

Weak form
$$\int_{\Omega} w \left[\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u - \epsilon \nabla u) \right] \mathrm{d}\mathbf{x} = 0$$

Group FEM formulation

Fletcher (1983)

$$u = \sum_j u_j \varphi_j, \quad \mathbf{v}u = \sum_j (\mathbf{v}_j u_j) \varphi_j$$

Galerkin semi-discretisation with mass lumping

$$M_L \frac{\mathrm{d}u}{\mathrm{d}t} = Ku$$

$$m_i \frac{\mathrm{d}u_i}{\mathrm{d}t} = \sum_{j \neq i} k_{ij} (u_j - u_i) + \delta_i u_i$$

$$k_{ij} = -\mathbf{v}_j \cdot \mathbf{c}_{ij} - \epsilon s_{ij}$$

$$\delta_i = \sum_j k_{ij} \approx \nabla \cdot \mathbf{v}$$

$$\mathbf{c}_{ij} = \int_{\Omega} \varphi_i \nabla \varphi_j \mathrm{d}\mathbf{x}$$

$$s_{ij} = \int_{\Omega} \nabla \varphi_i \cdot \nabla \varphi_j \mathrm{d}\mathbf{x}$$

Adaptive artificial diffusion $L = K + D$

$$d_{ij} = d_{ji} = \max\{0, -k_{ij}, -k_{ji}\}, \quad d_{ii} = -\sum_{j \neq i} d_{ij}$$

Edge-based elimination of negative off-diagonal entries

$$L := K \rightarrow \begin{aligned} l_{ii} &:= l_{ii} - d_{ij}, & l_{ij} &:= l_{ij} + d_{ij} \\ l_{ji} &:= l_{ji} + d_{ij}, & l_{jj} &:= l_{jj} - d_{ij} \end{aligned}$$

FEM-FCT formulation

Galerkin θ -scheme

$$Au^H = b^n + f(u^n, u^H)$$

$$A = M_L - \theta \Delta t L, \quad b^n = M_L u^n + (1 - \theta) \Delta t L u^n$$

Antidiffusive contribution

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

$$f(u^n, u^H) = \sum_{j \neq i} f_{ij}, \quad f_{ji} = -f_{ij}, \quad i \neq j$$

Antidiffusive flux decomposition

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

Implicit FEM-FCT algorithm

Kuzmin (2001)

$$Au^{n+1} = M_L \tilde{u}^n + f^*(u^n, u^H)$$

$$\begin{aligned} f^*(u^n, u^H) &= \sum_{j \neq i} \alpha_{ij} f_{ij} & \alpha_{ij} &= \alpha_{ij}(\tilde{u}^n, f_{ij}), \\ & & 0 &\leq \alpha_{ij} \leq 1 \end{aligned}$$

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

Positivity constraint $\Delta t \leq \frac{1}{1-\theta} \min_i \left\{ -\frac{m_i}{l_{ii}} \mid l_{ii} < 0 \right\}$

Iterative defect correction

Successive approximations

$$u^{(m+1)} = u^{(m)} + [A(u^{(m)})]^{-1} r^{(m)}$$

Practical implementation

$$A(u^{(m)}) \Delta u^{(m)} = r^{(m)}, \quad m = 0, 1, 2, \dots$$

$$u^{(m+1)} = u^{(m)} + \Delta u^{(m)}, \quad u^{(0)} = u^n$$

‘Upwind’ preconditioner $A(u^{(m)}) = M_L - \theta \Delta t L(u^{(m)})$

Defect vector with antidiffusion and low-order RHS

$$r^{(m)} = b^n - A(u^{(m)})u^{(m)} + f^*(u^n, u^{(m)})$$

$$b^n = M_L u^n + (1 - \theta) \Delta t L(u^n) u^n$$

Basic FEM-FCT algorithm $A(u^{(m)})u^{(m+1)} = b^{(m+1)}$

$$b_i^{(m+1)} = b_i^n + \sum_{j \neq i} \alpha_{ij}^{(m)} f_{ij}^{(m)} \quad \alpha_{ij}^{(m)} = \alpha_{ij}(\tilde{u}^n, f_{ij}^{(m)})$$

Principle: Let $b^{(m+1)} = B\tilde{u}$, $B \geq 0$ and $\tilde{u}$ positivity preserving auxiliary solution. Then we have

$$u^n \geq 0 \quad \Rightarrow \quad \tilde{u} \geq 0 \quad \Rightarrow \quad u^{(m+1)} \geq 0$$

⊖ amount of accepted antidiffusion depends on the magnitude of the time step Δt



Iterative FEM-FCT

Strategy: build accepted antidiffusion into $\tilde{u}$

$$M_L \tilde{u}^{(m)} = b^{(m)}, \quad b^{(0)} = b^n$$

Raw flux difference

$$\Delta f_{ij}^{(m)} = f_{ij}^{(m)} - g_{ij}^{(m)}, \quad \Delta f_{ij}^{(0)} = f_{ij}^{(0)}$$

Correction factors (Zalesak's limiter)

$$\alpha_{ij}^{(m)} = \alpha_{ij}(\tilde{u}^{(m)}, \Delta f_{ij}^{(m)}), \quad 0 \leq \alpha_{ij}^{(m)} \leq 1$$

Accepted antidiffusion

$$g_{ij}^{(m+1)} = g_{ij}^{(m)} + \alpha_{ij}^{(m)} \Delta f_{ij}^{(m)}, \quad g_{ij}^{(0)} = 0$$

Update of the RHS

$$b_i^{(m+1)} = b_i^{(m)} + \sum_{j \neq i} \alpha_{ij}^{(m)} \Delta f_{ij}^{(m)}$$

- ⊕ rejected antidiffusion can be ‘recycled’
- ⊕ no excessive flux limiting for large time steps



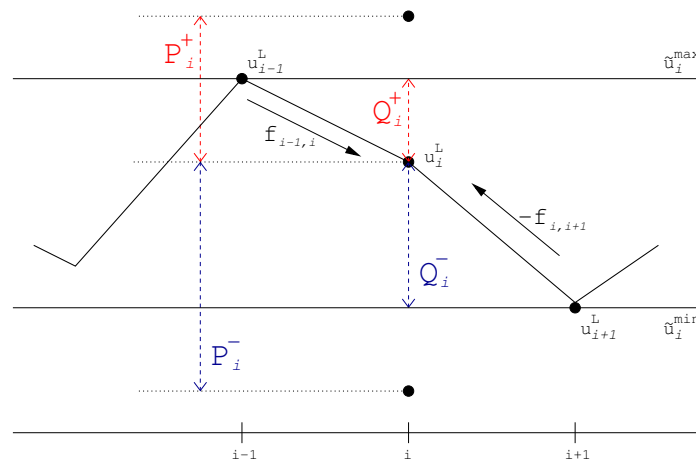
Zalesak's limiter

1. **Prelimiting:** $f_{ij} := 0$, if $f_{ij}(\tilde{u}_i - \tilde{u}_j) \leq 0$.
2. Positive/negative fluxes and upper/lower bounds

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

3. Nodal correction factors

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



4. **Postlimiting:** $R_i^\pm := 1$ at in-/outlet

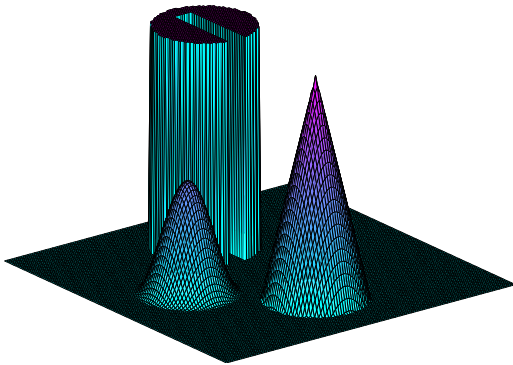


5. Final correction factors

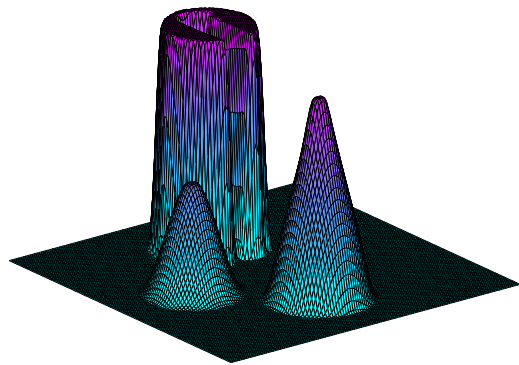
$$\alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\}, & \text{if } f_{ij} \geq 0 \\ \min\{R_j^+, R_i^-\}, & \text{if } f_{ij} < 0 \end{cases}$$

Solid body rotation

exact solution



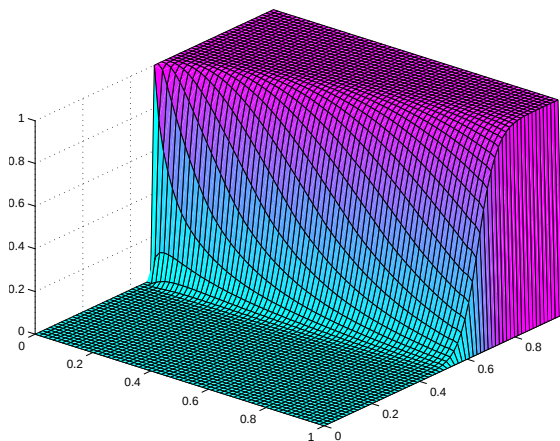
FEM-FCT



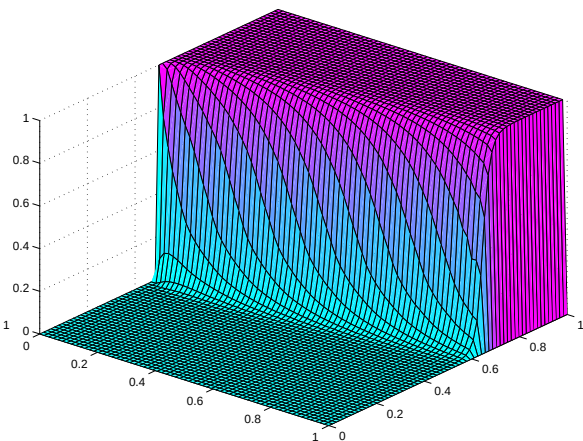
Crank-Nicolson, $\Delta t = 10^{-3}$, $128 \times 128 Q_1$ elements

Steady-state convection-diffusion

basic FEM-FCT



iterative FEM-FCT



Backward Euler, $\Delta t = 10^{-1}$, $\epsilon = 10^{-3}$, $64 \times 64 Q_1$ elements

Compressible Euler equations

Divergence form

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

$$U = (\rho, \rho \mathbf{v}, \rho E)^T$$

$$\mathbf{F} = (F^1, F^2, F^3)$$

$$F^1 = \begin{bmatrix} \rho v_1 \\ \rho v_1^2 + p \\ \rho v_1 v_2 \\ \rho v_1 v_3 \\ \rho H v_1 \end{bmatrix}, \quad F^2 = \begin{bmatrix} \rho v_2 \\ \rho v_1 v_2 \\ \rho v_2^2 + p \\ \rho v_2 v_3 \\ \rho H v_2 \end{bmatrix}, \quad F^3 = \begin{bmatrix} \rho v_3 \\ \rho v_1 v_3 \\ \rho v_2 v_3 \\ \rho v_3^2 + p \\ \rho H v_3 \end{bmatrix}$$

where $H = E + p/\rho$ and $p = (\gamma - 1)\rho (E - |\mathbf{v}|^2/2)$

Quasi-linear formulation

$$\frac{\partial U}{\partial t} + \mathbf{A} \cdot \nabla U = 0$$

Jacobian matrices

$$\mathbf{A} = (A^1, A^2, A^3)$$

$$F^d = A^d U, \quad A^d = \frac{\partial F^d}{\partial U}, \quad d = 1, 2, 3.$$

Mathematical challenges:

- hyperbolicity
- nonlinearity
- strong coupling



Galerkin discretisation

Group FEM formulation $\sum_j \varphi_j \equiv 1 \Rightarrow \mathbf{c}_{ii} = - \sum_{j \neq i} \mathbf{c}_{ij}$

$$\boxed{M_C \frac{dU}{dt} = KU} \quad (KU)_i = - \sum_{j \neq i} \mathbf{c}_{ij} \cdot (\mathbf{F}_j - \mathbf{F}_i)$$

$$\mathbf{F}_j - \mathbf{F}_i = \hat{\mathbf{A}}_{ij}(U_j - U_i) \quad \text{where} \quad \hat{\mathbf{A}}_{ij} = \mathbf{A}(\hat{\rho}_{ij}, \hat{\mathbf{v}}_{ij}, \hat{H}_{ij})$$

Roe mean values $\hat{\rho}_{ij} = \sqrt{\rho_i \rho_j}$

$$\hat{\mathbf{v}}_{ij} = \frac{\sqrt{\rho_i} \mathbf{v}_i + \sqrt{\rho_j} \mathbf{v}_j}{\sqrt{\rho_i} + \sqrt{\rho_j}}, \quad \hat{H}_{ij} = \frac{\sqrt{\rho_i} H_i + \sqrt{\rho_j} H_j}{\sqrt{\rho_i} + \sqrt{\rho_j}}$$

Quasi-linear formulation

$$(KU)_i = - \sum_{j \neq i} \mathbf{c}_{ij} \cdot \hat{\mathbf{A}}_{ij}(U_j - U_i) = \sum_{j \neq i} (\mathbf{A}_{ij} + \mathbf{B}_{ij})(U_j - U_i)$$

Cumulative Roe matrices

$$\begin{aligned} \mathbf{A}_{ij} &= \mathbf{a}_{ij} \cdot \hat{\mathbf{A}}_{ij}, & \mathbf{a}_{ij} &= - \frac{\mathbf{c}_{ij} - \mathbf{c}_{ji}}{2} \\ \mathbf{B}_{ij} &= \mathbf{b}_{ij} \cdot \hat{\mathbf{A}}_{ij}, & \mathbf{b}_{ij} &= - \frac{\mathbf{c}_{ij} + \mathbf{c}_{ji}}{2} \end{aligned}$$

Contribution of edge $\vec{i j}$

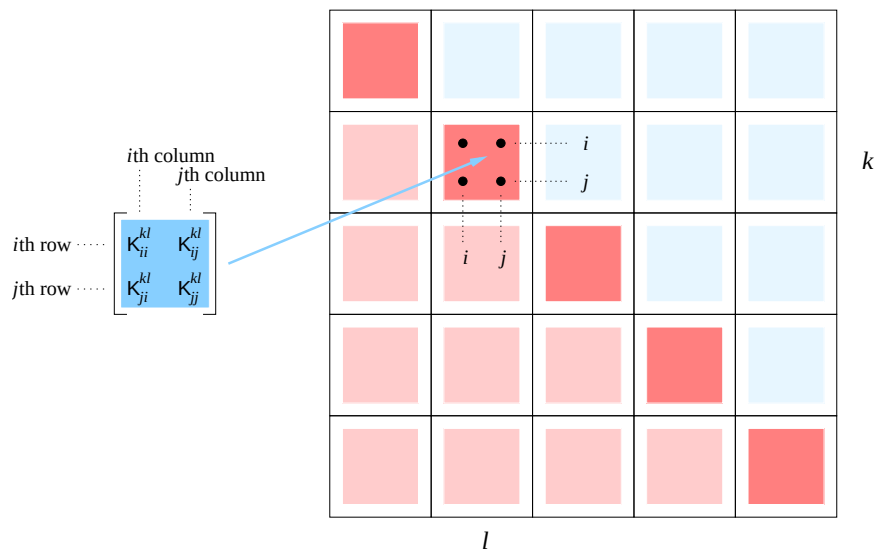
$$\begin{aligned} (\mathbf{A}_{ij} + \mathbf{B}_{ij})(U_j - U_i) &\longrightarrow (KU)_i \\ (\mathbf{A}_{ij} - \mathbf{B}_{ij})(U_j - U_i) &\longrightarrow (KU)_j \end{aligned}$$

Galerkin matrix assembly

Edge contribution to the operator K

$$K_{ii} = -A_{ij} - B_{ij} \quad K_{ij} = A_{ij} + B_{ij}$$

$$K_{ji} = -A_{ij} + B_{ij} \quad K_{jj} = A_{ij} - B_{ij}$$



Edge contribution to the operator L

$$L_{ii} = -A_{ij} - D_{ij} \quad L_{ij} = A_{ij} + D_{ij}$$

$$L_{ji} = -A_{ij} + D_{ij} \quad L_{jj} = A_{ij} - D_{ij}$$

Raw antidiffusive flux

$$F_{ij} = - \left(M_{ij} \frac{d}{dt} + D_{ij} - B_{ij} \right) (U_j - U_i), \quad F_{ji} = -F_{ij}$$

where $M_{ij} = m_{ij}I$ and D_{ij} is the tensorial dissipation

Artificial viscosity

LED-principle for systems: *all off-diagonal blocks of the global Jacobian matrix should be positive definite*

Characteristic decomposition

$$A_{ij} = R_{ij} \Lambda_{ij} R_{ij}^{-1}$$

$$\Lambda_{ij} = |\mathbf{a}_{ij}| \text{diag} \{ \lambda_1, \dots, \lambda_5 \}, \quad |\mathbf{a}_{ij}| = \sqrt{\mathbf{a}_{ij} \cdot \mathbf{a}_{ij}}$$

Eigenvalues of the cumulative Roe matrix A_{ij}

$$\lambda_1 = \hat{v}_{ij} - \hat{c}_{ij}, \quad \lambda_2 = \lambda_3 = \lambda_4 = \hat{v}_{ij}, \quad \lambda_5 = \hat{v}_{ij} + \hat{c}_{ij}$$

$$\hat{v}_{ij} = \frac{\mathbf{a}_{ij} \cdot \hat{\mathbf{v}}_{ij}}{|\mathbf{a}_{ij}|}, \quad \hat{c}_{ij} = \sqrt{(\gamma - 1) \left(\hat{H}_{ij} - \frac{|\hat{\mathbf{v}}_{ij}|^2}{2} \right)}$$

System upwinding (expensive)

$$D_{ij} = |A_{ij}| = R_{ij} |\Lambda_{ij}| R_{ij}^{-1}$$

Generalisation of Roe's approximate Riemann solver

Scalar dissipation (efficient)

$$D_{ij} = d_{ij} I \quad \text{where} \quad d_{ij} = |\mathbf{a}_{ij}| \max_i |\lambda_i|$$

is optimal for FEM-FCT since excessive artificial diffusion is removed by the flux limiter

Iterative defect correction

Successive approximations

$$U^{(m+1)} = U^{(m)} + [A(U^{(m)})]^{-1} R^{(m)}$$

Defect vector

$$R^{(m)} = B^{(m+1)} - A(U^{(m)})U^{(m)}$$

Right-hand side

$$\begin{aligned} \text{or} \quad B^{(m+1)} &= B^n + F^*(U^n, U^{(m)}) \\ B^{(m+1)} &= B^{(m)} + \Delta F^*(U^n, U^{(m)}) \end{aligned}$$

Initialisation

$$B^n = B^{(0)} = M_L U^n + (1 - \theta) \Delta t L(U^n) U^n$$

Raw antidiffusion

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

$$\begin{aligned} \Delta F(U^n, U^{(m)}) &= F(U^n, U^{(m)}) - G^{(m)} \\ G^{(m+1)} &= G^{(m)} + \Delta F^*(U^n, U^{(m)}), \quad G^{(0)} = 0 \end{aligned}$$

Synchronisation of correction factors

$$F_{ij}^* = f(\alpha_{ij}^1, \dots, \alpha_{ij}^5) F_{ij} \quad \text{Löhner (1987)}$$

Block-Jacobi preconditioner

Global linear system

$$\begin{bmatrix} A_{11}^{(m)} & A_{12}^{(m)} & A_{13}^{(m)} & A_{14}^{(m)} & A_{15}^{(m)} \\ A_{21}^{(m)} & A_{22}^{(m)} & A_{23}^{(m)} & A_{24}^{(m)} & A_{25}^{(m)} \\ A_{31}^{(m)} & A_{32}^{(m)} & A_{33}^{(m)} & A_{34}^{(m)} & A_{35}^{(m)} \\ A_{41}^{(m)} & A_{42}^{(m)} & A_{43}^{(m)} & A_{44}^{(m)} & A_{45}^{(m)} \\ A_{51}^{(m)} & A_{52}^{(m)} & A_{53}^{(m)} & A_{54}^{(m)} & A_{55}^{(m)} \end{bmatrix} \begin{bmatrix} \Delta u_1^{(m+1)} \\ \Delta u_2^{(m+1)} \\ \Delta u_3^{(m+1)} \\ \Delta u_4^{(m+1)} \\ \Delta u_5^{(m+1)} \end{bmatrix} = \begin{bmatrix} r_1^{(m)} \\ r_2^{(m)} \\ r_3^{(m)} \\ r_4^{(m)} \\ r_5^{(m)} \end{bmatrix}$$

Block-diagonal preconditioner

$$A_{kk}^{(m)} = M_L - \theta \Delta t L_{kk}^{(m)}, \quad A_{kl}^{(m)} = 0, \quad \forall l \neq k$$

Sequence of scalar subproblems

$$A_{kk}^{(m)} \Delta u_k^{(m)} = r_k^{(m)}, \quad k = 1, \dots, 5$$

$$u_k^{(m+1)} = u_k^{(m)} + \Delta u_k^{(m)}, \quad u_k^{(0)} = u_k^n$$

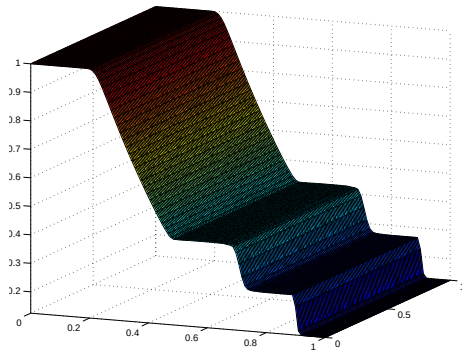
- ⊕ only 5 blocks need to be assembled/stored
- ⊕ equations can be solved separately/in parallel
- ⊖ poor convergence for large time steps



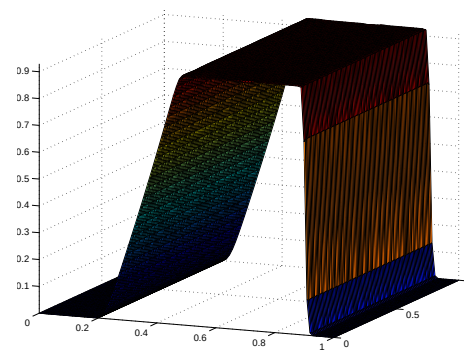
coupled solver (multigrid/BiCGSTAB with block-Gauss-Seidel smoother/preconditioner)

Shock tube problem

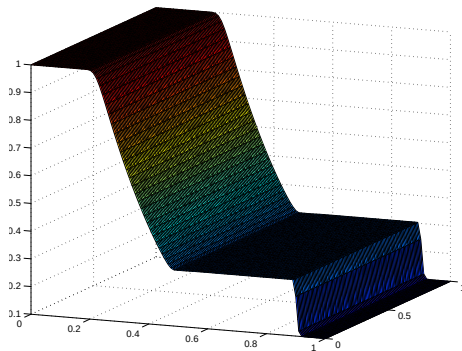
density



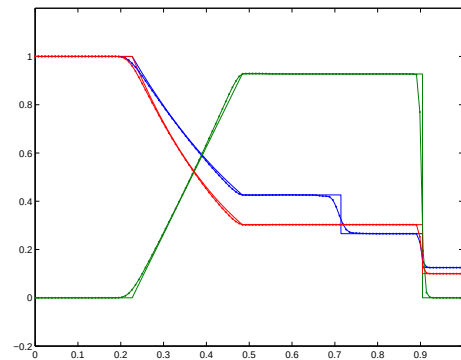
velocity



pressure

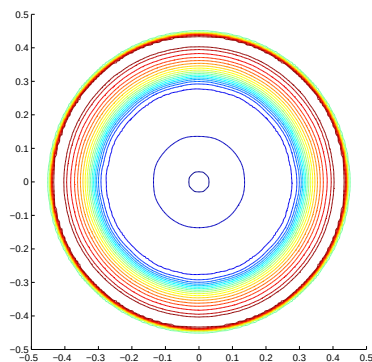


cutplane $y = 0.5$

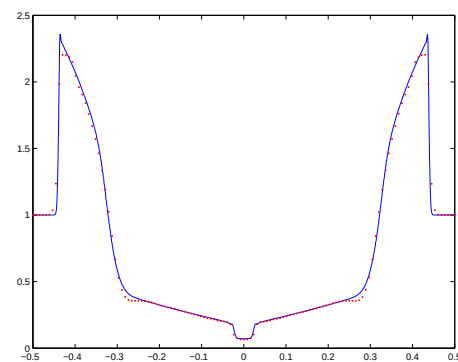


Radially symmetric Riemann problem

density



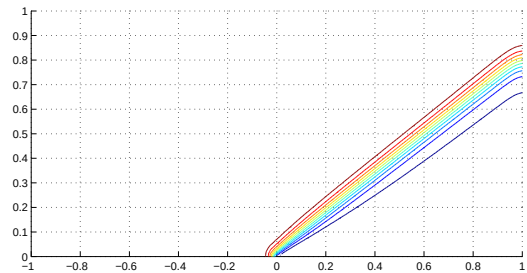
cutplane $y = 0$



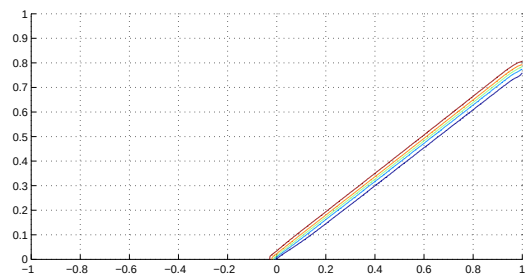
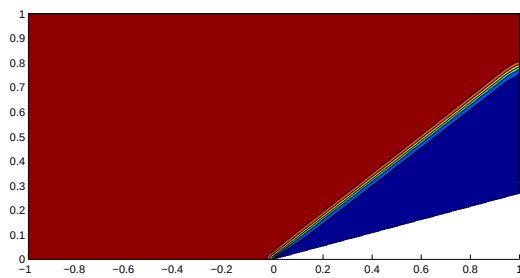
Crank-Nicolson, $\Delta t = 10^{-3}$, 128×128 Q_1 elements

Compression corner $M = 2.5, \theta = 15^\circ$

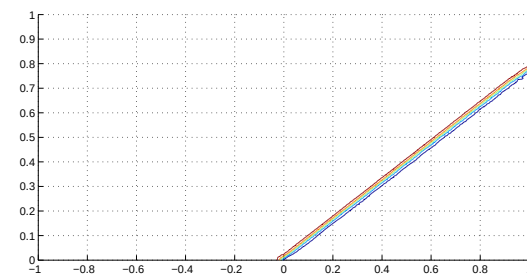
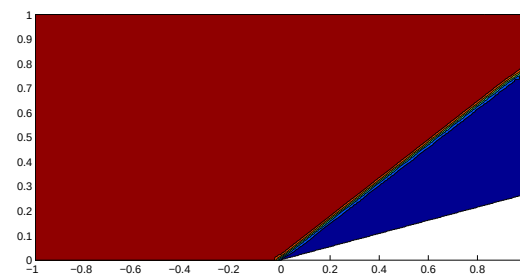
low-order method



FEM-FCT, basic limiter

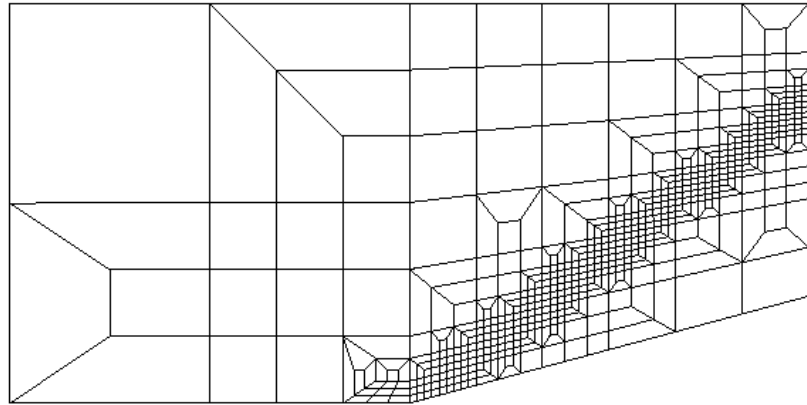


FEM-FCT, iterative limiter

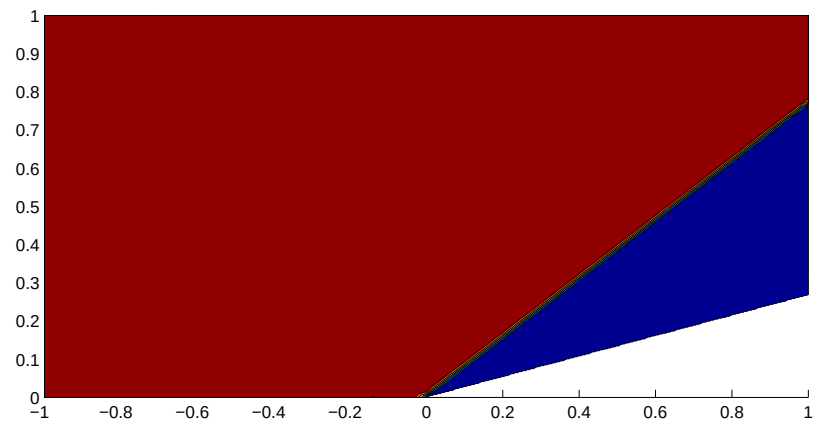


Backward Euler, $\Delta t = 10^{-2}$, $128 \times 128 Q_1$ elements

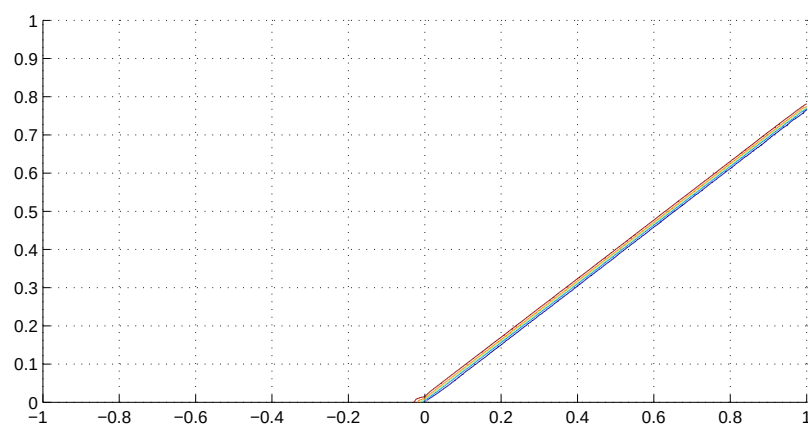
Compression corner $M = 2.5$, $\theta = 15^\circ$



coarse grid with local refinement



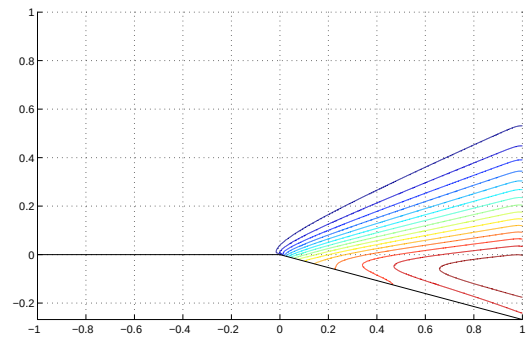
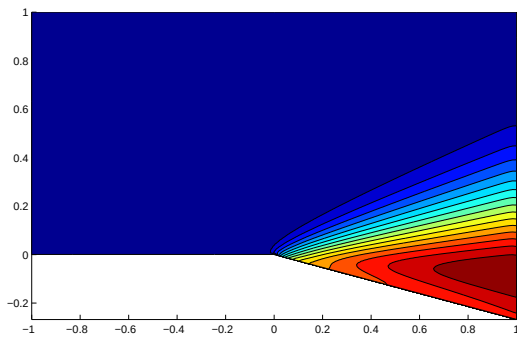
FEM-FCT, steady-state mach number distribution



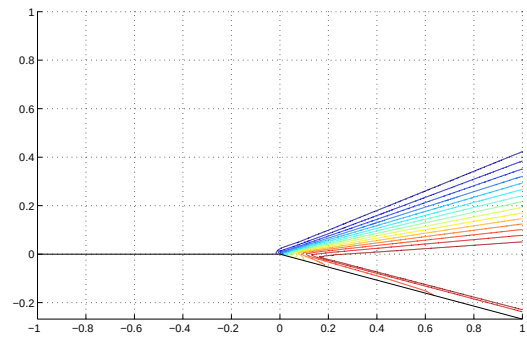
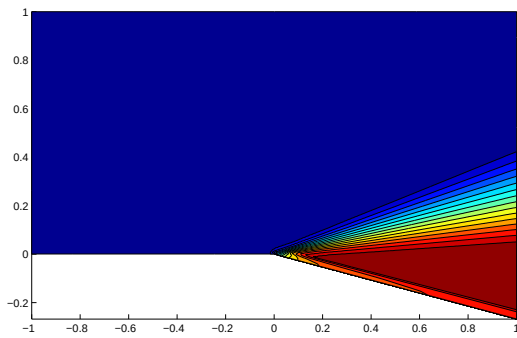
Backward Euler, $\Delta t = 10^{-2}$, iterative limiter

Prandtl-Meyer expansion $M = 2.5$, $\theta = 15^\circ$

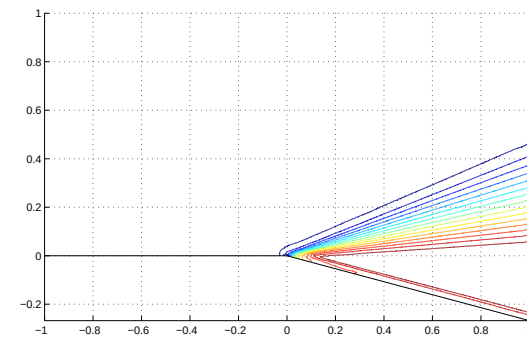
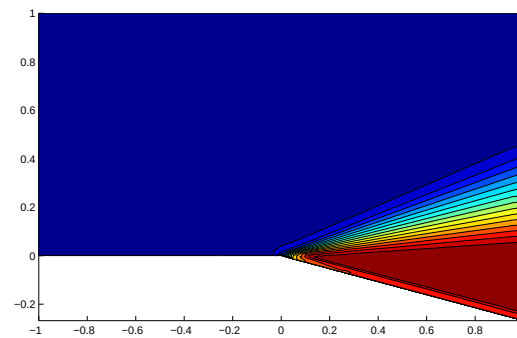
low-order method



FEM-FCT, basic limiter



FEM-FCT, iterative limiter



Backward Euler, $\Delta t = 10^{-2}$, 128×128 Q_1 elements

Conclusions

- Implicit FEM-FCT schemes can be derived on the basis of rigorous positivity criteria
- Discrete upwinding is performed by adding artificial diffusion so as to eliminate negative off-diagonal entries of the high-order operator
- In the case of hyperbolic systems scalar artificial dissipation proportional to the spectral radius of the Roe matrix can be utilised
- Flux correction can be performed within a defect correction preconditioned by the low-order operator
- Iterative limiting strategy prevents Zalesak's limiter from getting overly diffusive at large time steps

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University of Dortmund, September 29-30, 2003

<http://www.mathematik.uni-dortmund.de/lisiii/conf/fct30.html>

