UNIVERSITÄT DORTMUND

Implicit FEM-FCT algorithm for compressible flows

M. Möller, D. Kuzmin, S. Turek Institute of Applied Mathematics, University of Dortmund, Germany



- 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

- \ominus High-order methods: oscillatory
- \ominus Convergence to nonphysical weak solution
- \ominus Low-order methods: overdiffusive
- \ominus Non-symmetric, ill-conditioned matrices
- $\oplus \ {\rm High}\mbox{-resolution methods: } {\bf nonlinear}$

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

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

Objective: a *methodology* which is

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

FEM-FCT

or

FEM-TVD

Discrete positivity criteria

LED:
$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \sum_{j \neq i} c_{ij}(u_j - u_i), \quad c_{ij} \ge 0 \qquad \begin{array}{c} \text{Jameson} \\ (1993) \end{array}$$

e.g.
$$u_i = \max_{j \in S_i} u_j \implies u_j - u_i \le 0 \implies \frac{\mathrm{d}u_i}{\mathrm{d}t} \le 0$$

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Lemma. A discrete scheme of the form $Au^{n+1} = Bu^n, \quad u^n \ge 0$ 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)

$$u = \sum_{j} u_j \varphi_j, \qquad \mathbf{v} u = \sum_{j} (\mathbf{v}_j u_j) \varphi_j$$

Galerkin semi-discretisation with mass lumping

$$M_L rac{\mathrm{d} u}{\mathrm{d} t} = K u \qquad m_i rac{\mathrm{d} u_i}{\mathrm{d} t} = \sum_{j
eq i} k_{ij} (u_j - u_i) + \delta_i u_i$$

Adaptive artificial diffusion L = K + D

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

Edge-based elimination of negative off-diagonal entries

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

FEM-FCT formulation

Galerkin $\theta\text{-scheme}$

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

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

Antidiffusive contribution

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

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

Antidiffusive flux decomposition

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

Implicit FEM-FCT algorithm

Kuzmin (2001)

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

$$f^*(u^n, u^H) = \sum_{j \neq i} \alpha_{ij} f_{ij} \qquad \begin{array}{l} \alpha_{ij} = \alpha_{ij} (\tilde{u}^n, f_{ij}), \\ 0 \le \alpha_{ij} \le 1 \end{array}$$

Intermediate solution $\tilde{u}^n = u^L(t^{n+1-\theta})$: $M_L \tilde{u}^n = b^n$ Positivity constraint $\Delta t \leq \frac{1}{1-\theta} \min_i \left\{ -\frac{m_i}{l_{ii}} | l_{ii} < 0 \right\}$

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 $A(u^{(m)})u^{(m+1)} = b^{(m+1)}$

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

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

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

 \ominus amount of accepted antidiffusion depends on the magnitude of the time step Δt



Iterative FEM-FCT

Strategy: build accepted antidiffusion into \tilde{u}

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

Raw flux difference

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

Correction factors (Zalesak's limiter)

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

Accepted antidiffusion

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

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 $f_{ij}(\tilde{u}_i \tilde{u}_j) \le 0$.
- 2. Positive/negative fluxes and upper/lower bounds

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

3. Nodal correction factors



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

5. Final correction factors

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



Compressible Euler equations

Divergence form

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

$$U = (\rho, \rho \mathbf{v}, \rho E)^T$$
$$\mathbf{F} = (F^1, F^2, F^3)$$

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

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

Quasi-linear formulation

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

Jacobian matrices

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

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

Mathematical challenges:

- hyperbolicity
- nonlinearity
- strong coupling



Galerkin discretisation

Group FEM formulation $\sum_{j} \varphi_{j} \equiv 1 \Rightarrow \mathbf{c}_{ii} = -\sum_{j \neq i} \mathbf{c}_{ij}$ $M_{C} \frac{\mathrm{d}U}{\mathrm{d}t} = KU \qquad (KU)_{i} = -\sum_{j \neq i} \mathbf{c}_{ij} \cdot (\mathbf{F}_{j} - \mathbf{F}_{i})$

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

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

$$A_{ij} = \mathbf{a}_{ij} \cdot \hat{\mathbf{A}}_{ij}, \qquad \mathbf{a}_{ij} = -\frac{\mathbf{c}_{ij} - \mathbf{c}_{ji}}{2}$$
$$B_{ij} = \mathbf{b}_{ij} \cdot \hat{\mathbf{A}}_{ij}, \qquad \mathbf{b}_{ij} = -\frac{\mathbf{c}_{ij} + \mathbf{c}_{ji}}{2}$$

Contribution of edge \vec{ij}

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



Edge contribution to the operator L

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

Raw antidiffusive flux

$$\mathbf{F}_{ij} = -\left(\mathbf{M}_{ij}\frac{\mathbf{d}}{\mathbf{d}t} + \mathbf{D}_{ij} - \mathbf{B}_{ij}\right)(U_j - U_i), \quad \mathbf{F}_{ji} = -\mathbf{F}_{ij}$$

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

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

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

Eigenvalues of the cumulative Roe matrix A_{ij}

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

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

System upwinding

(expensive)

$$\mathbf{D}_{ij} = |\mathbf{A}_{ij}| = R_{ij} |\Lambda_{ij}| R_{ij}^{-1}$$

Generalisation of Roe's approximate Riemann solver

Scalar dissipation

(efficient)

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

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

or
$$B^{(m+1)} = B^{n} + F^{*}(U^{n}, U^{(m)})$$
$$B^{(m+1)} = B^{(m)} + \Delta F^{*}(U^{n}, U^{(m)})$$

Initialisation

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

Raw antidiffusion

$$F(U^{n}, U^{(m)}) = [(M_{C} - M_{L}) - (1 - \theta)\Delta t D(U^{n})]U^{n} - [(M_{C} - M_{L}) + \theta\Delta t D(U^{(m)})]U^{(m)}$$

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

Synchronisation of correction factors

$$\mathbf{F}_{ij}^* = f(\alpha_{ij}^1, \dots, \alpha_{ij}^5) \mathbf{F}_{ij} \qquad \text{Löhner (1987)}$$

Block-Jacobi preconditioner

Global linear system

$A_{11}^{(m)}$	$A_{12}^{(m)}$	$A_{13}^{(m)}$	$A_{14}^{(m)}$	$A_{15}^{(m)}$	$\left[\Delta u_1^{(m+1)}\right]$		$\left\lceil r_{1}^{(m)}\right\rceil$
$A_{21}^{(m)}$	$A_{22}^{(m)}$	$A_{23}^{(m)}$	$A_{24}^{(m)}$	$A_{25}^{(m)}$	$\Delta u_2^{(m+1)}$		$r_2^{(m)}$
$A_{31}^{(m)}$	$A_{32}^{(m)}$	$A_{33}^{(m)}$	$A_{34}^{(m)}$	$A_{35}^{(m)}$	$\Delta u_3^{(m+1)}$	=	$r_3^{(m)}$
$A_{41}^{(m)}$	$A_{42}^{(m)}$	$A_{43}^{(m)}$	$A_{44}^{(m)}$	$A_{45}^{(m)}$	$\Delta u_4^{(m+1)}$		$r_4^{(m)}$
$A_{51}^{(m)}$	$A_{52}^{(m)}$	$A_{53}^{(m)}$	$A_{54}^{(m)}$	$A_{55}^{(m)}$	$\Delta u_5^{(m+1)}$		$\left\lfloor r_{5}^{(m)} ight floor$

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

 $A_{kk}^{(m)} \Delta u_k^{(m)} = r_k^{(m)}, \qquad k = 1, \dots, 5$ $u_k^{(m+1)} = u_k^{(m)} + \Delta u_k^{(m)}, \quad u_k^{(0)} = u_k^n$

 \oplus only 5 blocks need to be assembled/stored

 \oplus equations can be solved separately/in parallel

 \ominus poor convergence for large time steps



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









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





Positivity proof for FEM-FCT

Representation of RHS

$$b_i = m_i \tilde{u}_i + \sum_{j \neq i} \alpha_{ij} f_{ij} \ge 0, \quad \text{if} \quad \tilde{u} \ge 0$$

Trivial case: $\sum_{j \neq i} \alpha_{ij} f_{ij} = 0 \implies b_i = m_i \tilde{u}_i \ge 0$

Nontrivial case: let $c_i = \frac{1}{Q_i} \sum_{j \neq i} \alpha_{ij} f_{ij}$ where

$$Q_{i} = \begin{cases} Q_{i}^{+} = \tilde{u}_{i}^{\max} - \tilde{u}_{i}, & \text{if } \sum_{j \neq i} \alpha_{ij} f_{ij} > 0\\ Q_{i}^{-} = \tilde{u}_{i}^{\min} - \tilde{u}_{i}, & \text{if } \sum_{j \neq i} \alpha_{ij} f_{ij} < 0 \end{cases}$$

$$b_i = m_i \tilde{u}_i + c_i (\tilde{u}_k - \tilde{u}_i)$$
$$= (m_i - c_i) \tilde{u}_i + c_i \tilde{u}_k$$

Requirements

1.
$$m_i \ge c_i \ge 0$$

2. $\alpha_{ij} \equiv 0$, if $Q_i = 0$

Zalesak's limiter: $Q_i^{\pm} = 0 \Rightarrow R_i^{\pm} = 0 \Rightarrow \alpha_{ij} = 0$ $\sum_{j \neq i} \alpha_{ij} f_{ij} \leq \sum_{j \neq i} \alpha_{ij} \max\{0, f_{ij}\} \leq m_i R_i^+ P_i^+ \leq m_i Q_i^+$ $\sum_{j \neq i} \alpha_{ij} f_{ij} \geq \sum_{j \neq i} \alpha_{ij} \min\{0, f_{ij}\} \geq m_i R_i^- P_i^- \geq m_i Q_i^-$ This implies $m_i \geq c_i$