An Iterative FEM-FCT Algorithm for the Compressible Euler Equations

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- State of the art: discretization techniques
- Discrete upwinding for scalar equations
- Iterative defect correction scheme
- Generalized FEM-FCT formulation

- Matrix assembly for the Euler equations
- Construction of artificial viscosities
- Solution strategies for coupled equations
- Implementation of boundary conditions

Algebraic Flux Correction of FCT-type

Scalar conservation law
$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0$$
 in Ω

1. Linear high-order scheme (e.g. Galerkin FEM)

$$M_C \frac{u^{n+1} - u^n}{\Delta t} = \theta K u^{n+1} + (1 - \theta) K u^n, \qquad \exists j \neq i : k_{ij} < 0$$

2. Linear low-order scheme
$$L = K + D$$

$$M_L \frac{u^{n+1} - u^n}{\Delta t} = \theta L u^{n+1} + (1 - \theta) L u^n, \qquad l_{ij} \ge 0, \ \forall j \neq i$$

3. Nonlinear high-resolution scheme
$$f_i = \sum_{j \neq i} f_{ij}^a$$

$$M_L \frac{u^{n+1} - u^n}{\Delta t} = \theta L u^{n+1} + (1 - \theta) L u^n + f(u^{n+1}, u^n)$$

Equivalent representation $Au^{n+1} = \overline{B(\tilde{u})\tilde{u}}$, where

 $A = M_L - \theta \Delta t L$ is an *M*-matrix and $b_{ij} \ge 0, \forall i, j$

Algebraic Design Criteria

Algebraic Constraint I: (semi-discrete level)

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \sum_{j \neq i} \sigma_{ij} (u_j - u_i), \quad \sigma_{ij} \ge 0 \qquad u_i = \left\{ \begin{array}{c} \max_j \\ \min_j \end{array} \right\} u_j \quad \Rightarrow \quad u_j - u_i \left\{ \begin{array}{c} \leq \\ \geq \end{array} \right\} 0 \quad \Rightarrow \quad \frac{\mathrm{d}u_i}{\mathrm{d}t} \left\{ \begin{array}{c} \leq \\ \geq \end{array} \right\} 0$$

In 1D, Jameson's (1993) LED property is equivalent to Harten's (1983) TVD conditions.

Algebraic Constraint II:(fully discrete level)A discrete scheme of the form $Au^{n+1} = Bu^n, \quad u^n \ge 0$ is positivity-preservingif A is an M-matrix ($a_{ij} \le 0, \forall j \ne i, \quad A^{-1} \ge 0$) and all entries of B are non-negative.

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

where
$$d_{ij} = d_{ji}$$
 and $\sum_j d_{ij} = \sum_i d_{ij} = 0.$

Flux decomposition of diffusive terms into antisymmetric fluxes

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

High- and Low-Order Schemes

Difference between high- and low-order scheme

$$P(u) = [M_L - M_C] \frac{\mathrm{d}u}{\mathrm{d}t} - [\underbrace{L - K}_D]u$$

Flux decomposition of raw antidiffusion

$$P_i = \sum_{j \neq i} f_{ij}, \qquad f_{ij} = -[m_{ij}\frac{d}{dt} + d_{ij}](u_j - u_i), \quad f_{ji} = -f_{ij}$$

Nonlinear system for an implicit time discretization (standard θ – scheme)

$$M_L \frac{u^{n+1} - u^n}{\Delta t} = \theta L u^{n+1} + (1 - \theta) L u^n + P(u^{n+1}, u^n)$$

Successive approximation $Au^{(m+1)} = b^{(m+1)}$ $u^{(0)} = u^n$, $m = 0, 1, 2, ...$
Preconditioner $A = M_L - \theta \Delta t L$ and load-vector $b^{(m+1)} = b^n + P(u^{(m)}, u^n)$
Low-order contribution $b^n = [M_L + (1 - \theta) \Delta t L] u^n$
Raw antidiffusion $P_i^{(m)} = \sum_{j \neq i} f_{ij}^{(m)}$ with antisymmetric fluxes
 $f_{ij}^{(m)} = [m_{ij} - (1 - \theta) \Delta t d_{ij}^n](u_j^n - u_i^n) - [m_{ij} + \theta \Delta t d_{ij}^{(m)}](u_j^{(m)} - u_i^{(m)}) = -f_{ji}^{(m)}$

Basic FEM-FCT Algorithm

 $Au^{(m+1)} = b^{(m+1)}$

By construction, $A = M_L - \theta \Delta t L$ is an M-matrix which is easy to 'invert' and satisfies Algebraic Constraint II.

Multiply the antidiffusive fluxes by 'some' correction factors $\alpha_{ij} \in [0, 1]$ so that there Strategy: exists a matrix $B(\tilde{u}) \ge 0$ and a positivity-preserving solution \tilde{u} such that $b^{(m+1)} = B(\tilde{u})\tilde{u}$.

Positivity transfer cycle

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

Auxiliary solution to the explicit subproblem $M_L \tilde{u}^n = b^n$ proves to be positivity-preserving for $\Delta t \leq \frac{1}{1-\theta} \min_{i} \{-m_i/l_{ii} | l_{ii} < 0\}, \quad 0 \leq \theta < 1$

 $\alpha_{ii}^{(m)} = \alpha_{ij}(\tilde{u}^n, f_{ii}^{(m)}), \quad 0 \le \alpha_{ij} \le 1 \qquad \text{Zalesak's limiter (1979)}$ **Correction factors**

Modified right-hand side

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

The admissible percentage of the antidiffusive flux depends *Remark:* on the magnitude of the time step Δt .



Iterative FEM-FCT Algorithm

Build accepted antidiffusion into \tilde{u} and limit only the rejected portion. Strategy: $M_L \tilde{u}^{(m)} = b^{(m)},$ $b^{(0)} = b^n$ **Variable** auxiliary solution $\Delta f_{ij}^{(m)} = f_{ij}^{(m)} - g_{ij}^{(m)},$ $\Delta f_{ij}^{(0)} = f_{ij}^{(0)}$ Rejected antidiffusive fluxes $\alpha_{ij}^{(m)} = \alpha_{ij}(\tilde{u}^{(m)}, \Delta f_{ij}^{(m)}), \qquad 0 \le \alpha_{ij}^{(m)} \le 1$ Correction factors $g_{ij}^{(m+1)} = g_{ij}^{(m)} + \alpha_{ij}^{(m)} \Delta f_{ij}^{(m)}, \qquad g_{ij}^{(0)} = 0$ Accepted antidiffusive fluxes $b_{i}^{(m+1)} = b_{i}^{(m)} + \sum_{j \neq i} \alpha_{ij}^{(m)} \Delta f_{ij}^{(m)}$ Modified right-hand side Consistency: $\alpha_{ij}^{(m)} \equiv 1 \implies b_i^{(m+1)} = b_i^n + \sum_{j \neq i} \left(g_{ij}^{(m)} + \Delta f_{ij}^{(m)} \right) = b_i^n + \sum_{j \neq i} f_{ij}^{(m)}$

<u>Remark:</u> The iterative flux limiter makes it possible to 'recycle' the rejected antidiffusion.

Zalesak's Flux Limiter

- 1. Positive/negative contributions $P_i = P_i^+ + P_i^-$, where $P_i^{\pm} = \sum_{j \neq i} \max_{\min} \{0, f_{ij}\}$
- 2. Maximum/minimum increment

$$Q_i^{\pm} = \frac{\max}{\min} \Delta u_{ij}^{\pm}, \quad \text{where} \quad \Delta u_{ij}^{\pm} = \frac{\max}{\min} \{0, \tilde{u}_j - \tilde{u}_i\}$$

3. Nodal correction factors

$$R_{i}^{\pm} = \begin{cases} \min\{1, m_{i}Q_{i}^{\pm}/P_{i}^{\pm}\}, & \text{if } P_{i}^{\pm} \neq 0\\ 1, & \text{if } P_{i}^{\pm} = 0 \end{cases}$$

4. Final correction factors

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

<u>Remark:</u> This choice of the correction factors guarantees that

$$\tilde{u}_i^{(m)} + Q_i^- \le \tilde{u}_i^{(m+1)} \le \tilde{u}_i^{(m)} + Q_i^+$$

so that no enhancement of local extrema takes place.

Solid Body Rotation





Compressible Euler Equations

Divergence form

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{0} \qquad \text{where} \quad \nabla \cdot \mathbf{F} = \sum_{d=1}^{3} \frac{\partial F^d}{\partial x_d}$$

Conservative variables and fluxes

$$U = \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ \rho E \end{bmatrix} \qquad \mathbf{F} = (F^1, F^2, F^3) = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + p\mathcal{I} \\ \rho H \mathbf{v} \end{bmatrix} \qquad H = E + \frac{p}{\rho}$$
$$\gamma = c_p/c_v$$

Equation of state $p = (\gamma - 1)\rho(E - 0.5|\mathbf{v}|^2)$ for a polytropic gas

Quasi-linear form $\frac{\partial U}{\partial t} + \mathbf{A} \cdot \nabla U = \mathbf{0}$ where $\mathbf{A} \cdot \nabla U = \sum_{d=1}^{3} A^{d} \frac{\partial U}{\partial x_{d}}$

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

High-Order Scheme

Group FEM formulation

$M_{\alpha} \frac{\mathrm{d}U}{\mathrm{d}U}$	$-K_{\mathrm{TT}}$
$MC \overline{\mathrm{d}t}$	$-\Lambda 0$

$$(K\mathbf{U})_{i} = -\sum_{j} \mathbf{c}_{ij} \cdot \mathbf{F}_{j} = -\sum_{j \neq i} \mathbf{c}_{ij} \cdot (\mathbf{F}_{j} - \mathbf{F}_{i})$$

due to the fact that $\sum_{j} \varphi_{j} \equiv 1 \implies \mathbf{c}_{ii} = -\sum_{j \neq i} \mathbf{c}_{ij}$

Roe averaging $\mathbf{F}_j - \mathbf{F}_i = \hat{\mathbf{A}}_{ij}(\mathbf{U}_j - \mathbf{U}_i)$ where $\hat{\mathbf{A}}_{ij} = \mathbf{A}(\hat{\rho}_{ij}, \hat{\mathbf{v}}_{ij}, \hat{H}_{ij})$

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

Quasi-linear formulation

$$(K\mathbf{U})_i = -\sum_{j\neq i} \mathbf{c}_{ij} \cdot \hat{\mathbf{A}}_{ij} (\mathbf{U}_j - \mathbf{U}_i) = \sum_{j\neq i} (\mathbf{A}_{ij} + \mathbf{B}_{ij}) (\mathbf{U}_j - \mathbf{U}_i)$$

Cumulative Roe matrices

Contribution of edge $i \vec{j}$

$$A_{ij} = \mathbf{a}_{ij} \cdot \hat{\mathbf{A}}_{ij} = -A_{ji}, \qquad \mathbf{a}_{ij} = 0.5 \ (\mathbf{c}_{ij} - \mathbf{c}_{ji}) \qquad (A_{ij} + B_{ij})(\mathbf{U}_i - \mathbf{U}_j) \longrightarrow (K\mathbf{U})_i$$
$$B_{ij} = \mathbf{b}_{ij} \cdot \hat{\mathbf{A}}_{ij} = -B_{ji}, \qquad \mathbf{b}_{ij} = 0.5 \ (\mathbf{c}_{ij} + \mathbf{c}_{ji}) \qquad (A_{ij} - B_{ij})(\mathbf{U}_i - \mathbf{U}_j) \longrightarrow (K\mathbf{U})_j$$

Galerkin Matrix Assembly

Edge contribution to the operator K

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

Edge contribution to the operator *L*

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

Structure of the global matrix



Raw antidiffusive flux

$$\mathbf{F}_{ij} = -[\mathbf{M}_{ij}\frac{\mathrm{d}}{\mathrm{d}t} + \mathbf{D}_{ij} + \mathbf{B}_{ij}](\mathbf{U}_j - \mathbf{U}_i), \qquad \mathbf{F}_{ji} = -\mathbf{F}_{ij}$$

where $M_{ij} = m_{ij}I$ is a block of M_C and D_{ij} is the tensorial artificial diffusion.

<u>Remark:</u> Depending on the solution strategy (segregated/coupled), only 'a few' blocks of the global matrix need to be assembled and stored.

Design of Artificial Viscosities

LED principle for systems:(semi-discrete level)Render all off-diagonal matrix blocks L_{ij} positive semi-definiteCharacteristic decomposition $A_{ij} = |\mathbf{a}_{ij}| R_{ij} \Lambda_{ij} R_{ij}^{-1}$ $|\mathbf{a}_{ij}| = \sqrt{\mathbf{a}_{ij} \cdot \mathbf{a}_{ij}}$ where R_{ij} is the matrix of right eigenvectors and the eigenvalues of A_{ij}

are given by $\Lambda_{ij} = \text{diag}\{\hat{v}_{ij} - \hat{c}_{ij}, \hat{v}_{ij}, \hat{v}_{ij}, \hat{v}_{ij}, \hat{v}_{ij} + \hat{c}_{ij}\}$

Characteristic velocities $\hat{v}_{ij} = \frac{\mathbf{a}_{ij}}{|\mathbf{a}_{ij}|} \cdot \hat{\mathbf{v}}_{ij}, \qquad \hat{c}_{ij} = \sqrt{(\gamma - 1)(\hat{H}_{ij} - 0.5 |\hat{\mathbf{v}}_{ij}|^2)}$

System upwinding (expensive)

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

Generalization of Roe's approximate Riemann solver (1981) to multidimensions Scalar dissipation (efficient) $D_{ij} = d_{ij}I$ where $d_{ij} = |\mathbf{a}_{ij}| \max_i |\lambda_i|$

Optimal choice for FCT since artificial diffusion is removed by the flux limiter

Iterative Defect Correction

(Preconditioned) defect correction

Practical implementation

 $A(\mathbf{U}^{(m)}) \Delta \mathbf{U}^{(m+1)} = \mathbf{R}^{(m)}, \quad m = 0, 1, \dots$

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

$$U^{(m+1)} = U^{(m)} + [A(U^{(m)})]^{-1} R^{(m)}, \quad m = 0, 1, \dots$$
$$R^{(m)} = B^n - A(U^{(m)}) U^{(m)} + F(U^{(m)}, U^n)$$

 $A_{kl}^{(m)} := \delta_{kl} A_{kl}^{(m)}$

How to solve this system?

Block-Jacobi method

$$\begin{bmatrix} A_{11}^{(m)} & A_{12}^{(m)} & A_{13}^{(m)} & A_{14}^{(m)} & A_{15}^{(m)} \\ A_{21}^{(m)} & A_{22}^{(m)} & A_{23}^{(m)} & A_{24}^{(m)} & A_{25}^{(m)} \\ A_{31}^{(m)} & A_{32}^{(m)} & A_{33}^{(m)} & A_{34}^{(m)} & A_{35}^{(m)} \\ A_{41}^{(m)} & A_{42}^{(m)} & A_{43}^{(m)} & A_{44}^{(m)} & A_{45}^{(m)} \\ A_{51}^{(m)} & A_{52}^{(m)} & A_{53}^{(m)} & A_{54}^{(m)} & A_{55}^{(m)} \end{bmatrix} \begin{bmatrix} \Delta U_{1}^{(m+1)} \\ \Delta U_{2}^{(m+1)} \\ \Delta U_{2}^{(m+1)} \\ \Delta U_{3}^{(m+1)} \\ \Delta U_{4}^{(m+1)} \\ \Delta U_{5}^{(m+1)} \end{bmatrix} = \begin{bmatrix} R_{1}^{(m)} \\ R_{2}^{(m)} \\ R_{3}^{(m)} \\ R_{4}^{(m)} \\ R_{5}^{(m)} \end{bmatrix}$$

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

- \oplus only 5 blocks need to be assembled and stored
- \oplus equations can be solved separately or in parallel
- \ominus poor/no convergence for large time steps due to increasing stiffness of the equations for Mach numbers near 0 or 1 \longrightarrow local preconditioning

Implementation of Characteristic Boundary Conditions

Numbers of PBC vs. NBC $N_v = N_p + N_n$ depend on the local Mach number $M = |v_n|/c$

For all $\mathbf{x}_i \in \Gamma$ do

1. Nullify
$$a_{ij}^{kl} := 0 \quad \forall j \neq i, \ \forall l \neq k$$

and update $U_i^* = U_i^{(m)} + \text{diag}\{A_{ii}^{-1}\}R_i^{(m)}$

2. Transform U_i^* into W_i^* and apply PBC for the incoming Riemann invariants

3. Transform
$$\mathrm{W}_i^{**}$$
 to U_i^{**} and nullify $\mathrm{R}_i^{(m)}:=0$

N_p/N_n	1D	2D	3D
subsonic inflow	2/1	3/1	4/1
subsonic outflow	3/0	4/0	5/0
supersonic inflow	1/2	1/4	1/4
supersonic outflow	0/3	0/4	0/5

Variable transformations



- \oplus Values U_i^{**} represent Dirichlet boundary conditions for the end-of-step solution $U_i^{(m+1)}$
- \oplus No *ad hoc* extrapolation of data from the interior
- ⊕ Easy to implement as a 'black-box' module



Crank-Nicolson time-stepping, $\Delta t = 10^{-3}$, 16, 384 Q_1 elements at t = 0.231

Radially Symmetric Riemann Problem



Compression Corner $M_{\infty} = 2.5, \ \theta = 15^{\circ}$





Backward Euler time-stepping, $\Delta t = 10^{-2}$, 16, 384 Q_1 elements

Compression Corner $M_{\infty} = 2.5, \ \theta = 15^{\circ}$





Backward Euler time-stepping, $\Delta t = 10^{-2}$, 10, 016 Q_1 elements

Prandtl-Meyer Expansion $M_{\infty} = 2.5, \ \theta = 15^{\circ}$



Backward Euler time-stepping, $\Delta t = 10^{-2}$, 16, 384 Q_1 elements

Algebraic Flux Correction: FCT vs. TVD

- Both node-oriented flux limiters act at the algebraic level which makes them applicable to 'arbitrary' discretizations in time (explicit/implicit) and space (FD/FV/FE)
- Fully discrete FCT-type schemes, which are positivity preserving by construction, are to be recommended for time dependent problems
- TVD-type methods are preferable for the treatment of stationary flows. They are derived at the semi-discrete level but preserve positivity only upon convergence

Outstanding tasks

- Extension of the methodology to higher-order finite elements
- Robust and efficient iterative solvers for nonsymmetric algebraic systems
- Understanding of clipping and terracing phenomina
- Adaptive grid refinement for flux limiting schemes