High-resolution finite element schemes for (magneto)hydrodynamics

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Outline

1. High-resolution scheme
   - Finite element approximation
   - Flux-correction algorithm
2. Applications
   - Idealized Z-pinch implosion model
   - Ideal MHD equations
3. Efficient implementation
   - Blocking and parallelization

Finite element approximation

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

- Weak formulation

$$\int_\Omega W \frac{\partial U}{\partial t} - \nabla W \cdot \mathbf{F}(U)\,\mathrm{d}\mathbf{x} + \int_\Gamma W\,\mathbf{n}\cdot\mathbf{F}(U)\,\mathrm{d}s = 0, \quad \forall W \in \mathcal{W}$$

- Group representation[1]

$$U(\mathbf{x},t) \approx \sum_j \varphi_j(\mathbf{x})U_j(t), \qquad \mathbf{F}(U) \approx \sum_j \varphi_j(\mathbf{x})\mathbf{F}_j(t), \quad \mathbf{F}_j = \mathbf{F}(U_j)$$

- Semi-discrete high-order scheme

$$\boxed{\sum_j m_{ij}\frac{\mathrm{d}U_j}{\mathrm{d}t} - \sum_j \mathbf{c}_{ji}\cdot\mathbf{F}_j + \sum_j \mathbf{s}_{ij}\cdot\mathbf{F}_j = 0}$$

$$m_{ij} = \int_\Omega \varphi_i\varphi_j\,\mathrm{d}\mathbf{x}, \qquad \mathbf{c}_{ji} = \int_\Omega \nabla\varphi_i\varphi_j\,\mathrm{d}\mathbf{x}, \qquad \mathbf{s}_{ij} = \int_\Gamma \varphi_i\varphi_j\mathbf{n}\,\mathrm{d}s$$

[1] C.A.J. Fletcher, CMAME 1983, 37(2), pp. 225–244

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- Semi-discrete high-order scheme

$$\sum_j m_{ij} \frac{\mathrm{d}U_j}{\mathrm{d}t} - \sum_j \mathbf{c}_{ji} \cdot \mathbf{F}_j + \sum_j \mathbf{s}_{ij} \cdot \mathbf{F}_j = 0$$

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Finite element approximation, cont'd

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

- Semi-discrete high-order scheme[2]

$$\sum_j m_{ij} \frac{\mathrm{d}U_j}{\mathrm{d}t} - \sum_j \mathbf{c}_{ji} \cdot \mathbf{F}_j = 0, \qquad -\mathbf{c}_{ii} = \sum_{j \neq i} \mathbf{c}_{ij}$$

[2] D. Kuzmin, M. M, S. Turek, IJNMF 2003, 42(3), pp. 265–295

Finite element approximation, cont'd

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

- Semi-discrete high-order scheme[2]

$$\sum_j m_{ij} \frac{\mathrm{d}U_j}{\mathrm{d}t} + \sum_{j \neq i} G_{ij} = 0 \qquad G_{ij} = \mathbf{c}_{ij} \cdot \mathbf{F}_i - \mathbf{c}_{ji} \cdot \mathbf{F}_j$$

  - Efficient *edge-based* assembly of residual/right-hand side vector

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  - Efficient *edge-based* assembly of residual/right-hand side vector

- Semi-discrete low-order scheme

$$m_i \frac{\mathrm{d}U_i}{\mathrm{d}t} + \sum_{j \neq i} G_{ij} + D_{ij}(U_j - U_i) = 0 \qquad m_i = \sum_j m_{ij}$$

  - Flexibility in the choice of D_{ij} (Roe-/Rusanov-type)
  - Low-order scheme must satisfy physical constraints

[2] D. Kuzmin, M. M, S. Turek, IJNMF 2003, 42(3), pp. 265–295

Linearized FCT algorithm[3]

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

- Conservative flux decomposition $\qquad m_i(U_i^H - U_i^L) = \sum_{j\neq i} \dot{F}_{ij}$

$$\dot{F}_{ij} = m_{ij}\left(\frac{\mathrm{d}U_i}{\mathrm{d}t} - \frac{\mathrm{d}U_j}{\mathrm{d}t}\right) + D_{ij}(U_i - U_j), \qquad \dot{F}_{ji} = -\dot{F}_{ij}$$

- **Predictor:** Compute the low-order solution U^L and $\dot{U}^L \approx \frac{\mathrm{d}U}{\mathrm{d}t}$

  and linearize the raw antidiffusive flux $F_{ji}^L = -F_{ij}^L$

$$\boxed{F_{ij}^L = \Delta t\left[m_{ij}(\dot{U}_i^L - \dot{U}_j^L) + D_{ij}(U_i^L - U_j^L)\right]}$$

- **Corrector:** Apply the limited *conservative* antidiffusive fluxes

$$\boxed{m_i U_i = m_i U_i^L + \sum_{j\neq i} \alpha_{ij} F_{ij}^L} \qquad \alpha_{ji} = \alpha_{ij} \in [0,1]$$

[3] D. Kuzmin, JCP 2009, 228(7), pp. 2517–2534

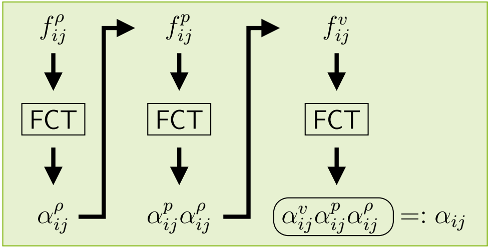
Flux limiting for systems

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

- Zalesak's flux limiter[4] is applicable to scalar variables only

$$f_{ij}^L,\ u_i^L \rightarrow \boxed{\text{FCT}} \rightarrow u_i^{\min} \leq u_i^L + \frac{1}{m_i}\sum_{j\neq i} \alpha_{ij} f_{ij}^L \leq u_i^{\max}$$

- Apply limiter to a set of control variables one after the other[5]



Nodal transformation

- $f_{ij}^\rho = \mathcal{T}_i^\rho F_{ij}^L$
- $f_{ij}^p = \mathcal{T}_i^p (\alpha_{ij}^\rho F_{ij}^L)$
- $f_{ij}^v = \mathcal{T}_i^v (\alpha_{ij}^p \alpha_{ij}^\rho F_{ij}^L)$

Flux correction: $\alpha_{ij} F_{ij}^L$

[4]S. Zalesak, JCP 1979, 31(3), pp. 335–362

[5]D. Kuzmin, M. M, J.N. Shadid, M. Shashkov, JCP 2010, 229(23), pp. 8766–8779

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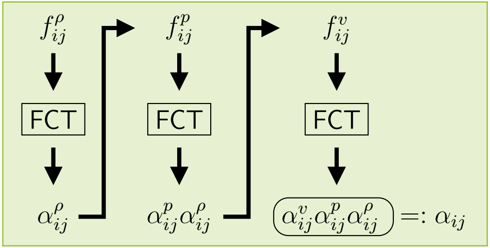

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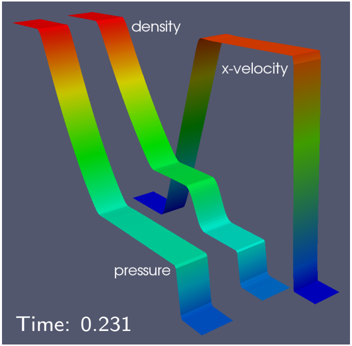
Benchmark: Sod's shock tube problem

- Transient compressible Euler equations in 2D
- Rusanov-type dissipation
- FCT: $\alpha_{ij} = \alpha_{ij}^{p}\alpha_{ij}^{\rho}$
- $10n \times n$ grid, Q_1 FEs



numerical convergence-order

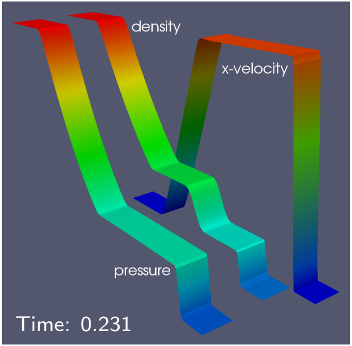
$$\kappa_u = \log \frac{\|u_{2h}-u_{4h}\|_1}{\|u_h-u_{2h}\|_1} / \log 2$$

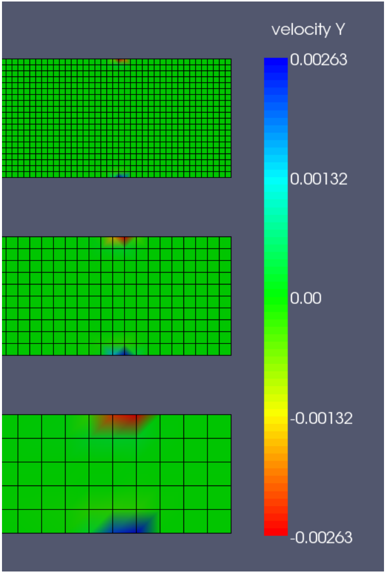
	Crank Nicolson time stepping			
	FCT		Low-order	
n_{fine}	κ_ρ	κ_p	κ_ρ	κ_p
20	0.624	1.027	0.193	0.623
40	0.970	1.003	0.421	0.671
80	1.079	1.005	0.575	0.701
160	1.073	1.005	0.624	0.730

	Backward Euler time stepping			
	FCT		Low-order	
n_{fine}	κ_ρ	κ_p	κ_ρ	κ_p
20	0.671	0.982	0.190	0.619
40	0.980	0.950	0.416	0.669
80	0.977	0.947	0.575	0.701
160	0.981	0.945	0.624	0.730

Benchmark: Sod's shock tube problem

Omitting the group FE representation in the boundary integral may lead to boundary errors!





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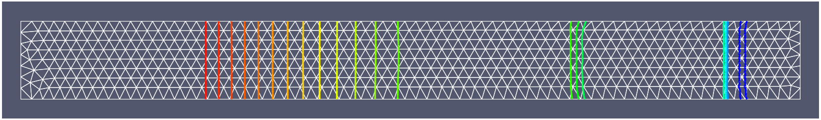


Coarse mesh with contour plot of density variable at time $t = 0.231$

	Crank Nicolson time stepping				Backward Euler time stepping			
	FCT		Low-order		FCT		Low-order	
#trias	κ_ρ	κ_p	κ_ρ	κ_p	κ_ρ	κ_p	κ_ρ	κ_p
18,176	0.925	0.876	0.364	0.665	0.955	0.841	0.357	0.662
72,704	0.874	0.800	0.539	0.679	0.820	0.732	0.536	0.679
290,816	0.806	0.934	0.614	0.718	0.765	0.875	0.616	0.719
1,163,264	0.948	0.966	0.641	0.739	0.889	0.905	0.642	0.740

Linearized FCT algorithm yields accurate and non-oscillatory solutions using P_1 and Q_1 finite elements on structured and unstructured meshes, respectively.

Idealized Z-pinch implosion model[6]

- Generalized Euler system coupled with scalar tracer equation

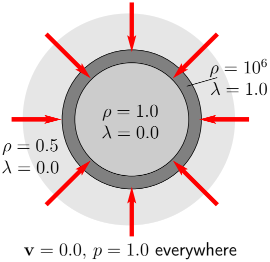
$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho\mathbf{v} \\ \rho E \\ \rho\lambda\end{bmatrix} + \nabla\cdot\begin{bmatrix}\rho\mathbf{v} \\ \rho\mathbf{v}\otimes\mathbf{v}+p\mathcal{I} \\ \rho E\mathbf{v}+p\mathbf{v} \\ \rho\lambda\mathbf{v}\end{bmatrix} = \begin{bmatrix}0 \\ \mathbf{f} \\ \mathbf{f}\cdot\mathbf{v} \\ 0\end{bmatrix}$$

- Equation of state

$$p = (\gamma-1)\rho(E-0.5|\mathbf{v}|^2)$$

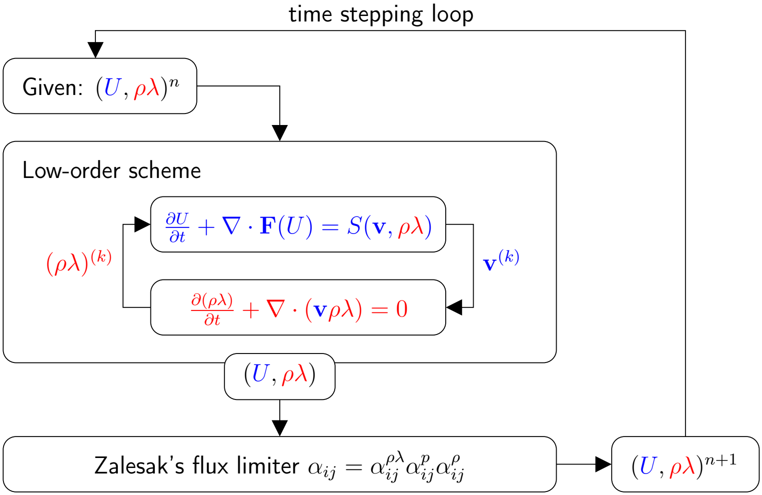
- Non-dimensional Lorentz force

$$\mathbf{f} = (\rho\lambda)\left(\frac{I(t)}{I_{\max}}\right)^2\frac{\hat{\mathbf{e}}_r}{r_{\text{eff}}}, \quad 0\le\lambda\le 1$$

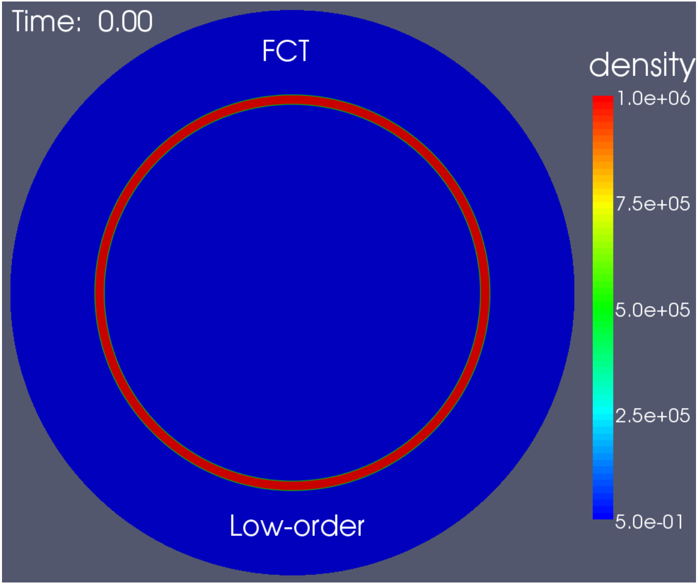


[6] J.W. Banks, J.N. Shadid, IJNMF 2009, 61(7), pp. 725–751

Coupled solution algorithm



Benchmark: Idealized Z-pinch implosion



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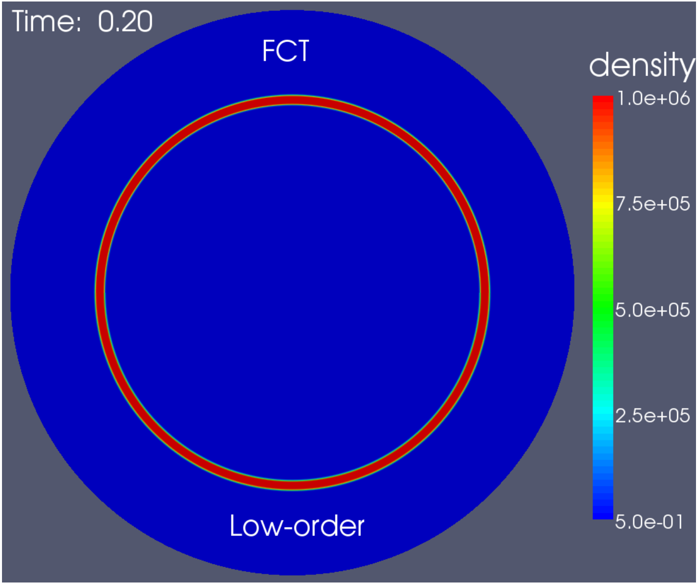

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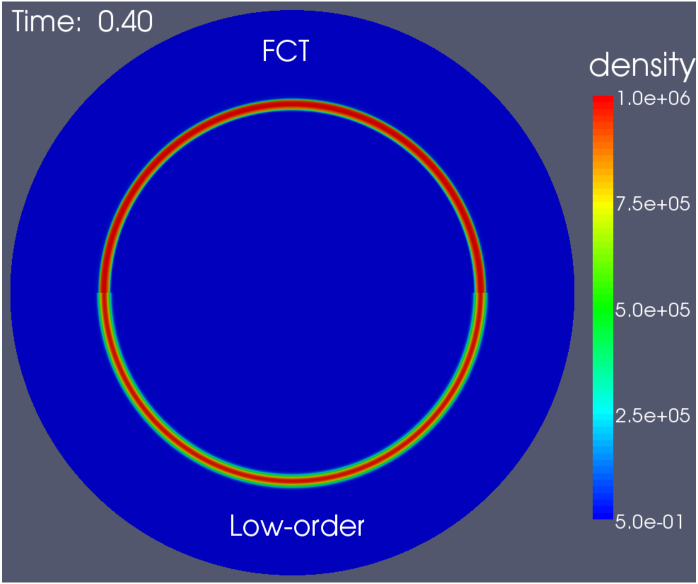

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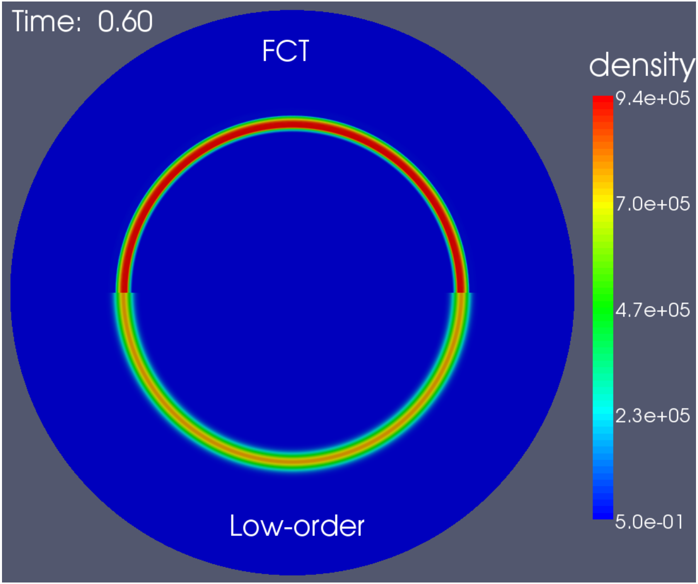

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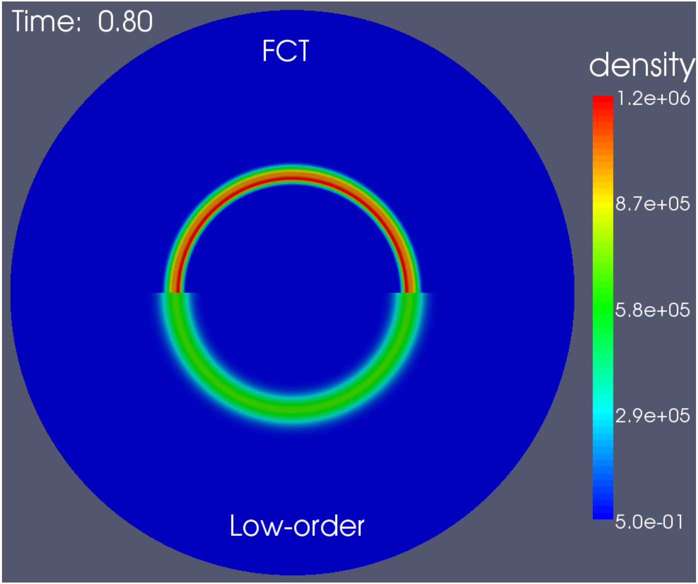

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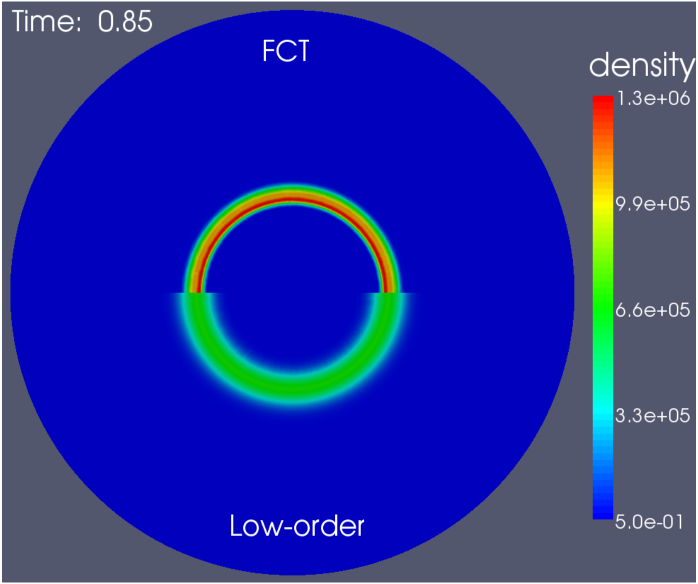

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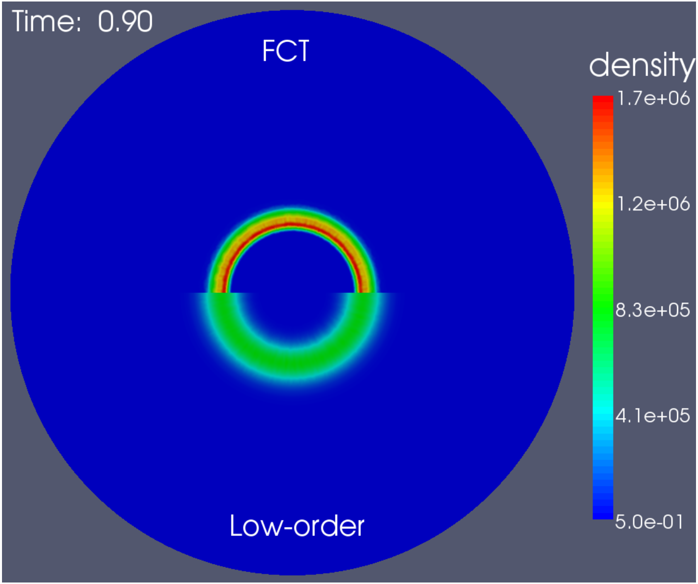

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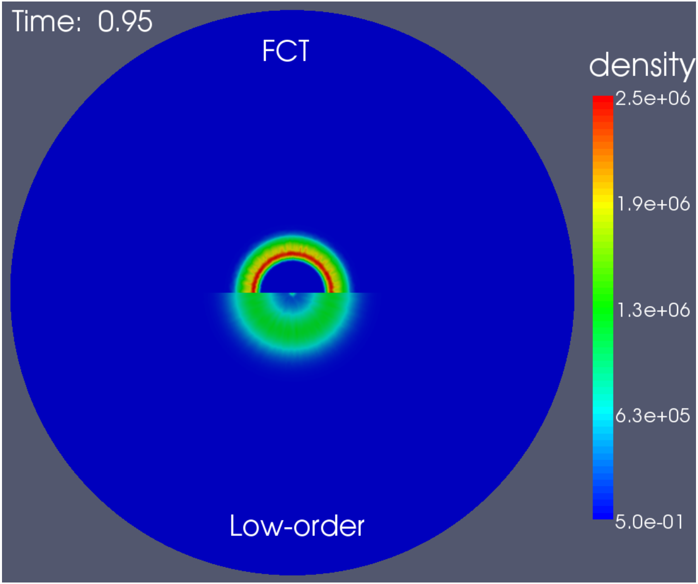

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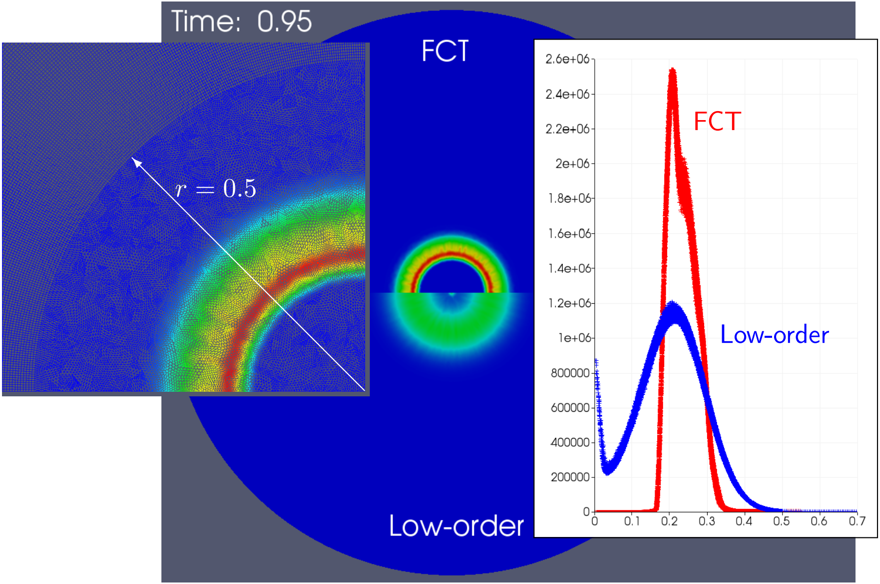


Ideal MHD equations

- Idealized MHD equations

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho\mathbf{v}\\ \mathbf{B}\\ \rho E\end{bmatrix}+\nabla\cdot\begin{bmatrix}\rho\mathbf{v}\\ \rho\mathbf{v}\otimes\mathbf{v}+p\mathcal{I}-\mathbf{B}\otimes\mathbf{B}\\ \mathbf{v}\otimes\mathbf{B}-\mathbf{B}\otimes\mathbf{v}\\ \rho E\mathbf{v}+p\mathbf{v}-(\mathbf{B}\cdot\mathbf{v})\mathbf{B}\end{bmatrix}=0$$

  subject to $\nabla\cdot\mathbf{B}=0$

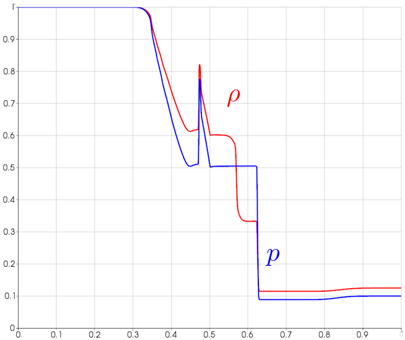
- Divergence involution in 1D: $\partial_x B_x = 0 \;\Rightarrow\; B_x = const$
- Hyperbolic conservation laws for 7 variables: ρ, $\mathbf{v}$, B_y, B_z, ρE
- Roe matrix (for arbitrary γ) by Cargo and Gallice[7]
- FCT limiter is applied to control variables ρ, p, B_y and B_z

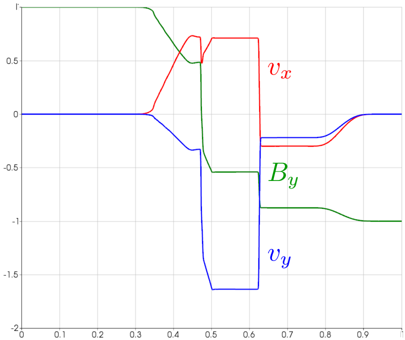
[7] P. Cargo, G. Gallice, JCP 1997, 136(2), pp.446–466

Benchmark: Shock tube problem

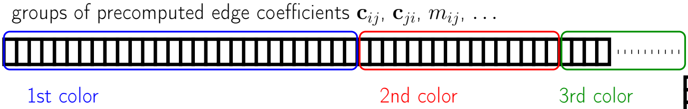
- $\gamma = 1.4, \quad B_x = 0.75, \quad t_{\text{fin}} = 0.1,$ 800 grid points

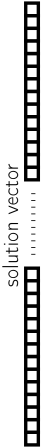
$$(\rho, \mathbf{v}, B_y, B_z, p)^T = \begin{cases} (1.0 \quad ,0.0, \quad 1.0, 0.0, 1.0)^T & \text{if } x \le 0.5 \\ (0.125, 0.0, -1.0, 0.0, 0.1)^T & \text{if } x > 0.5 \end{cases}$$



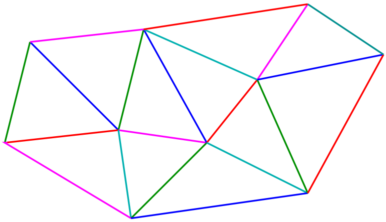


Parallel edge-based assembly





Perform edge-coloring of the FE sparsity graph such that all endpoints of all edges in one group are different and can be treated simultaneously.



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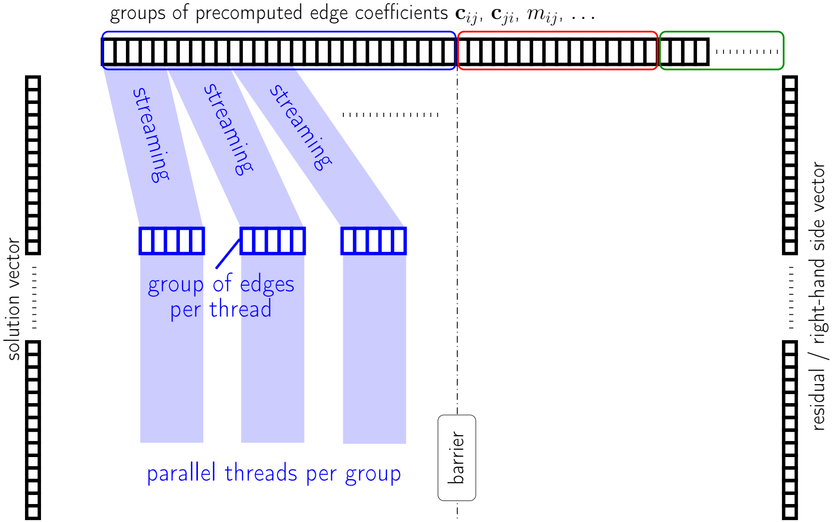

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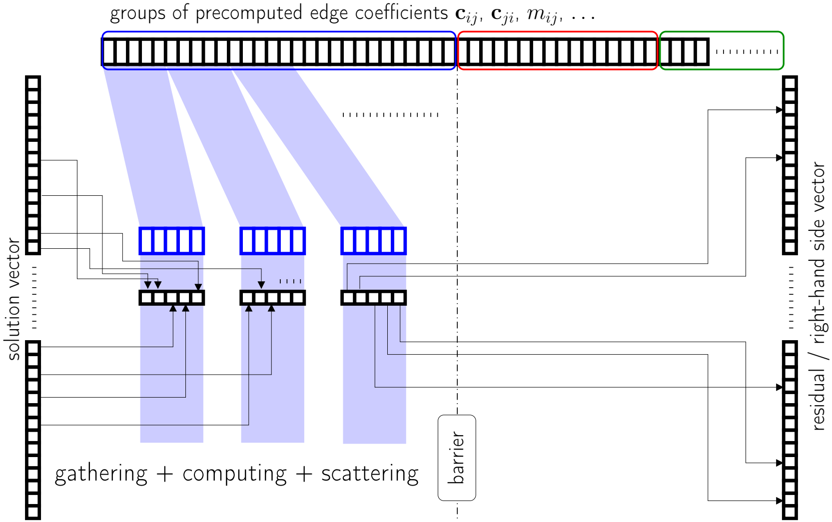
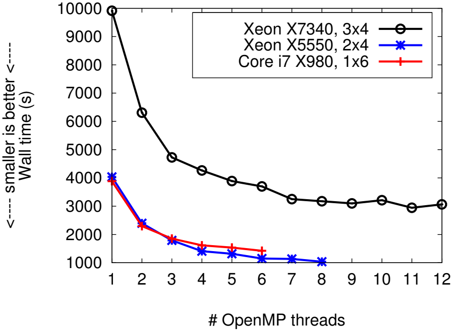


Computational efficiency

- 2D-Shock tube problem
- Roe-type dissipation
- FCT: $\alpha_{ij} = \alpha_{ij}^p \alpha_{ij}^\rho$
- 290,816 triangles
- 2,310 time steps BE
- 800 edges per thread



Edge-based formulation leads to an efficient assembly of vectors/matrices

Conclusions

- Linearized flux correction algorithm
  - ensures boundedness of physical quantities
  - preserves symmetry on unstructured grids
  - is applicable to 'challenging' applications
  - admits an efficient edge-based assembly
- Future research
  - extension to multidimensional MHD equations
  - treatment of the $\nabla \cdot \mathbf{B} = 0$ involution

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Thank you for your attention!

References

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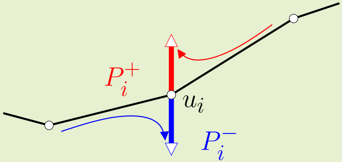
2. D. Kuzmin, M. M, S. Turek, *Multidimensional FEM-FCT schemes for arbitrary time-stepping*. IJNMF 2003, 42(3), pp. 265-295.
3. D. Kuzmin, *Explicit and implicit FEM-FCT algorithms with flux linearization*. JCP 2009, 228(7), pp. 2517–2534.
4. S.T. Zalesak, *Fully multidimensional flux-corrected transport algorithms for fluids*. JCP 1979, 31(3), pp. 335–362.
5. D. Kuzmin, M. M, J.N. Shadid, M. Shashkov, *Failsafe flux limiting and constrained data projections for equations of gas dynamics*. JCP 2010, 229(23), pp. 8766–8779.
6. J.W. Banks, J.N. Shadid, *An Euler system source term that develops prototype Z-pinch implosions intended for the evaluation of shock-hydro methods*. IJNMF 2009, 61(7), pp. 725–751.
7. P. Cargo, G. Gallice, *Roe matrices for ideal MHD and systematic construction of Roe matrices for systems of conservation laws*. JCP 1997, 136(2), pp.446–466.

Zalesak's flux limiter[5]

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



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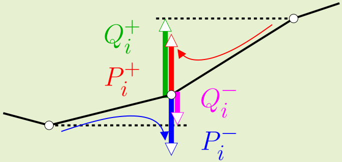

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- Limit antidiffusive flux if it exceeds the distance to upper/lower bounds

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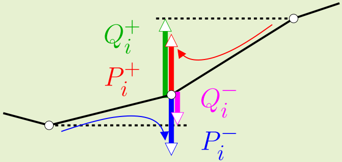


- Consider sums of positive/negative antidiffusive fluxes into each node
- Limit antidiffusive flux if it exceeds the distance to upper/lower bounds

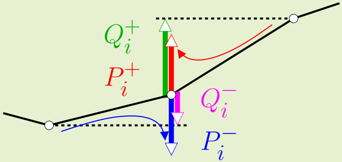
- Compute nodal correction factors

$$R_i^+ = \min\{1, Q_i^+/P_i^+\} \quad \text{and} \quad R_i^- = \min\{1, Q_i^-/P_i^-\}$$

[5] S. Zalesak, JCP 1979, 31(3), pp. 335–362

Zalesak's flux limiter[5]

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



- Consider sums of positive/negative antidiffusive fluxes into each node
- Limit antidiffusive flux if it exceeds the distance to upper/lower bounds

- Compute nodal correction factors

$$R_i^+ = \min\{1, Q_i^+/P_i^+\} \quad \text{and} \quad R_i^- = \min\{1, Q_i^-/P_i^-\}$$

- Limit antidiffusive flux for edge ij by

$$\alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\} & \text{for positive fluxes} \\ \min\{R_i^-, R_j^+\} & \text{for negative fluxes} \end{cases}$$

[5] S. Zalesak, JCP 1979, 31(3), pp. 335–362

Extended version of Zalesak's FCT limiter

Input: auxiliary solution u^L and antidiffusive fluxes f_{ij}^u, where $f_{ji}^u \neq f_{ij}^u$

1. Sums of positive/negative antidiffusive fluxes into node i

$$P_i^+ = \sum_{j\neq i} \max\{0, f_{ij}^u\}, \qquad P_i^- = \sum_{j\neq i} \min\{0, f_{ij}^u\}$$

2. Upper/lower bounds based on the local extrema of u^L

$$Q_i^+ = m_i(u_i^{\max} - u_i^L), \qquad Q_i^- = m_i(u_i^{\min} - u_i^L)$$

3. Correction factors $\alpha_{ij}^u = \alpha_{ji}^u$ to satisfy the FCT constraints

$$\alpha_{ij}^u = \min\{R_{ij}, R_{ji}\}, \quad R_{ij} = \begin{cases} \min\{1, Q_i^+/P_i^+\} & \text{if } f_{ij}^u \geq 0 \\ \min\{1, Q_i^-/P_i^-\} & \text{if } f_{ij}^u < 0 \end{cases}$$

Node-based transformation of control variables

- Conservative variables: density, momentum, total energy

$$U_i = [\rho_i, (\rho\mathbf{v})_i, (\rho E)_i], \qquad F_{ij} = \left[f_{ij}^{\rho}, \mathbf{f}_{ij}^{\rho v}, f_{ij}^{\rho E}\right], \qquad F_{ji} = -F_{ij}$$

- Primitive variables $V = TU$: density, velocity, pressure

$$V_i = [\rho_i, \mathbf{v}_i, p_i], \qquad \mathbf{v}_i = \frac{(\rho\mathbf{v})_i}{\rho_i}, \qquad p_i = (\gamma - 1)\left[(\rho E)_i - \frac{|(\rho\mathbf{v})_i|^2}{2\rho_i}\right]$$

$$G_{ij} = \left[f_{ij}^{\rho}, \mathbf{f}_{ij}^{v}, f_{ij}^{p}\right] = T(U_i)F_{ij}, \qquad T(U_j)F_{ji} = G_{ji} \neq -G_{ij}$$

- Raw antidiffusive fluxes for the velocity and pressure

$$\mathbf{f}_{ij}^{v} = \frac{\mathbf{f}_{ij}^{\rho v} - \mathbf{v}_i f_{ij}^{\rho}}{\rho_i}, \qquad f_{ij}^{p} = (\gamma - 1)\left[\frac{|\mathbf{v}_i|^2}{2} f_{ij}^{\rho} - \mathbf{v}_i \cdot \mathbf{f}_{ij}^{\rho v} + f_{ij}^{\rho E}\right]$$