

High-resolution finite element schemes for coupled problems

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- Generalized Euler system coupled with scalar tracer equation

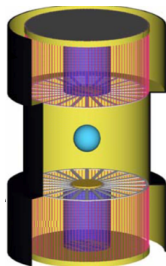
$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ \rho E \\ \rho \lambda \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + p \mathcal{I} \\ \rho E \mathbf{v} + p \mathbf{v} \\ \rho \lambda \mathbf{v} \end{bmatrix} = \begin{bmatrix}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

- Non-dimensional Lorentz force

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

$$I(t) = \sqrt{12(1-t^4)} t^2$$

$$r_{\text{eff}} = \max\{r/R_0, r_{\min}\}$$



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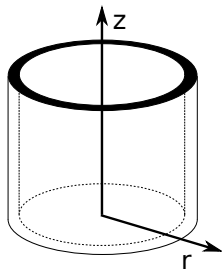
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Outline

- 1 High-resolution schemes for scalar conservation laws
- 2 High-resolution schemes for hyperbolic systems
- 3 Coupled solution algorithm for phenomenological model
- 4 Mesh adaptation for transient flows
- 5 Conclusions and Outlook

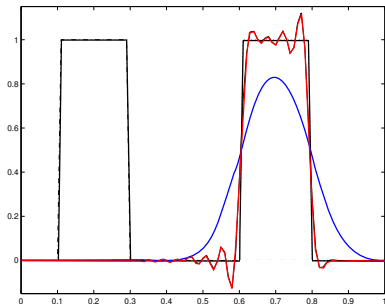
Numerical troubles

Convection in 1D

$$\begin{cases} \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} = 0, & v > 0 \\ u(x, 0) = u_0(x), & \forall x \in (0, 1) \\ u(0, t) = 0, & \forall t \geq 0 \end{cases}$$

finite difference approximation

backward Euler time stepping



- Qualitative properties: nonnegativity, no creation of new extrema
- Underresolved approximations: spurious wiggles, numerical diffusion

Design criteria I

- Model problem $M \frac{du}{dt} = Cu, \quad M = \text{diag}\{m_i\}, \quad C = \{c_{ij}\}$

Local extremum diminishing scheme, *Jameson '93*

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

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Proof: maximum u_i at node i implies $u_i \geq u_j, \quad \forall j \neq i$

$$c_{ij} (u_j - u_i) \leq 0, \quad \forall j \neq i \quad \Rightarrow \quad \frac{du_i}{dt} \leq 0$$

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- General form $m_i \frac{du_i}{dt} = \sum_{j \neq i} c_{ij} (u_j - u_i) + u_i \sum_j c_{ij}$

Design criteria II

Positivity-preserving scheme

If A is a monotone matrix (i.e. $A^{-1} \geq 0$) and $B \geq 0$ then

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

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- Sufficient conditions for regular matrix A to be monotone
 - A has positive diagonal coefficients $a_{ii} > 0, \quad \forall i$
 - A has no positive off-diagonal entries $a_{ij} \leq 0, \quad \forall j \neq i$
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- Two-level θ -scheme $M \frac{u^{n+1} - u^n}{\Delta t} = \theta C u^{n+1} + (1 - \theta) C u^n$

Constraints on $A = M - \theta \Delta t C$ and $B = M + (1 - \theta) \Delta t C$
($0 \leq \theta \leq 1$) yield computable bounds on the time step Δt .

Galerkin finite element scheme

- Continuity equation $\int_{\Omega} w \left[\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) \right] d\mathbf{x} = 0, \quad \forall w$

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■ Galerkin FEM $M_C \frac{du}{dt} = K u, \quad M_C = \{m_{ij}\}, \quad K = \{k_{ij}\}$

$$m_{ij} = \int_{\Omega} \varphi_i \varphi_j d\mathbf{x}, \quad k_{ij} = -\mathbf{c}_{ij} \cdot \mathbf{v}_j, \quad \mathbf{c}_{ij} = \int_{\Omega} \varphi_i \nabla \varphi_j d\mathbf{x}$$

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Lumped mass high-order scheme $M_L \frac{du}{dt} = K u$

$$m_i \frac{du_i}{dt} = \sum_{j \neq i} k_{ij} (u_j - u_i) + u_i \sum_j k_{ij}, \quad m_i = \sum_j m_{ij}$$

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For P_1/Q_1 FEs $m_i > 0, \forall i$ but $k_{ij} < 0$ for some $j \neq i$. **⚡LED**

Discrete upwind scheme

Low-order scheme

$$M_L \frac{du}{dt} = Lu, \quad L = K + D$$

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- Properties of discrete diffusion operators $D = \{d_{ij}\}$

$$d_{ij} = d_{ji}, \quad \sum_j d_{ij} = \sum_i d_{ij} = 0 \quad \Rightarrow \quad d_{ii} = - \sum_{j \neq i} d_{ij}$$

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- Choice of artificial diffusion coefficients

$$d_{ij} = \max\{-k_{ij}, 0, -k_{ji}\}$$

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Linear monotone methods are at most first order accurate!

Algebraic flux correction

- Residual difference $f = (M_L - M_C) \frac{du}{dt} - Du$

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- Enforcing positivity constraints $\bar{f}_{ij} = \alpha_{ij} f_{ij}, \quad 0 \leq \alpha_{ij} \leq 1$
 - high-order approximation ($\alpha_{ij} = 1$) to be used in smooth regions
 - low-order approximation ($\alpha_{ij} = 0$) to be used near steep fronts

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 - high-order approximation ($\alpha_{ij} = 1$) to be used in smooth regions
 - low-order approximation ($\alpha_{ij} = 0$) to be used near step fronts
- High-resolution scheme $M_L \frac{du}{dt} = Lu + \bar{f}(u), \quad \bar{f}_i = \sum_{j \neq i} \bar{f}_{ij}$

Roadmap of nonlinear FEM-FCT schemes

Nonlinear algebraic system for the two-level θ -scheme, $0 < \theta \leq 1$

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

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- 2 Compute successive approximations to u^{n+1} until convergence
 - Apply Zalesak's limiter to constrain antidiffusive fluxes

$$M_L \bar{u} = M_L \tilde{u} + \Delta t \bar{f}(u^{(m)}, u^n)$$

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$$M_L \bar{u} = M_L \tilde{u} + \Delta t \bar{f}(u^{(m)}, u^n)$$

- Solve the linear system for the new solution $u^{(m+1)} \approx u^{n+1}$

$$[M_L - \theta \Delta t L]u^{(m+1)} = M_L \bar{u}$$

Roadmap of linearized FEM-FCT schemes

Linearization of antidiffusive fluxes

$$f = (M_L - M_C)\dot{u}^L - Du^L, \quad \dot{u}^L \approx \frac{du}{dt}, \quad u^L \approx u^{n+1}$$

Roadmap of linearized FEM-FCT schemes

Linearization of antidiffusive fluxes

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- 1 Compute a provisional low-order solution

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

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$$M_C\dot{u}^L = Ku^L \quad \text{or} \quad M_L\dot{u}^L = Lu^L$$

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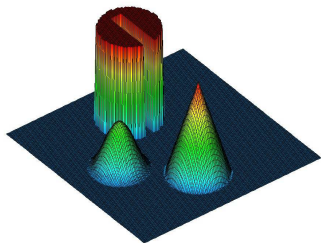
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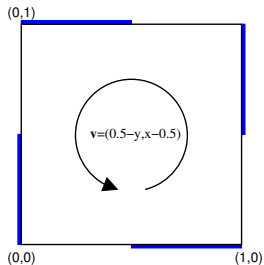
Solid body rotation

Crank-Nicolson time-stepping, Q_1 elements, $h = 1/128$, $\Delta t = 10^{-3}$

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0 \quad \text{in } \Omega = (0, 1) \times (0, 1), \quad u = 0 \quad \text{on } \Gamma_D$$

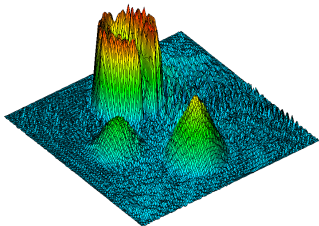


initial/exact solution $t = 2\pi k$

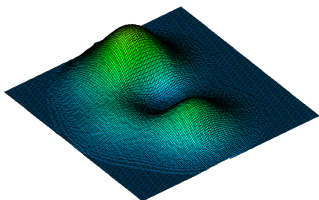


domain and velocity

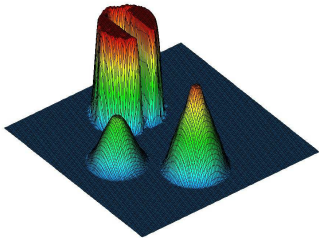
Solid body rotation $t = 2\pi$



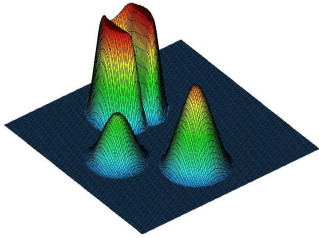
high-order solution



low-order solution



nonlinear FEM-FCT solution



linearized FEM-FCT solution

Remarks

- High-resolution schemes for scalar conservation can be based on the Galerkin method by enforcing mathematical constraints a posteriori
- FEM-FCT schemes based on flux linearization provide an efficient alternative to the nonlinear flux corrected transport algorithm
- Algebraic flux correction can be generalized to hyperbolic systems

Design criteria III

Reminder: LED criterion for scalar equations

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

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Generalized LED criterion for hyperbolic systems

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- Condition for matrix C_{ij} to be positive semi-definite

$$x^T C_{ij} x \geq 0, \quad \forall x \quad \Leftrightarrow \quad \text{all eigenvalues of } C_{ij} \text{ are non-negative}$$

Hyperbolic conservation laws

Divergence form

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F} = 0, \quad \nabla \cdot \mathbf{F} = \sum_d \frac{\partial F^d}{\partial x_d}$$

Quasi-linear form

$$\frac{\partial U}{\partial t} + \mathbf{A} \cdot \nabla U = 0, \quad A^d = \frac{\partial F^d}{\partial U}$$

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- Group finite element formulation

Quasi-linear form

$$\frac{\partial U}{\partial t} + \mathbf{A} \cdot \nabla U = 0, \quad A^d = \frac{\partial F^d}{\partial U}$$

$$U = \sum_j U_j \varphi_j, \quad \mathbf{F} = \sum_j \mathbf{F}_j \varphi_j$$

Hyperbolic conservation laws

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- Group finite element formulation
- Lumped mass Galerkin method

Quasi-linear form

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$$U = \sum_j U_j \varphi_j, \quad \mathbf{F} = \sum_j \mathbf{F}_j \varphi_j$$

$$M_L \frac{dU}{dt} = KU, \quad K = \{K_{ij}\}$$

Hyperbolic conservation laws

Divergence form

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- Decomposition of the right-hand side into edge contributions

$$\mathbf{c}_{ii} = - \sum_{j \neq i} \mathbf{c}_{ij} \Rightarrow (KU)_i = - \sum_{j \neq i} \mathbf{c}_{ij} \cdot (\mathbf{F}_j - \mathbf{F}_i)$$

Upwinding for the Euler equations

- Representation based on homogeneity property $F^d = A^d U, \quad \forall d$

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- Eigenvalues of matrix $K_{ij} = R_{ij} \Lambda_{ij} R_{ij}^{-1}, \quad \Lambda_{ij} \in \mathbb{R}^5$

$$\lambda_1 = v_{ij} + |\mathbf{c}_{ij}| c_j, \quad \lambda_{2,3,4} = v_{ij}, \quad \lambda_5 = v_{ij} - |\mathbf{c}_{ij}| c_j$$

$$v_{ij} = -\mathbf{c}_{ij} \cdot \mathbf{v}_j, \quad c_j = \sqrt{(\gamma - 1) \left(E_j + p_j / \rho_j - \frac{1}{2} |\mathbf{v}_j|^2 \right)}$$

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- Rusanov-type artificial viscosities $L_{ij} = K_{ij} + D_{ij}, \quad D_{ij} = d_{ij} \mathbf{I}$

$$d_{ij} = \max\{|v_{ij}| + |\mathbf{c}_{ij}| c_j, |v_{ji}| + |\mathbf{c}_{ji}| c_i\}, \quad v_{ji} = -\mathbf{c}_{ji} \cdot \mathbf{v}_i$$

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- High-resolution scheme $M_L \frac{dU}{dt} = LU + \bar{F}(U)$

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Choosing the 'best' strategy is quite an art which requires a good knowledge of the physics of the problem to be solved.

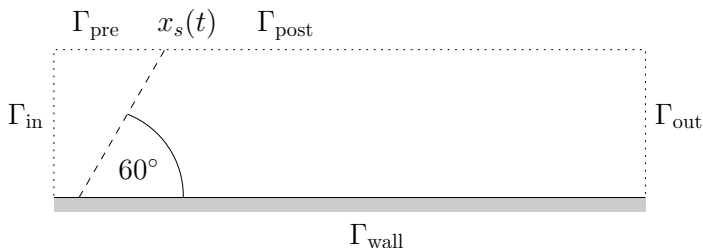
Double Mach reflection

Pre- and post-shock initial conditions in $\Omega = (0, 4) \times (0, 1)$

$$\begin{bmatrix} \rho_{\text{pre}} \\ u_{\text{pre}} \\ v_{\text{pre}} \\ p_{\text{pre}} \end{bmatrix} = \begin{bmatrix} 8.0 \\ 8.25 \cos(30^\circ) \\ -8.25 \sin(30^\circ) \\ 116.5 \end{bmatrix} \quad \begin{bmatrix} \rho_{\text{post}} \\ u_{\text{post}} \\ v_{\text{post}} \\ p_{\text{post}} \end{bmatrix} = \begin{bmatrix} 1.4 \\ 0.0 \\ 0.0 \\ 1.0 \end{bmatrix}$$

Time-dependent boundary conditions $x_s(t) = \frac{1}{6} + \frac{1+20t}{\sqrt{3}}$

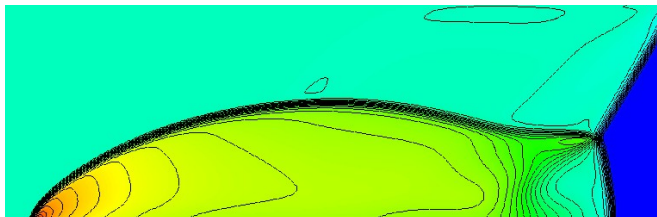
$$\Gamma_{\text{pre}} = \{x < x_s(t), y = 1\}, \quad \Gamma_{\text{post}} = \{x \geq x_s(t), y = 1\}$$



Double Mach reflection, density profile at $t=0.2$



Characteristic FEM-FCT vs. low-order solution



Remarks

- High-resolution schemes for hyperbolic systems can be based on a generalized local extremum diminishing criterion
- Flux correction can be performed in characteristic variables
- Conservative flux limiting based on a set of indicator variables requires the synchronization of correction factors

Idealized Z-pinch implosion model revisited

- Generalized Euler system coupled with scalar transport equation

$$\frac{\partial U}{\partial t} + \nabla \cdot \mathbf{F}(U) = S(U, \xi), \quad \frac{\partial \xi}{\partial t} + \nabla \cdot (\xi \mathbf{v}) = 0$$

- Conservative variables, fluxes and source term

$$U = \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ \rho E \end{bmatrix}, \quad \xi = \rho \lambda, \quad \mathbf{F} = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + p \mathcal{I} \\ \rho E \mathbf{v} + p \mathbf{v} \end{bmatrix}, \quad S = \begin{bmatrix} 0 \\ \mathbf{f} \\ \mathbf{f} \cdot \mathbf{v} \end{bmatrix}$$

- EOS for an ideal gas and non-dimensional Lorentz force term

$$p = (\gamma - 1) \rho \left(E - \frac{1}{2} |\mathbf{v}|^2 \right), \quad \mathbf{f} = \xi \left(\frac{I(t)}{I_{\max}} \right)^2 \frac{\hat{\mathbf{e}}_r}{r_{\text{eff}}}$$

Coupled solution algorithm

For $n = 0, 1, \dots, \bar{n} - 1$

time-stepping loop

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- Update the low-order solution to the Euler system

For $l = 0, 1, \dots, \bar{l} - 1$

defect correction loop

$$\frac{U^{(k+1,l+1)} - U^n}{\Delta t} + \theta \nabla \cdot \mathbf{F}(U^{(k+1,l+1)}) + (1 - \theta) \nabla \cdot \mathbf{F}(U^n) = \theta S(\mathbf{v}^{(k+1,l+1)}, \xi^{(k)}) + (1 - \theta) S(\mathbf{v}^n, \xi^n)$$

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- Apply synchronized FCT correction to $U^L = U^{(\bar{k}, \bar{l})}$, $\xi^L = \xi^{(\bar{k})}$

Finishing touches

- Uniform dissipation for the Euler system and the tracer equation

$$D_{ij} = d_{ij}I, \quad d_{ij} = \max\{|-\mathbf{c}_{ij} \cdot \mathbf{v}_j| + |\mathbf{c}_{ij}| c_j, |-\mathbf{c}_{ji} \cdot \mathbf{v}_i| + |\mathbf{c}_{ji}| c_i\}$$

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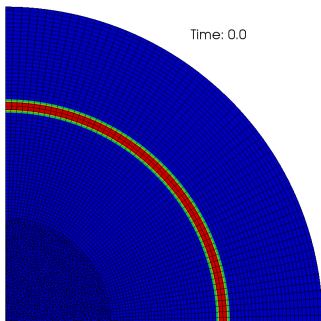
Idealized Z-pinch implosion

Non-dimensional initial conditions

▶ movie

$$\rho' = \begin{cases} 1.0 & \text{if } r < R_0 \\ 10^6 & \text{if } r \in [R_0, R_0 + \Delta] \\ 0.5 & \text{if } r > R_0 + \Delta \end{cases} \quad \xi' = \begin{cases} 10^6 & \text{if } r \in [R_0, R_0 + \Delta] \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{v}' = 0.0, \quad p' = 1.0, \quad R_0 = 1, \quad \Delta = 0.05, \quad r_{\text{eff}} = 10^{-4}, \quad I_{\text{max}} = 1.0$$



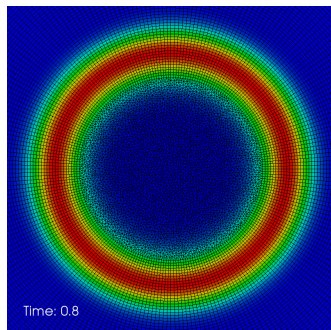
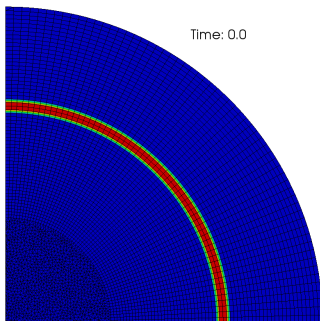
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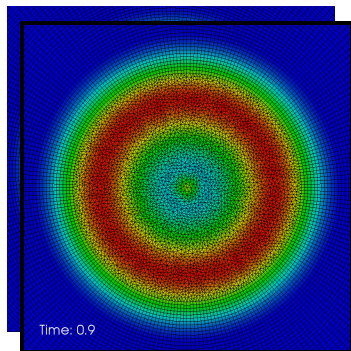
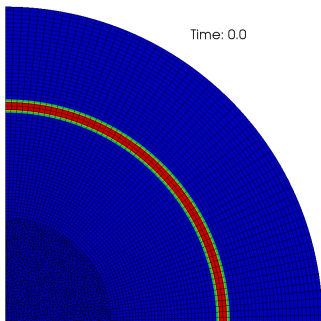
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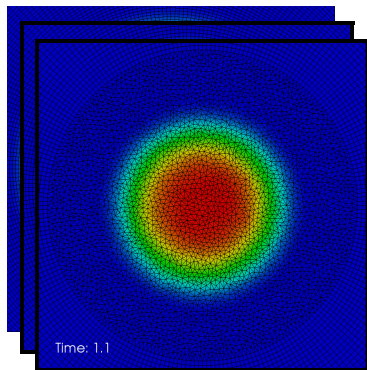
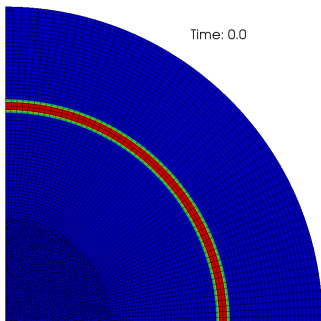
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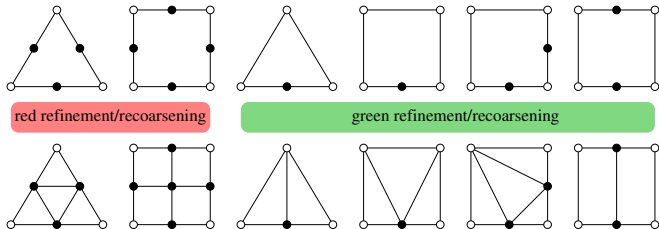


Dynamic mesh adaptation

Conformal refinement algorithm

Bank, et al. '83

- 1 subdivide marked elements regularly (red rule)
- 2 eliminate 'hanging nodes' by transition cells (green rule)

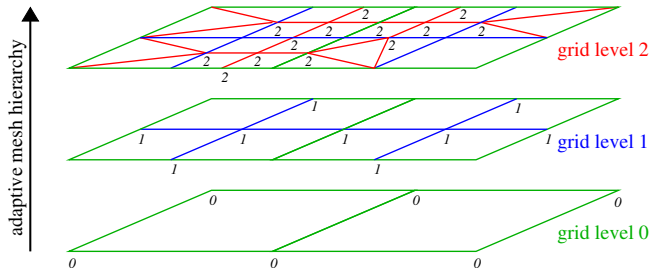


Dynamic mesh adaptation, cont'd

- Vertex-locking algorithm is used to reverse mesh refinement
- Nodal generation function provides all necessary information:
element type, inter-element relationship, refinement level, ...

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Solid body rotation

Crank-Nicolson scheme, P_1/Q_1 elements, $h_{\min} = 1/512$, $\Delta t = 10^{-3}$

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0 \quad \text{in } \Omega = (0, 1) \times (0, 1), \quad u = 0 \quad \text{on } \Gamma_D$$

Conclusions and Outlook

- Algebraic flux correction techniques can be used to compute highly accurate and symmetric solutions to prototypical Z-pinch implosions
- Globally coupled solution strategy makes it possible to treat the Euler system and the scalar tracer equation one after the other
- Mesh adaptation is a handy tool to compensate the artificial diffusion of the low-order method in the vicinity of steep fronts

Future plans for the Z-pinch implosions model

- Analysis of the coupled solution vs. operator splitting approach
- Mesh adaptation based on reliable error indicators/estimators

Constraints on the time step size

Two-level θ -time stepping scheme, $0 \leq \theta \leq 1$

$$m_i \frac{u_i^{n+1} - u_i^n}{\Delta t} = \theta \sum_j c_{ij} u_j^{n+1} + (1 - \theta) \sum_j c_{ij} u_j^n, \quad c_{ij} \geq 0, \quad \forall j \neq i$$

- System matrices $A = M_L - \theta \Delta t C, \quad B = M_L + (1 - \theta) \Delta t C$
- Off-diagonal entries $a_{ij} = -\theta \Delta t c_{ij} \leq 0, \quad b_{ij} = (1 - \theta) \Delta t c_{ij} \geq 0$
- Diagonal coefficient $a_{ii} = m_i - \theta \Delta t c_{ii} > \theta \Delta t \sum_{j \neq i} c_{ij} \geq 0, \quad \forall i$
- Diagonal coefficient $b_{ii} = m_i + (1 - \theta) \Delta t c_{ii} \geq 0, \quad \forall i$

Zalesak's multidimensional FCT limiter

Input: raw antidiffusive fluxes f_{ij} , auxiliary solution \tilde{u}

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

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

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$$Q_i^+ = \frac{m_i}{\Delta t} (\tilde{u}_i^{\max} - \tilde{u}_i), \quad Q_i^- = \frac{m_i}{\Delta t} (\tilde{u}_i^{\min} - \tilde{u}_i)$$

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- 3 Correction factors for the pair of fluxes f_{ij} and $f_{ji} = -f_{ij}$

$$R_i^\pm = \min \left\{ 1, \frac{Q_i^\pm}{P_i^\pm} \right\}, \quad \alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\} & \text{if } f_{ij} \geq 0 \\ \min\{R_i^-, R_j^+\} & \text{if } f_{ij} < 0 \end{cases}$$

Mesh genealogy

Triangulation $\mathcal{T}_m(\mathcal{E}_m, \mathcal{V}_m)$, $m = 0, 1, 2, \dots$ consists of

$$\mathcal{E}_m = \{\Omega_k : k = 1, \dots, N_E\} \quad \text{and} \quad \mathcal{V}_m = \{v_i : i = 1, \dots, N_V\}$$

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- nodal **generation function** $g : \mathcal{V}_m \rightarrow \mathbb{N}_0$ is defined recursively

$$g(v_i) := \begin{cases} 0 & \text{if } v_i \in \mathcal{V}_0 \\ \max_{v_j \in \Gamma_{kl}} g(v_j) + 1 & \text{if } v_i \in \Gamma_{kl} := \bar{\Omega}_k \cap \bar{\Omega}_l \\ \max_{v_j \in \partial\Omega_k} g(v_j) + 1 & \text{if } v_i \in \Omega_k \setminus \partial\Omega_k \end{cases}$$

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Mesh genealogy

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- represents number of subdivisions \Rightarrow prescribe maximum depth
- characterizes elements and their relation to neighboring cells

Mesh re-coarsening

Re-coarsening algorithms (vertex-based approach)

- 1 'lock' **vertices** step-by-step which must not be removed
- 2 delete 'free' vertices/elements and restore **macro cells**

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 - v_i belongs to an element which is marked for refinement
 - v_i belongs to a red element which should not be coarsened
 - there is an edge ij such that $g(v_i) < g(v_j)$ for some $v_j \in \mathcal{V}_m$

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 - 3 vertices are locked to preclude the creation of **blue elements**

Mesh re-coarsening

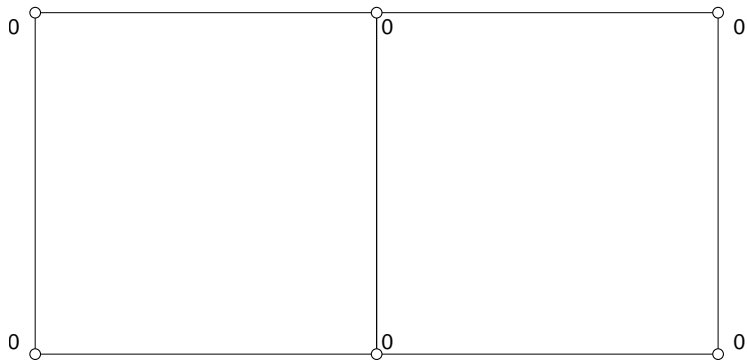
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Result: Vertex v_i is locked if $d(v_i) \leq 0$; otherwise it can be deleted.
All vertices of the initial mesh are locked by construction!

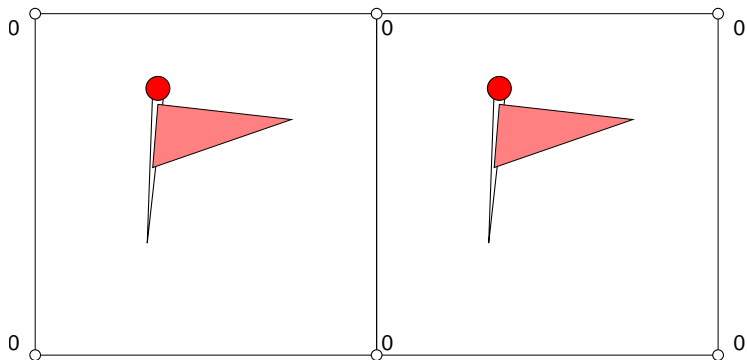
Step-by-step illustration

Refinement algorithm: initial mesh



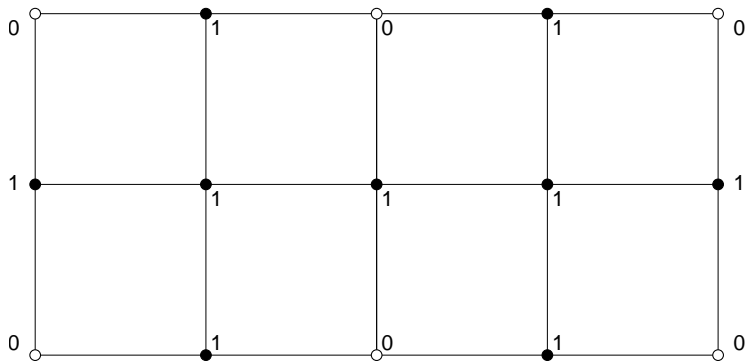
Step-by-step illustration

Refinement algorithm: mark elements for **regular refinement**



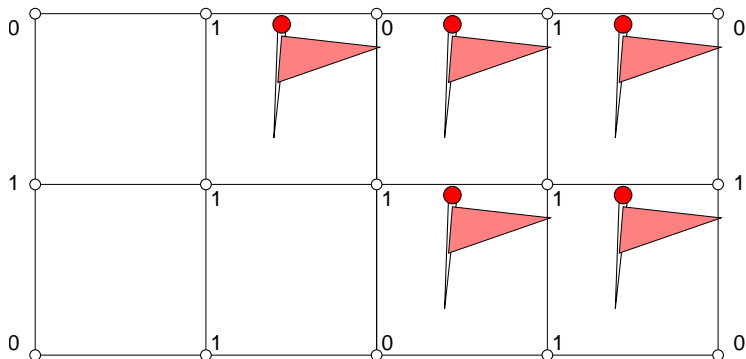
Step-by-step illustration

Refinement algorithm: perform regular refinement



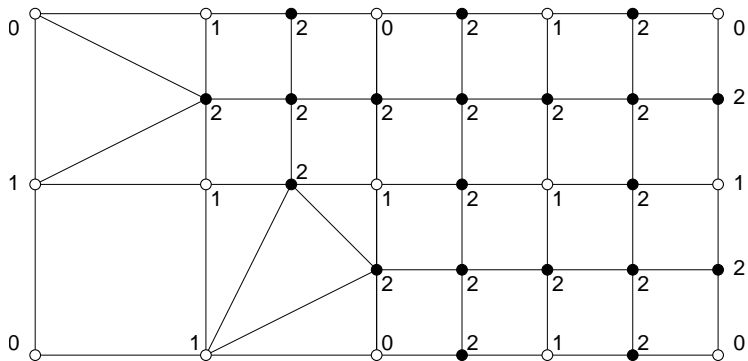
Step-by-step illustration

Refinement algorithm: mark elements for **regular refinement**



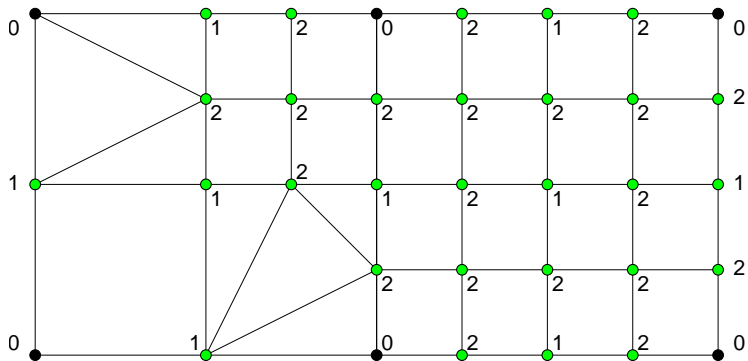
Step-by-step illustration

Refinement algorithm: perform regular refinement + transition cells



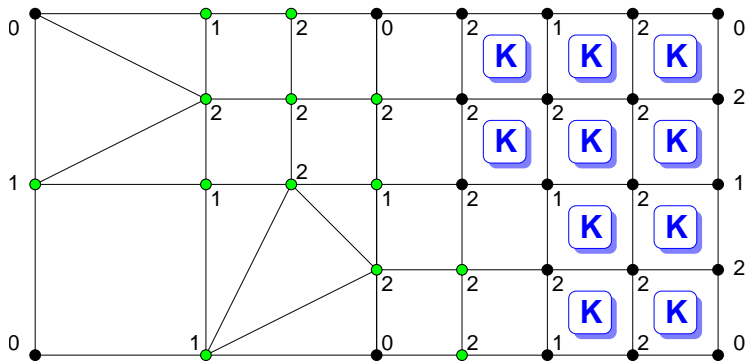
Step-by-step illustration

Re-coarsening algorithm: vertices from initial mesh are locked



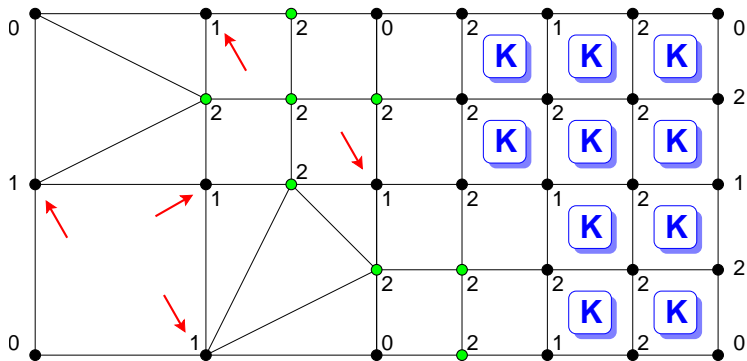
Step-by-step illustration

Re-coarsening algorithm: keep cells and lock connected vertices



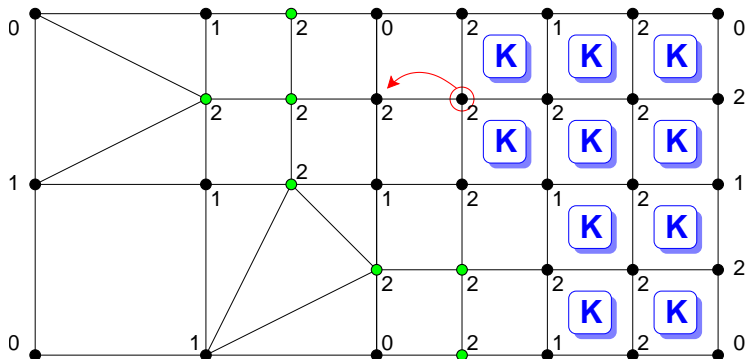
Step-by-step illustration

Re-coarsening algorithm: lock vertices if there are younger neighbors



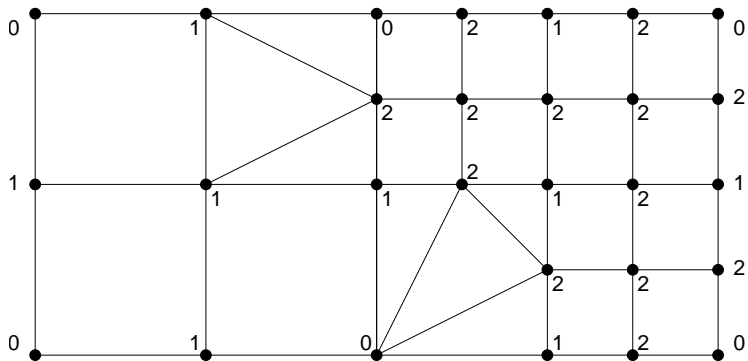
Step-by-step illustration

Re-coarsening algorithm: lock vertices to preclude blue elements



Step-by-step illustration

Re-coarsening algorithm: remove vertices and update elements



Dynamic mesh adaptation for the Euler equations
