An Explicit, Positivity-Preserving Flux-Corrected Transport Scheme for the Transport Equation Using Continuous Finite Elements

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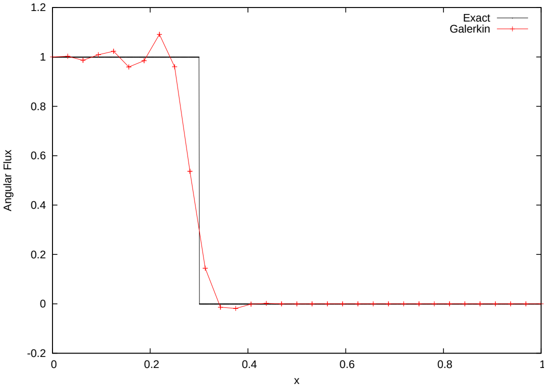
Motivation

- Numerical solution of transport equation prone to spurious oscillations and negativities in regions of discontinuities and sharp gradients:



Objective and Plan

- The **Objective** is to obtain a solution to the transport equation that
  - uses CFEM - not a traditional discretization for transport, but recent efforts have used CFEM for shock hydrodynamics
  - is non-negative
  - is free of spurious oscillations
  - has high-order accuracy (2nd order)
- The **Plan** is the following:
  - Use a low-order, monotone, non-negative scheme in conjunction with a high-order scheme via the flux-corrected transport (FCT) algorithm to produce a high-order, non-negative scheme
    - monotonicity not guaranteed but demonstrated for most cases

Problem Formulation

- Model transport equation:

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(\mathbf{x},t) + \Sigma(\mathbf{x})\psi(\mathbf{x},t) = q(\mathbf{x},t) \qquad (1)$$

$$\Sigma(\mathbf{x}) \geq 0, \qquad q(\mathbf{x},t) \geq 0$$

- Define problem:

$$\psi(\mathbf{x},0) = \psi^0(\mathbf{x}) \quad \forall\mathbf{x}\in\mathcal{D} \qquad (2)$$

$$\psi(\mathbf{x},t) = \psi^{inc}(\mathbf{x}) \quad \forall\mathbf{x}\in\partial\mathcal{D}^{inc} \qquad (3)$$

- CFEM solution:

$$\psi_h(\mathbf{x},t) = \sum_{j=1}^{N} U_j(t)\varphi_j(\mathbf{x}), \quad \varphi_j(\mathbf{x})\in P_h^1 \qquad (4)$$

Temporal Discretization

- Fully explicit temporal schemes used here:
  - Forward Euler (FE)
  - Explicit Strong Stability Preserving Runge-Kutta methods, which can be expressed as a number of FE steps
- Forward Euler scheme:

$$\mathbf{M}^C \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + \mathbf{A}\mathbf{U}^n = \mathbf{b}^n \tag{5}$$

$$M^C_{i,j} \equiv \int\limits_{S_{i,j}} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x}) d\mathbf{x} \tag{6}$$

$$A_{i,j} \equiv v \int\limits_{S_{i,j}} \left(\mathbf{\Omega} \cdot \nabla\varphi_j(\mathbf{x}) + \Sigma(\mathbf{x})\varphi_j(\mathbf{x})\right) \varphi_i(\mathbf{x}) d\mathbf{x} \tag{7}$$

$$b^n_i \equiv v \int\limits_{S_i} q(\mathbf{x}, t^n)\varphi_i(\mathbf{x}) d\mathbf{x} \tag{8}$$

Low-Order Scheme
Definition

- Lump mass matrix and add artificial viscosity:

$$\mathbf{M}^L\frac{\mathbf{U}^{L,n+1}-\mathbf{U}^n}{\Delta t}+(\mathbf{A}+\mathbf{D}^L)\mathbf{U}^n=\mathbf{b}^n \tag{9}$$

$$D^L_{i,j}=\sum_{K\subset S_{i,j}}\nu^L_K b_K(\varphi_j,\varphi_i) \tag{10}$$

$$b_K(\varphi_j,\varphi_i)\equiv\begin{cases}-\frac{1}{n_K-1}|K| & i\neq j,\quad i,j\in\mathcal{I}(K)\\ |K| & i=j,\quad i,j\in\mathcal{I}(K)\\ 0 & i\notin\mathcal{I}(K)\,|\,j\notin\mathcal{I}(K)\end{cases} \tag{11}$$

$$\nu^L_K\equiv\max_{i\neq j\in\mathcal{I}(K)}\frac{\max(0,A_{i,j})}{-\sum\limits_{T\subset S_{i,j}}b_T(\varphi_j,\varphi_i)} \tag{12}$$

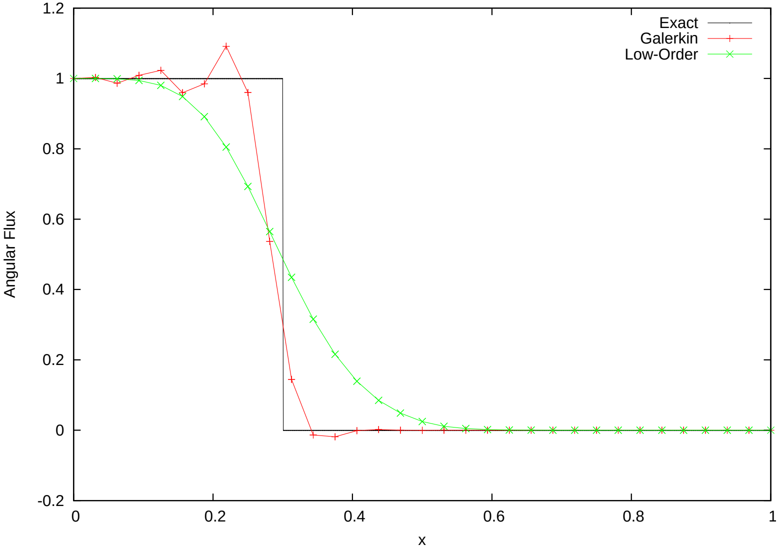
- These definitions make $(\mathbf{A}+\mathbf{D}^L)$ an M-matrix, which has the following desirable consequences for the low-order solution $\mathbf{U}^{L,n+1}$:
  - monotonicity
  - non-negativity
  - satisfaction of a discrete maximum principle (DMP):

$$W_i^-(\mathbf{U}^n) \leq U_i^{L,n+1} \leq W_i^+(\mathbf{U}^n) \qquad \forall i \tag{13}$$

$$W_i^\pm(\mathbf{U}^n) \equiv U^n_{\substack{\max\\\min},i}\left(1 - \frac{\Delta t}{m_i}\sum_j A^L_{i,j}\right) + \frac{\Delta t}{m_i} b_i^n \tag{14}$$

- Undesirable consequence: first-order accuracy

Low-Order Scheme
Results Example



- Add high-order artificial viscosity:

$$\mathbf{M}^C \frac{\mathbf{U}^{H,n+1} - \mathbf{U}^n}{\Delta t} + (\mathbf{A} + \mathbf{D}^{H,n})\mathbf{U}^n = \mathbf{b}^n \tag{15}$$

$$D_{i,j}^{H,n} = \sum_{K \subset S_{i,j}} \nu_K^{H,n} b_K(\varphi_j, \varphi_i) \tag{16}$$

$$\nu_K^{H,n} = \min(\nu_K^L, \nu_K^{E,n}) \tag{17}$$

- The entropy-based artificial viscosity $\nu_K^{E,n}$ is proportional to local "entropy" production.

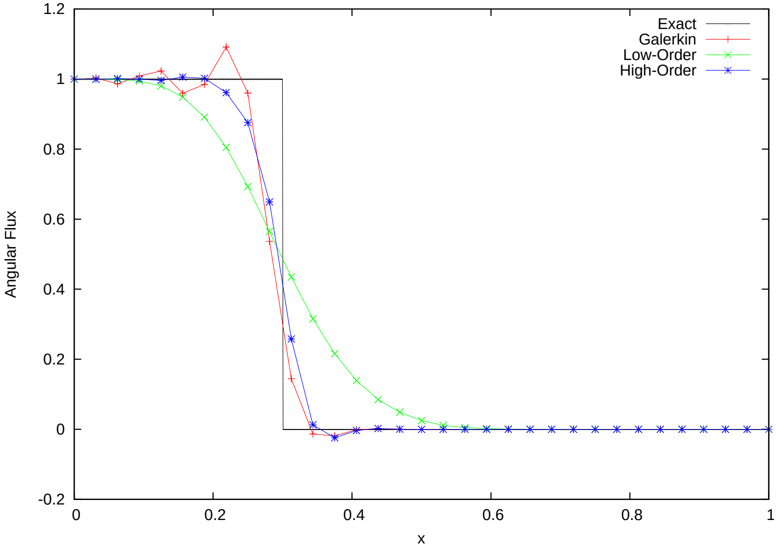
- One chooses a convex entropy function $E(\psi)$ such as $E(\psi) = \frac{1}{2}\psi^2$ and manipulates the transport equation to get an entropy residual:

$$R_K(\psi) = \left\| \frac{\partial E}{\partial t} + \frac{dE}{d\psi}\left(\mathbf{\Omega}\cdot\nabla\psi + \sigma\psi - q\right)\right\|_{L^\infty(K)} \tag{18}$$

- Entropy-based artificial viscosity is proportional to an entropy residual $R_K^n(\psi_h)$:

$$\nu_K^{E,n} = \frac{c_E R_K^n(\psi_h) + c_J \max\limits_{F\in\partial K} J_F(\psi_h^n)}{\|E(\psi_h^n) - \bar{E}(\psi_h^n)\|_{L^\infty(\mathcal{D})}} \tag{19}$$

High-Order Scheme
Results Example



Flux Corrected Transport (FCT) Scheme

- Initially developed in 1973 for finite difference discretizations of transport/conservation law problems and recently applied to finite element method
- Works by adding conservative fluxes to satisfy physical bounds on the solution
- Employs low-order scheme and high-order scheme
- Defines a *correction*, or *antidiffusion*, flux, which when added to the low-order scheme, produces the high-order scheme
- Limits this correction flux to enforce the physical bounds imposed

- Define a correction flux $\mathbf{f}$:

$$\begin{aligned}
\mathbf{f}\text{ Def.:}\quad & \mathbf{M}^L\frac{\mathbf{U}^{H,n+1}-\mathbf{U}^n}{\Delta t}+(\mathbf{A}+\mathbf{D}^L)\mathbf{U}^n=\mathbf{b}^n+\mathbf{f}^n\\
\text{Low-order:}\quad & \mathbf{M}^L\frac{\mathbf{U}^{L,n+1}-\mathbf{U}^n}{\Delta t}+(\mathbf{A}+\mathbf{D}^L)\mathbf{U}^n=\mathbf{b}^n\\
\text{High-order:}\quad & \mathbf{M}^C\frac{\mathbf{U}^{H,n+1}-\mathbf{U}^n}{\Delta t}+(\mathbf{A}+\mathbf{D}^{H,n})\mathbf{U}^n=\mathbf{b}^n
\end{aligned}$$

- Thus $\mathbf{f}$ is

$$\mathbf{f}^n\equiv-(\mathbf{M}^C-\mathbf{M}^L)\frac{\mathbf{U}^{H,n+1}-\mathbf{U}^n}{\Delta t}+(\mathbf{D}^L-\mathbf{D}^{H,n})\mathbf{U}^n \quad (20)$$

- Decompose $\mathbf{f}$ into internodal fluxes $F_{i,j}$: $f_i = \sum_j F_{i,j}$:

$$F_{i,j} = -M^C_{i,j}\left(\frac{dU_j}{dt}^{H,n+1} - \frac{dU_i}{dt}^{H,n+1}\right) + (D^L_{i,j} - D^H_{i,j})(U^n_j - U^n_i) \quad (21)$$

- The FCT scheme limits these fluxes with a limiter $\mathcal{L}$:

$$\mathbf{M}^L\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + \mathbf{A}^L\mathbf{U}^n = \mathbf{b} + \mathcal{L}[\mathbf{F}] \quad (22)$$

- The limiter $\mathcal{L}$ enforces the discrete maximum principle:

$$W^-_i(\mathbf{U}^n) \leq U^{n+1}_i \leq W^+_i(\mathbf{U}^n) \qquad \forall i \quad (23)$$

- Each correction flux $F_{i,j}$ has an associated limiting coefficient $\mathcal{L}_{i,j}$: $\mathcal{L}[\mathbf{F}]_i = \sum\limits_j \mathcal{L}_{i,j} F_{i,j}$:

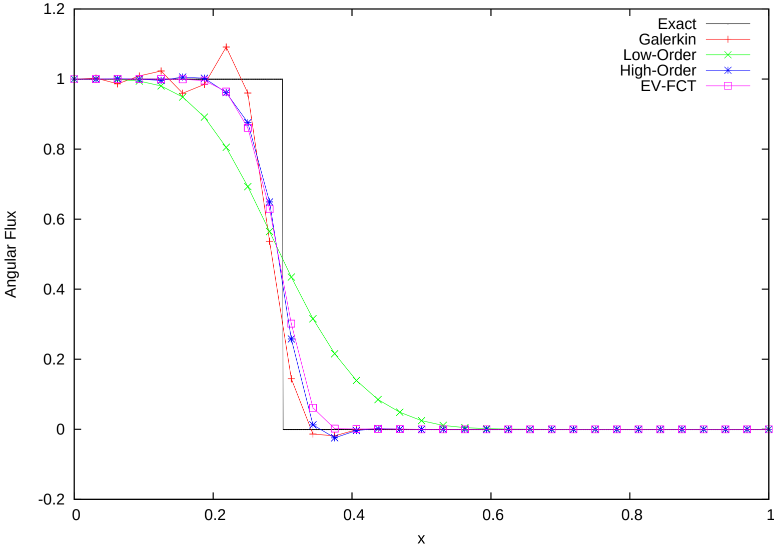
$$P_i^+ \equiv \sum_j \max(0, F_{i,j}) \qquad P_i^- \equiv \sum_j \min(0, F_{i,j}) \tag{24}$$

$$Q_i^\pm \equiv m_i \frac{W_i^\pm - U_i^n}{\Delta t} + \sum_j A_{i,j}^L U_j^n - b_i \tag{25}$$

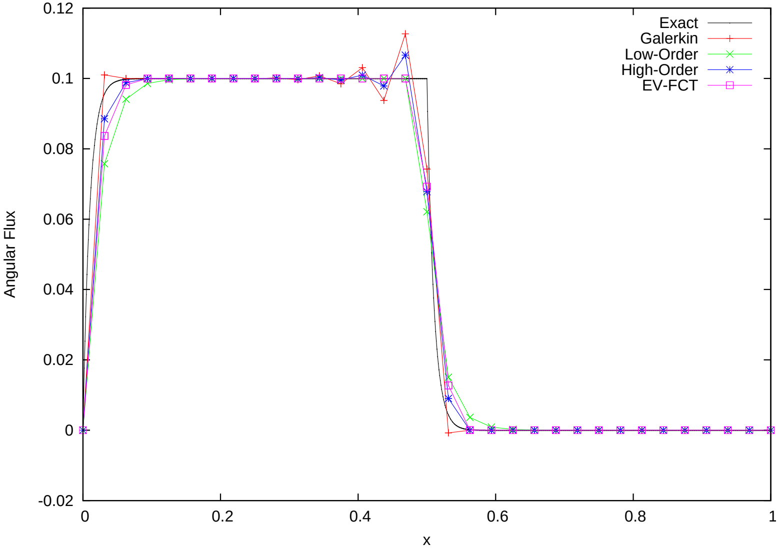
$$R_i^\pm \equiv \begin{cases} 1 & P_i^\pm = 0 \\ \min\left(1, \frac{Q_i^\pm}{P_i^\pm}\right) & P_i^\pm \neq 0 \end{cases} \tag{26}$$

$$\mathcal{L}_{i,j} \equiv \begin{cases} \min(R_i^+, R_j^-) & F_{i,j} \geq 0 \\ \min(R_i^-, R_j^+) & F_{i,j} < 0 \end{cases} \tag{27}$$

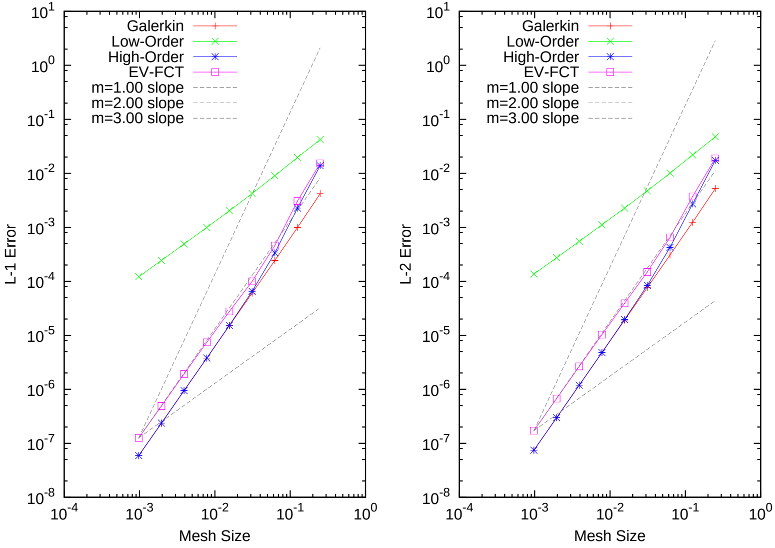
Flux Corrected Transport (FCT) Scheme
Results Example



Results
Source Problem Results

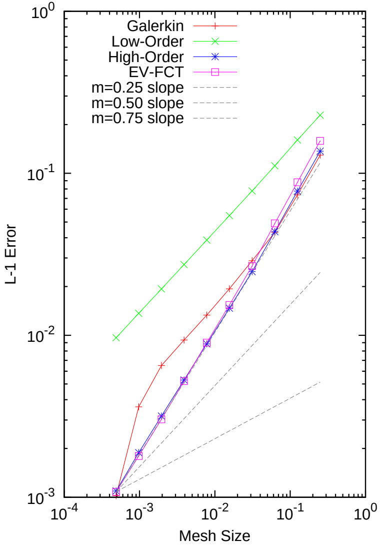


Results
Smooth Problem Convergence Results (Using FE)



Results

Non-smooth Problem Convergence Results (Using SSPRK33)



Conclusions

- guaranteed non-negative, DMP-satisfying scheme
- monotonicity for problems tested, but not guaranteed
- theoretical convergence rates observed
- future work:
  - implicit time discretizations
  - steady-state
  - more complicated physics

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