A Positivity-preserving Scheme for Radiation Transport

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INTRODUCTION

Flux-Corrected Transport (FCT) algorithms, initially developed by Boris and Book [**borisbook**], aim at addressing the issue of solution negativities and spurious oscillations for conservation laws.

Recently, the concept of FCT has been applied to continuous finite element discretizations.

The present work aims to extend this approach to radiative transport:

$$\frac{1}{v(E)}\frac{\partial\psi}{\partial t} + \boldsymbol{\Omega}\cdot\nabla\psi(\mathbf{x},E,\boldsymbol{\Omega},t) + \Sigma_t(\mathbf{x},E)\psi(\mathbf{x},E,\boldsymbol{\Omega},t) = \int_0^\infty dE'\int_{4\pi} d\Omega'\Sigma_s(\mathbf{x},E'\to E,\boldsymbol{\Omega}'\to\boldsymbol{\Omega})\psi(\mathbf{x},E',\boldsymbol{\Omega}',t) + S_{ext}(\mathbf{x},E,\boldsymbol{\Omega},t) \quad (1)$$

Here, we use a simplified model which lumps scattering and external sources and consider a single direction and energy:

$$\boxed{\frac{\partial u}{\partial t} + \nabla\cdot(\mathbf{v}u(\mathbf{x},t)) + \sigma(\mathbf{x})u(\mathbf{x},t) = q(\mathbf{x},t)} \quad (2)$$

where $\mathbf{v}$ is a given velocity field.

CFEM DISCRETIZATION

Testing with each FEM basis function $\varphi_i(\mathbf{x})$ gives a linear system:

$$\mathbf{M}^C\frac{d\mathbf{U}}{dt} + \mathbf{A}\mathbf{U}(t) = \mathbf{b}, \quad (3)$$

$$M^C_{i,j} \equiv \int_{S_{i,j}} \varphi_j\varphi_i dV, \qquad A_{i,j} = \int_{S_{i,j}} (\mathbf{v}\cdot\nabla\varphi_j + \sigma\varphi_j)\,\varphi_i dV, \qquad b_i \equiv \int_{S_i} q\varphi_i dV. \quad (4)$$

To discretize Eqn. 1 in time, fully explicit temporal discretization schemes are used, such as explicit Euler,

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

and 3rd-order SSP (SSP3) explicit methods.

LOW-ORDER SCHEME

A **monotonicity-preserving, positivity-preserving low-order** scheme is defined by lumping the mass matrix and adding a low-order diffusion operator:

$$\mathbf{M}^L\frac{\mathbf{U}^{L,n+1}-\mathbf{U}^n}{\Delta t} + \left(\mathbf{A}+\mathbf{D}^L\right)\mathbf{U}^n = \mathbf{b}, \quad (6)$$

where the diffusion matrix $\mathbf{D}^L$ entries are computed using a local low-order viscosity and viscous bilinear form:

$$D^L_{i,j} = \sum_{K\subset S_{i,j}} \nu^L_K b_K(\varphi_j,\varphi_i). \quad (7)$$

The local viscous bilinear form for an element K takes a graph-theoretic approach introduced by Guermond [1]:

$$b_K(\varphi_j,\varphi_i) \equiv \begin{cases} -\frac{1}{n_K-1}V_K & i\neq j, \quad i,j\in\mathcal{I}(K), \\ V_K & i=j, \quad i,j\in\mathcal{I}(K), \\ 0 & i\notin\mathcal{I}(K) \quad | \quad j\notin\mathcal{I}(K), \end{cases} \quad (8)$$

where V_K is the volume of cell K, $\mathcal{I}(K) \equiv \{j\in\{1,\dots,N\} : |S_j\cap K| \neq 0\}$ is the set of indices corresponding to degrees of freedom in the support of cell K, and $n_K \equiv \mathrm{card}(\mathcal{I}(K))$. The local low-order viscosity is defined as the following:

$$\nu^L_K \equiv \max_{i\neq j\in\mathcal{I}(K)} \frac{\max(0,A_{i,j})}{-\sum\limits_{T\subset S_{i,j}} b_T(\varphi_j,\varphi_i)}, \quad (9)$$

If the CFL condition $\Delta t \leq \frac{M^L_{i,i}}{A^L_{i,i}}$ is satisfied for all i, then the explicit low-order scheme given in Eqn. 4 **satisfies the following discrete maximum principle**:

$$U^n_{\min,i}\left(1-\frac{\Delta t}{M^L_{i,i}}\sum_j A^L_{i,j}\right) + \frac{\Delta t}{M^L_{i,i}}b_i \leq U^{L,n+1}_i \leq U^n_{\max,i}\left(1-\frac{\Delta t}{M^L_{i,i}}\sum_j A^L_{i,j}\right) + \frac{\Delta t}{M^L_{i,i}}b_i \quad \forall i, \quad (10)$$

where $U^n_{\min,i} = \min\limits_{j\in\mathcal{I}(S_i)} U^n_j$, $U^n_{\max,i} = \max\limits_{j\in\mathcal{I}(S_i)} U^n_j$ and $\mathcal{I}(S_i)$ is the set of indices of degrees of freedom in the support of degree of freedom i.

HIGH-ORDER SCHEME

The high-order scheme is based on the concept of **entropy viscosity** introduced by Guermond [2, 3] which, by itself, does not guaranteed monotonicity-preserving or positivity-preserving.

The high-order scheme has the form

$$\mathbf{M}^C\frac{\mathbf{U}^{H,n+1}-\mathbf{U}^n}{\Delta t} + \left(\mathbf{A}+\mathbf{D}^{H,n}\right)\mathbf{U}^n = \mathbf{b}, \quad (11)$$

where the high-order diffusion operator $\mathbf{D}^H$ is computed in the same manner as its low-order counterpart, but employs a high-order viscosity definition based on an entropy viscosity bounded by the low-order viscosity: $\boxed{\nu^{H,n}_K = \min(\nu^L_K,\nu^{E,n}_K).}$

To compute the entropy viscosity ν^E, one first selects a convex entropy functional $E(u)$, e.g., $E(u) = \frac{1}{2}u^2$.

The entropy viscosity is designed **to add viscosity in regions of entropy production**, such as shocks, and avoids adding viscosity elsewhere.

Thus, the entropy viscosity is selected proportional to the entropy residual R^n_K:

$$\boxed{\nu^{E,n}_K = c_E\frac{R^n_K(u^n_h,u^{n-1}_h)}{\|E(u^n_h)-\bar{E}(u^n_h)\|_{L^\infty(\mathcal{D})}},} \quad (12)$$

where $\bar{E}(u^n_h)$ is the average entropy over the domain, and c_E is a tunable normalization parameter, usually ~ 1.

The entropy residual evaluated with explicit Euler is the following:

$$\boxed{R^n_K(u^n_h,u^{n-1}_h) = \left\|\frac{E(u^n_h)-E(u^{n-1}_h)}{\Delta t^n} + \left.\frac{dE}{du}\right|_{u^n_h}[\boldsymbol{\Omega}\cdot\nabla u^n_h + \sigma u^n_h - q]\right\|_{L^\infty(K)}.} \quad (13)$$

FCT SCHEME

- **FCT** blends the low-order and high-order schemes to produce a scheme that is high-order, positivity-preserving, **Discrete-Maximum-Principle-satisfying**.
- **Anti-diffusive fluxes** $\mathbf{F}$ are defined such that their application to the low-order scheme would reproduce the high-order scheme solution.
  - However, these fluxes $\mathbf{F}$ are then **limited** to satisfy physical bounds (bounds of the low-order scheme discrete maximum principle) imposed on the FCT solution.
- Since $\mathbf{M}^C-\mathbf{M}^L$ and $\mathbf{D}^L-\mathbf{D}^H$ are symmetric and feature zero row- and column-sums, a valid decomposition for the antidiffusive fluxes is

$$\boxed{F_{i,j} = -M^C_{i,j}\left(\frac{U^{H,n+1}_j-U^n_j}{\Delta t} - \frac{U^{H,n+1}_i-U^n_i}{\Delta t}\right) + (D^L_{i,j}-D^H_{i,j})(U^n_j-U^n_i).} \quad (14)$$

The FCT scheme is the following, where the operator $\mathbf{L}$ denotes the **limiter operation**:

$$\boxed{\mathbf{M}^L\frac{\mathbf{U}^{n+1}-\mathbf{U}^n}{\Delta t} + \mathbf{A}^L\mathbf{U}^n = \mathbf{b} + \mathbf{L}\cdot\mathbf{F},} \quad (15)$$

where the notation $\mathbf{L}\cdot\mathbf{F}$ denotes row-wise dot products: $\boxed{(\mathbf{L}\cdot\mathbf{F})_i = \sum_j L_{i,j}F_{i,j}}$. The limiting coefficients $L_{i,j}$ are given by the multidimensional limiter of Zalesak [4]:

$$F^+_i \equiv \sum_j \max(0,F_{i,j}) \qquad F^-_i \equiv \sum_j \min(0,F_{i,j}), \quad (16)$$

$$Q^\pm_i \equiv M^L_{i,i}\frac{W^\pm_i-U^n_i}{\Delta t} + \sum_j A^L_{i,j}U^n_j - b_i, \quad (17)$$

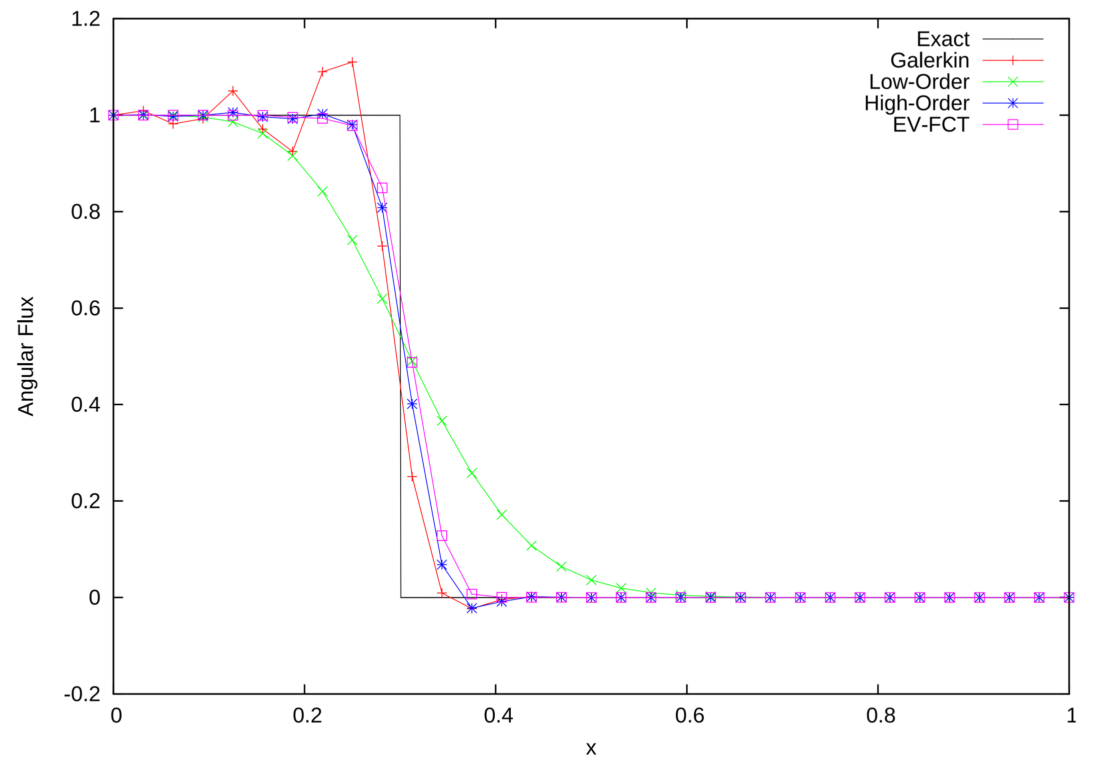
$$L^\pm_i \equiv \begin{cases} 1 & F^\pm_i = 0 \\ \min\left(1,\frac{Q^\pm_i}{P^\pm_i}\right) & F^\pm_i \neq 0 \end{cases}, \quad (18)$$

$$L_{i,j} \equiv \begin{cases} \min(L^+_i,L^-_j) & F_{i,j}\geq 0 \\ \min(L^-_i,L^+_j) & F_{i,j}<0 \end{cases}, \quad (19)$$

where $W^\pm_i$ are the **upper and lower discrete maximum principle bounds** given in Eqn. 8.

RESULTS

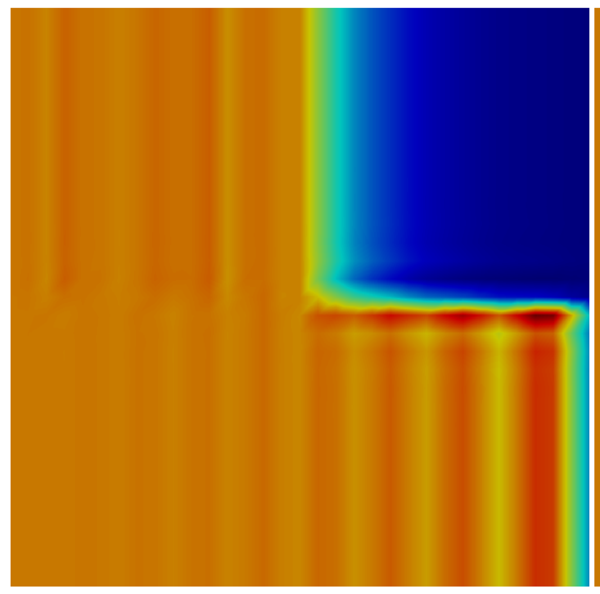
- At time 0, normally incident radiation impinges on the left side of a vacuum filled domain
- Expected result: propagation of a Heaviside wave front in a void to the right.
- The **standard Galerkin** FEM scheme produces unphysical oscillations and negativities
- These are remedied with the **FCT scheme** *without* introducing the amount of diffusion required by the **low-order scheme**.
- The high-order scheme based on entropy viscosity *without FCT* mitigates the formation of oscillations but ultimately still produces some negativities

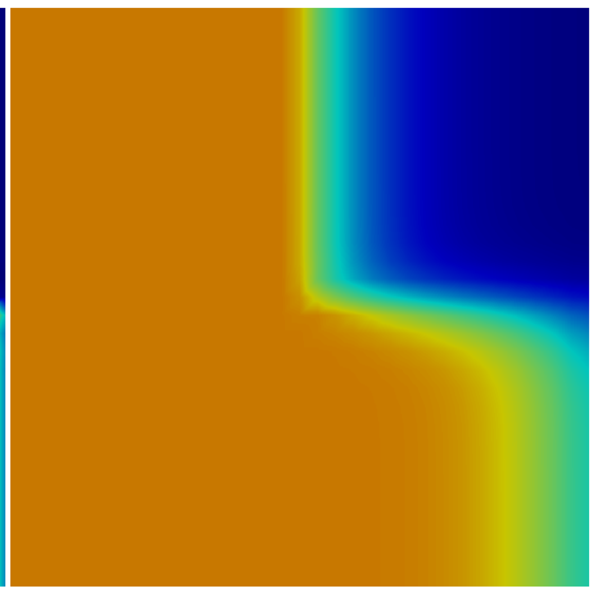


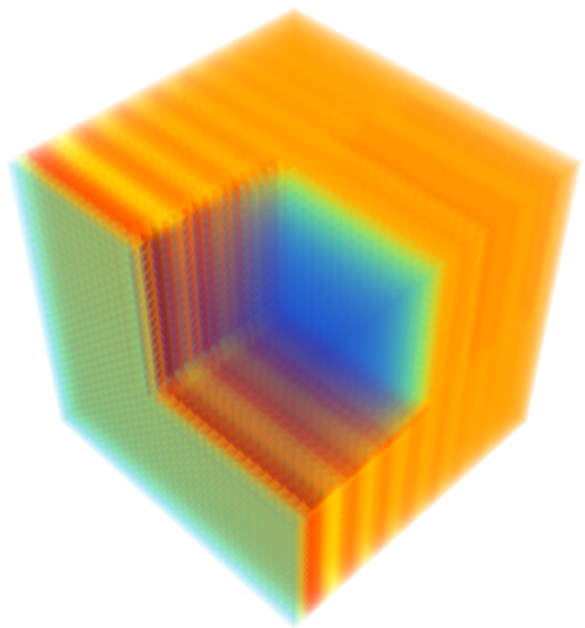
Multidimensional test cases:

A 2×2 material layout (2D) and $2\times 2\times 2$ layout (3D) where one material is a pure absorber and all other materials are void.

Radiation normally incident on one side (2D) or face (3D).


Galerkin


FCT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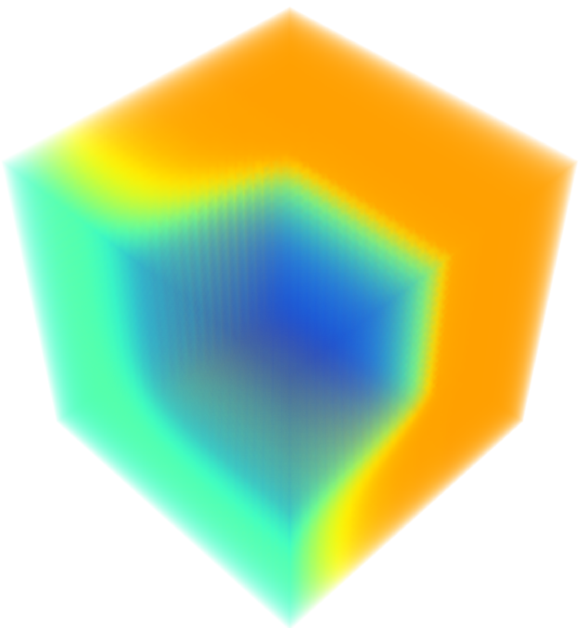
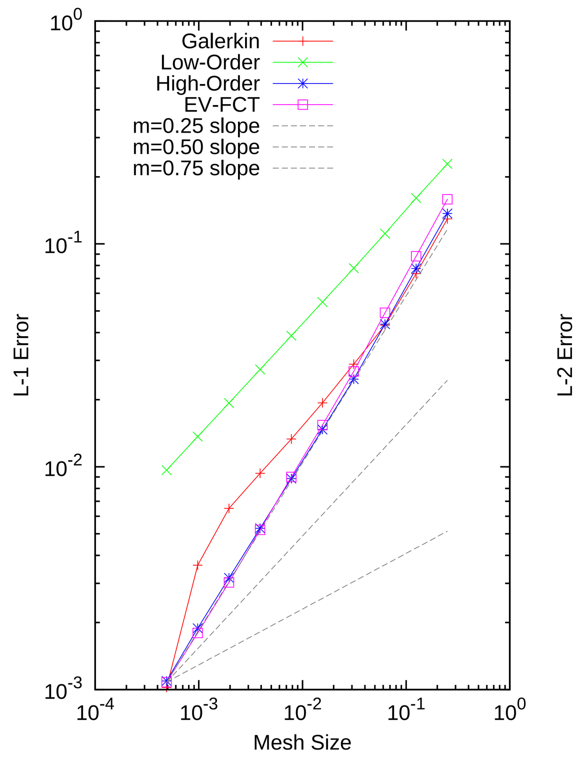
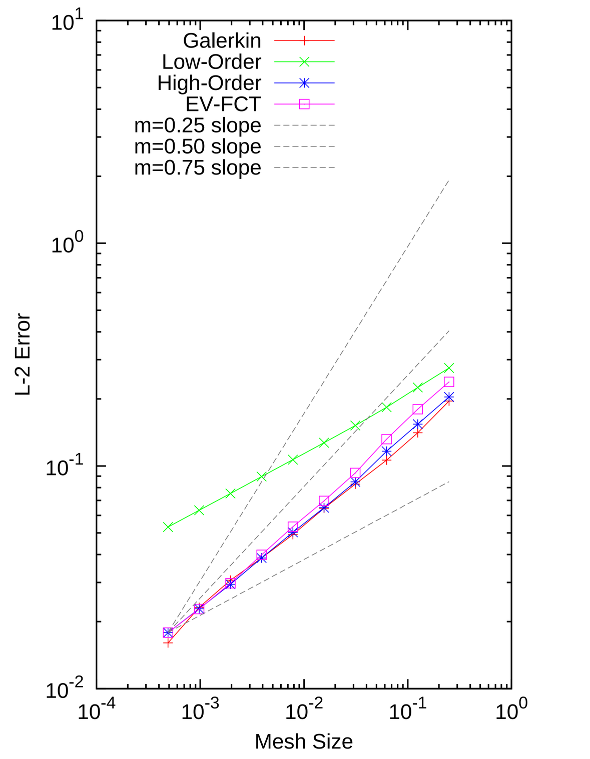

FCT

The figure below shows the convergence results for the void problem, which because the solution is discontinuous, the theoretical convergence rates for the high-order scheme are $\frac{3}{4}$ and $\frac{3}{8}$ for L-1 and L-2 error, respectively. The FCT scheme is shown here to achieve these convergence rates.





CONCLUSIONS

The numerical solutions **using FCT for radiation transport** exhibit the following properties.

Solutions

- are guaranteed non-negative
- are not guaranteed to be monotone, but rarely not monotone in practice
- satisfy a discrete maximum principle
- are 2nd-order accurate

Current and future work includes

- **FCT for radiation transport implicit time discretizations**
- conservation law *systems* (e.g., shallow water)

REFERENCES

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[4] Steven T. Zalesak. "Fully Multidimensional Flux-Corrected Transport Algorithms for Fluids". In: *Journal of Computational Physics* 31 (1979), pp. 335–362.