Limiting techniques and hp-adaptivity for high-order finite elements

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- Discrete maximum principles for high-order finite elements
- Flux-corrected transport: limiters for numerical solutions
- Built-in residual correction: limiters for artificial diffusion
- Partition of unity methods: limiters for basis functions

Galerkin discretization

- Scalar conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f}(u, \nabla u) = 0, \qquad u(\mathbf{x}, t) \in [u^{\min}, u^{\max}]$$

- Finite element approximation

$$u_h(\mathbf{x}, t) = \sum_{j=1}^{N_{\text{dof}}} u_j(t)\varphi_j(\mathbf{x}), \qquad M\frac{\mathrm{d}u}{\mathrm{d}t} + Au = b$$

- Bernstein basis functions

$$\varphi_i^e = \frac{p!\lambda_1^{p_{i,1}} \cdot \ldots \cdot \lambda_{d+1}^{p_{i,d+1}}}{p_{i,1}! \cdot \ldots \cdot p_{i,d+1}!} \geq 0, \qquad \sum_{i=1}^{d+1} \varphi_i^e \equiv 1$$

Bound-preserving schemes

- Discrete maximum principles

$$\min_{j\in\mathcal{N}^e} u_j \le u_h(\mathbf{x}) \le \max_{j\in\mathcal{N}^e} u_j \qquad \forall \mathbf{x}\in K^e$$

$$u^{\min} \le u_j^{\min} \le u_j \le u_j^{\max} \le u^{\max}$$

- Modification of discrete operators

$$M \to \bar{M} := \mathrm{diag}\{m_i\}, \qquad m_i = \sum_{j=1}^{N_{\mathrm{dof}}} m_{ij} > 0$$

$$A \to \bar{A} := A - D, \qquad d_{ij} = \begin{cases} \max\{a_{ij}, 0, a_{ji}\} & \text{if } j \ne i \\ -\sum_{k\ne i} d_{ik} & \text{if } j = i \end{cases}$$

- Nonlinear antidiffusive corrections

Flux-corrected transport[1]

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- Algebraic splitting of a high-order scheme

$$\bar{M}\frac{\mathrm{d}u}{\mathrm{d}t} + \bar{A}u = f(u) := (\bar{M} - M)\frac{\mathrm{d}u}{\mathrm{d}t} - Du$$

- Bound-preserving low-order approximation

$$\bar{M}\frac{\mathrm{d}\bar{u}}{\mathrm{d}t} + \bar{A}\bar{u} = 0, \qquad t \in (t^n, t^{n+1})$$

- Bound-preserving antidiffusive correction

$$u_i^{n+1} = \bar{u}_i^{n+1} + \frac{\Delta t}{m_i}\sum_{e\in\mathcal{E}_i}\alpha^e f_i^e(\bar{u}^{n+1}), \qquad f_i = \sum_{e\in\mathcal{E}_i} f_i^e$$

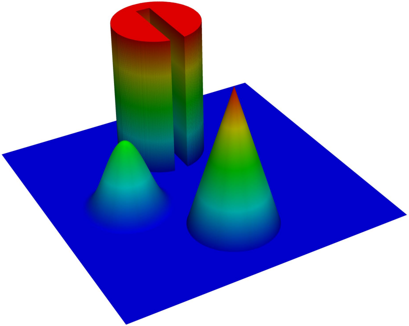
$$\alpha^e \in [0,1] \quad \text{s.t.} \quad \bar{u}_i^{\min} \le u_i^{n+1} \le \bar{u}_i^{\max}$$

[1] Boris & Book (1972)

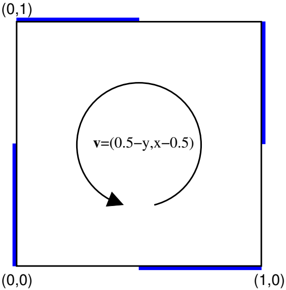
Example: FCT limiting

Solid body rotation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad \mathbf{v} = (0.5 - y, x - 0.5)$$



initial/exact solution

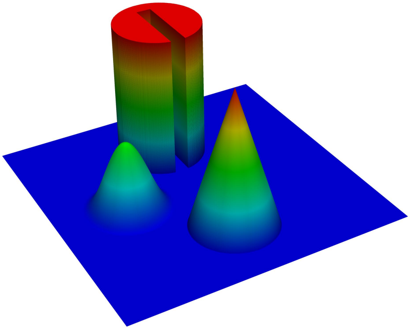


domain and velocity

Example: FCT limiting

Solid body rotation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad \mathbf{v} = (0.5 - y, x - 0.5)$$



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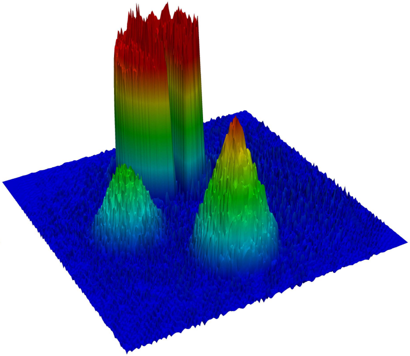
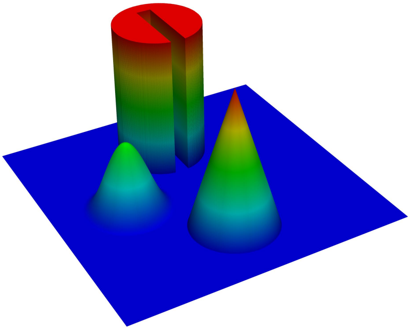


standard CG(2) scheme

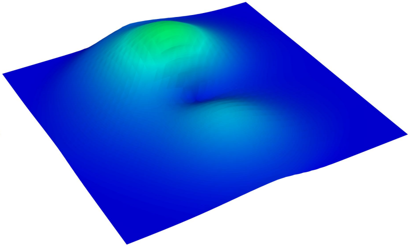
Example: FCT limiting

Solid body rotation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad \mathbf{v} = (0.5 - y, x - 0.5)$$



initial/exact solution

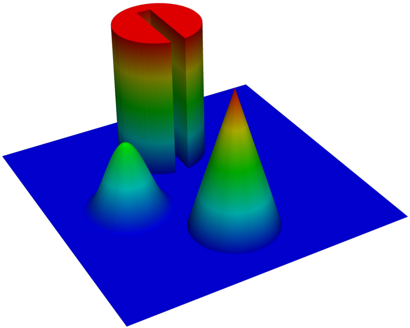


modified CG(2) scheme

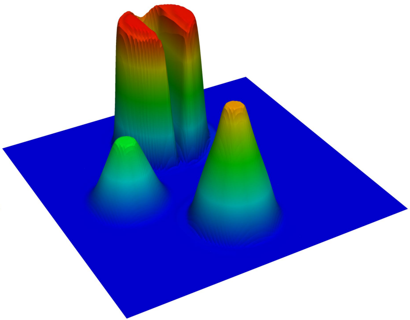
Example: FCT limiting

Solid body rotation

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0, \qquad \mathbf{v} = (0.5 - y, x - 0.5)$$



initial/exact solution



limited CG(2) scheme

Summary: FCT limiting

- Simple and efficient, easy to implement in existing codes
- Applicable to high-order Bernstein elements but careful localization is required to achieve optimal accuracy
- Levels of numerical diffusion depend on the time step Δt
- Definition of f_i^e in terms of $\bar{u}$ gives rise to splitting errors
- Not a good method for stationary transport problems: lack of convergence, dependence on the pseudo-time step

Algebraic residual correction

- Constrained nonlinear approximation

$$\bar{M}\frac{\mathrm{d}u}{\mathrm{d}t} + \bar{A}u = \bar{f}\left(u, \frac{\mathrm{d}u}{\mathrm{d}t}\right), \qquad \bar{f}_i = \sum_{e\in\mathcal{E}_i} \bar{f}_i^e$$

$$\bar{f}_i^e(u,\dot{u}) = \dot{\alpha}^e f(0,\dot{u}) + \alpha^e f(u,0)$$

- Local extremum diminishing (LED) property

$$u_i^{\max} := \max_{j\in\mathcal{N}_i} u_j = u_i \quad \Rightarrow \quad \bar{f}_i \le 0$$

$$u_i^{\min} := \min_{j\in\mathcal{N}_i} u_j = u_i \quad \Rightarrow \quad \bar{f}_i \ge 0$$

- Iterative solution of nonlinear systems

Gradient-based limiters

- Limited nodal gradients

$$\mathbf{g}_i \approx \nabla u(\mathbf{x}_i)$$

  - $\alpha_i \mathbf{g}_i = 0$ if $u_i = u_i^{\max}$ or $u_i = u_i^{\min}$
  - $\alpha_i \mathbf{g}_i = \nabla u_h(\mathbf{x}_i)$ if u_h is linear
  - $\alpha_i \mathbf{g}_i$ is Lipschitz continuous

$$\alpha_i := \min\left\{1, \frac{\gamma_i \min\{u_i^{\max} - u_i, u_i - u_i^{\min}\}}{\max\{u_i^{\max} - u_i, u_i - u_i^{\min}\} + \epsilon h}\right\}$$

- Element-based correction factors

$$\alpha^e = \min\left\{1, \min_{i \in \mathcal{N}^e} \frac{|2\alpha_i \mathbf{g}_i|^2}{|\nabla u_h^e|^2 + \epsilon}\right\}$$

- Built-in high-order stabilization

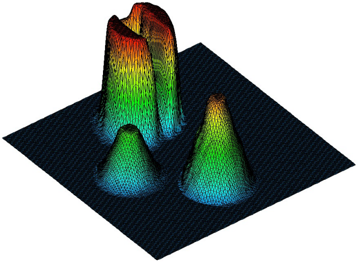
Example: iterative limiting

Unsteady convection

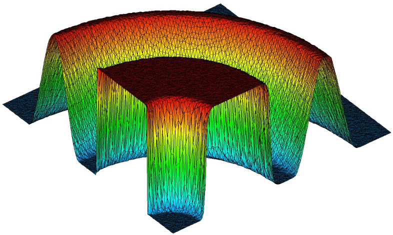
$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0$$

Steady convection

$$\nabla \cdot (\mathbf{v}u) = 0$$



$$\mathbf{v} = (0.5 - y, x - 0.5)$$



$$\mathbf{v}(x, y) = (y, -x)$$

Summary: iterative limiting

- Applicable to stationary and time-dependent problems
- Backed by a theoretical framework[2] which provides
  - proofs of existence, uniqueness, and boundedness
  - *a priori* error estimates for constrained schemes
- Extension to high-order Bernstein elements is possible
- Only converged solutions to nonlinear discrete problems are guaranteed to be bound-preserving
- Design of efficient iterative solvers is a difficult task
  - Anderson acceleration for fixed-point iterations
  - Newton methods for differentiable regularizations

[2] Barrenechea et al. (2016, 2017)

Partition of unity FEM

- High-order finite element space

$$V_{H,p} = \mathrm{span}\{\varphi_1^H, \ldots, \varphi_{N_{\mathrm{dof}}}^H\}$$

- Piecewise-linear approximation

$$V_{h,1} = \mathrm{span}\{\varphi_1^L, \ldots, \varphi_{N_{\mathrm{dof}}}^L\}$$

- Adaptive finite element bases

$$\varphi_i = \alpha_h \varphi_i^H + (1-\alpha_h)\varphi_i^L, \qquad i = 1, \ldots, N_{\mathrm{dof}}$$

- Continuous blending functions

$$\alpha_h = \sum_{i=1}^{N_{\mathrm{dof}}} \alpha_i \varphi_i^L, \qquad \alpha_i \in [0,1]$$

Partition of unity FEM

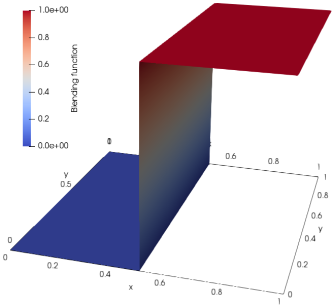
Continuous hp-adaptivity

$$v_h = \alpha_h \sum_{j=1}^{N_{\rm dof}} v_j \varphi_j^H + (1-\alpha_h) \sum_{j=1}^{N_{\rm dof}} v_j \varphi_j^L \qquad \forall v_h \in V_h(\alpha_h)$$

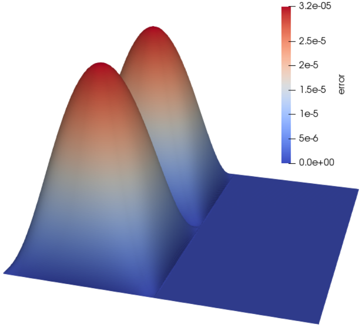
- seamless blending of $V_{H,p} = V_h(1)$ and $V_{h,1} = V_h(0)$
- no hanging h or p nodes due to continuity of $\alpha_h \in V_{h,1}$
- automatic h refinement in elements where $\alpha_h < 1$
- flexibility in the definition of blending functions α_h
- use of limiters only in ‘bad’ elements where $\alpha_h = 0$

Example: PUFEM limiting

Poisson's equation: $p = 2,\ H = 2h, \quad N_{\mathrm{dof}} = 321^2$



(a) Blending function α_h



(b) Error $|u(\mathbf{x}) - u_h(\mathbf{x})|$

Example: PUFEM limiting

Poisson's equation, manufactured solution

$$-\Delta u = f, \qquad u(x,y) = \sin(2\pi x)\sin(2\pi y)$$

N_{dof}	$\|\|e\|\|_{0,\Omega}$		$\|\|e\|\|_{1,\Omega}$	
21^2	3.49E-3	–	2.87E-1	–
41^2	8.63E-4	2.01	1.42E-1	1.01
81^2	2.15E-4	2.00	7.12E-2	1.00
161^2	5.38E-5	2.00	3.56E-2	1.00
321^2	1.34E-5	2.00	1.78E-2	1.00
641^2	3.36E-6	2.00	8.90E-3	1.00

convergence history in $\Omega = (0,1)\times(0,1)$

Example: PUFEM limiting

Poisson's equation, manufactured solution

$$-\Delta u = f, \qquad u(x,y) = \sin(2\pi x)\sin(2\pi y)$$

N_{dof}	$\|\|e\|\|_{0,\Omega_1}$		$\|\|e\|\|_{1,\Omega_1}$	
21^2	3.42E-3	–	2.83E-1	–
41^2	8.59E-4	1.99	1.42E-1	0.99
81^2	2.14E-4	1.99	7.12E-2	0.99
161^2	5.38E-5	1.99	3.56E-2	0.99
321^2	1.34E-5	1.99	1.78E-2	0.99
641^2	3.36E-6	1.99	8.90E-3	0.99

convergence history in $\Omega_1 = \{(x,y) \in \Omega : x < 0.5 - h\}$

Example: PUFEM limiting

Poisson's equation, manufactured solution

$$-\Delta u = f, \qquad u(x,y) = \sin(2\pi x)\sin(2\pi y)$$

N_{dof}	$\|\|e\|\|_{0,\Omega_2}$		$\|\|e\|\|_{1,\Omega_2}$	
21^2	6.55E-4	–	4.35E-2	–
41^2	8.56E-5	2.93	1.12E-2	1.95
81^2	1.09E-5	2.97	2.84E-3	1.97
161^2	1.38E-6	2.98	7.17E-4	1.98
321^2	1.73E-7	2.99	1.79E-4	1.99
641^2	2.17E-8	2.99	4.51E-5	1.99

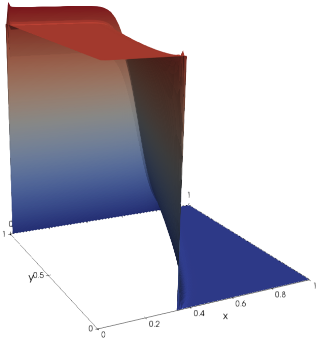
convergence history in $\Omega_2 = \{(x,y) \in \Omega : x > 0.5 + h\}$

Example: PUFEM limiting

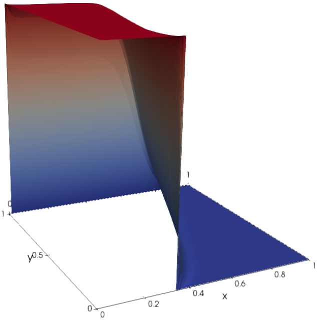
Steady advection-diffusion

$$\alpha_i(x,y) = \begin{cases} 1, & \text{if } 2h \le y \le 0.8 \\ 0, & \text{otherwise} \end{cases}$$

$$\mathbf{v} \cdot \nabla u - \epsilon \Delta u = 0, \qquad \mathbf{v} = (1,3), \qquad \epsilon = 0.01$$



(a) $V_{2h,2} = V_h(1)$



(b) $V_h(\alpha_h)$

Summary

- High-order finite element schemes are generally not bound-preserving
- Discrete maximum principles can be enforced by using appropriate basis functions and adding a certain amount of artificial diffusion
- Construction of accuracy-preserving correction schemes and limiters for high-order finite elements is more difficult than for $\mathbb{P}_1/\mathbb{Q}_1$
- The PU approach makes it possible to use standard high-order FEM in smooth regions and limited $\mathbb{P}_1/\mathbb{Q}_1$ approximations elsewhere
- Time discretizations can also be adjusted using continuous blending functions to combine different schemes in a conservative manner

Composite time stepping

- Time-dependent conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f}(u) = 0 \qquad \text{in } \Omega \subset \mathbb{R}^d, \quad d \in \{1,2,3\}$$

- Discretization in space and time

$$\int_\Omega \varphi_i \left(\frac{u_h^{n+1} - u_h^n}{\Delta t} \right) \mathrm{d}\mathbf{x} = \int_\Omega \nabla \varphi_i \cdot \mathbf{f}(u_h^{n+\theta}) \, \mathrm{d}\mathbf{x} - \int_{\partial\Omega} \varphi_i \mathbf{f}(u_h^{n+\theta}) \cdot \mathbf{n} \, \mathrm{d}s$$

$$u_h^{n+\theta} := \theta_h^n u_h^{n+1} + (1 - \theta_h^n) u_h^n, \qquad \theta_h = \sum_{i=1}^{N_{\mathrm{dof}}} \theta_i \varphi_i, \quad \theta_i \in [0,1]$$

- Discrete conservation property

Example: θ_h scheme

- 1D diffusion equation

$$\frac{\partial u}{\partial t} - d\frac{\partial^2 u}{\partial x^2} = 0, \qquad d = 10^{-2}, \quad \Omega = (0,1)$$

- Exact solution

$$u(x,t) = \frac{5}{7\sigma(t)} \exp\left\{ - \left(\frac{x - 0.5}{l\sigma(t)} \right)^2 \right\}$$

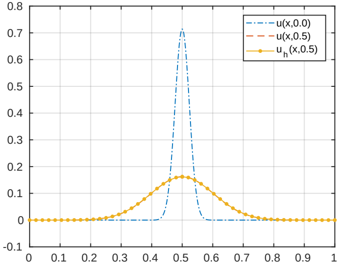
- Blending function

$$\theta_h(x) := \begin{cases} 1 & \text{if } |x - 0.5| \leq h \\ 2 - \frac{1}{h}|x - 0.5| & \text{if } h \leq |x - 0.5| \leq 2h \\ 0 & \text{if } |x - 0.5| \geq 2h \end{cases}$$

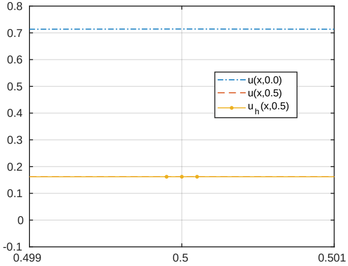
Example: θ_h scheme

Galerkin-$\mathbb{P}_1$-θ_h discretization, $\quad h = \frac{1}{50},\ \Delta t = \frac{1}{4}h^2$

Two small cut cells: $\quad \begin{array}{c} [\frac{1}{2} - h, \frac{1}{2} - \epsilon] \cup [\frac{1}{2} - \epsilon, \frac{1}{2}] \\ [\frac{1}{2}, \frac{1}{2} + \epsilon] \cup [\frac{1}{2} + \epsilon, \frac{1}{2} + h] \end{array} \qquad \epsilon = 10^{-4}$



(a) solution at $T = 0.5$



(b) cut cell region

References

- C. Lohmann, D. Kuzmin, J.N. Shadid, S. Mabuza, Flux-corrected transport algorithms for continuous Galerkin methods based on high order Bernstein finite elements. *J. Comput. Phys.* **344** (2017) 151-186.
- D. Kuzmin, Gradient-based limiting and stabilization of continuous Galerkin methods. *Ergebnisber. Angew. Math.* **589**, TU Dortmund University, 2018.
- D. Kuzmin, M. Quezada de Luna, C. Kees, A partition of unity approach to adaptivity and limiting in continuous finite element methods. In preparation.