The discrete maximum principle for FEM discretisations of the convection-diffusion equation

Gabriel R. Barrenechea

Department of Mathematics and Statistics, University of Strathclyde, Scotland

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This talk gathers contributions made in collaboration with:

1. Erik Burman (UCL, UK)
2. Volker John (WIAS, Germany)
3. Fotini Karakatsani (Chester, UK)
4. Petr Knobloch (Charles University, Czech Republic)
5. Richard Rankin (Nottingham, China)

Outline

Outline of the talk :

1. Introduction: classical results on the discrete maximum principle.
2. Nonlinear discretisations: general results.
3. Blending stabilised finite element methods.
4. Algebraic Flux Correction schemes.
5. Concluding remarks.

Introduction: The discrete maximum principle

The Continuous Maximum Principle :

Theorem

Let u be the weak solution of the problem ($\varepsilon > 0$)

$$\begin{aligned} -\varepsilon\Delta u + \boldsymbol{b}\cdot\nabla u &= g && \text{in } \Omega\,, \\ u &= 0 && \text{on } \partial\Omega\,. \end{aligned}$$

Then, if $g \geq 0$ in Ω, $u \geq 0$ in Ω, and has no interior minima.

The Finite Element Method : Find $u_h \in \mathbb{P}_1(\Omega)$such that

$$\varepsilon\,(\nabla u_h, \nabla v_h)_\Omega + (\boldsymbol{b}\cdot\nabla u_h, v_h)_\Omega = (g, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

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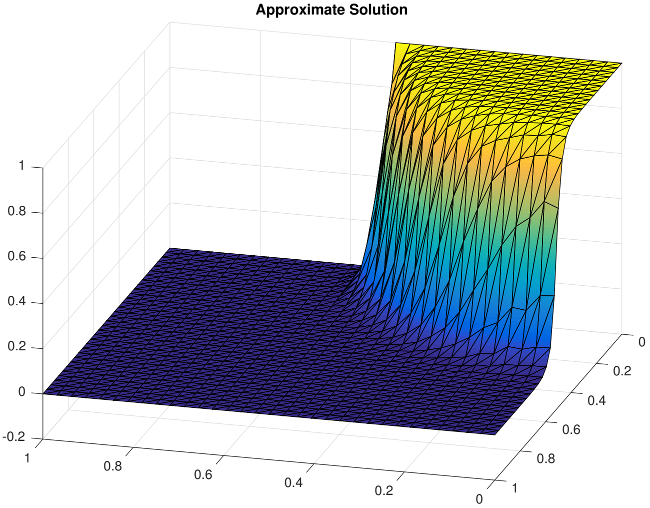

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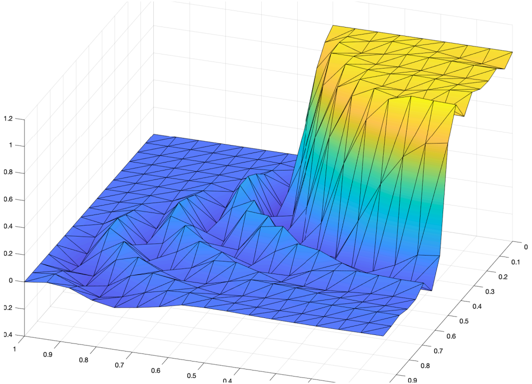

Figure 2: Rotating convection problem: Galerkin solution.

Introduction: The discrete maximum principle

The matrix form : Find $\mathrm{U} \in \mathbb{R}^N$ such that

$$\mathbb{A}\mathrm{U} = \mathrm{G}$$

where $\mathbb{A} = (a_{ij})_{i,j=1}^N$, with

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Desired result : Prove that $\mathbb{A}^{-1} \geq 0$. This is very difficult in general.

Sufficient Conditions (Ciarlet (1970, FDM); Ciarlet & Raviart (1973, FEM)):

- $a_{ii} > 0$ for every i;
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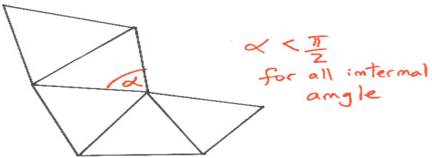

Figure 3: An acute mesh

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This means that the conforming $\mathbb{P}_1$ FEM satisfies the DMP for the convection-diffusion equation only on acute, very refined meshes.

Different solutions

The first idea: Artificial diffusion. Add an artificial viscosity of a size proportional to h.[1]

Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$a(u_h, v_h) + s(u_h, v_h) = (g, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

The matrix : In this case, we have

$$a_{ij} = (\varepsilon + \alpha\|\boldsymbol{b}\|_\infty h)\ell_{ij} + c_{ij} \leq 0$$

if the mesh is acute, and α is large enough.

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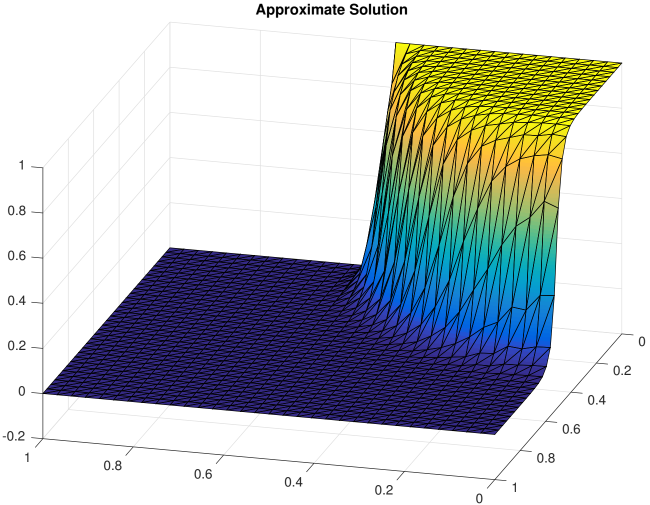
Data: $\varepsilon = 10^{-5}$, $\boldsymbol{b} = (-y, x)$, $g = 0$.



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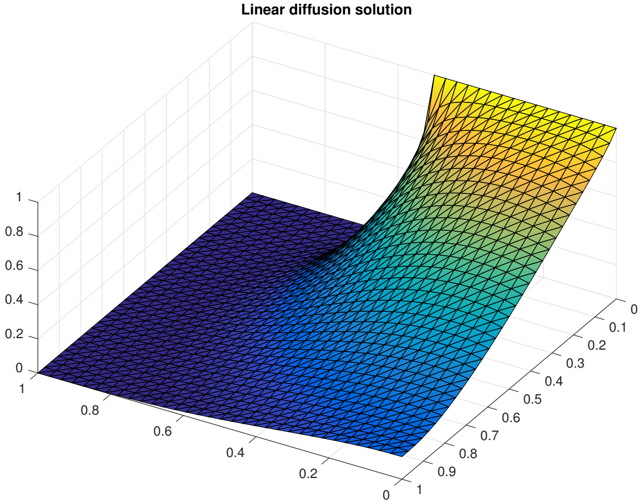

Solution: nonlinear diffusion

Back to the proof:

Theorem

Let us suppose that $a_{ij} \leq 0$ for all $i \neq j$ and let us define $S_i = \{j \in \{1, ..., N\} : a_{ij} \neq 0\}$. Then

$$(g, \phi_i)_\Omega \geq 0 \Longrightarrow u_h(\boldsymbol{x}_i) \geq \min\{u_h(\boldsymbol{x}_j) : j \in S_i \setminus \{i\}\} .$$

Proof: Let us suppose that $u_h(x_i)$ is a strict local minimum. Then,

$$0 \leq (g, \phi_i)_\Omega = \sum_{j=1}^{N} a_{ij} u_h(\boldsymbol{x}_j)$$

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Main Conclusion : The validity of the maximum principle does not need $a_{ij} \leq 0$ for all $i \neq j$, but only for the rows in which there is a local extremum.

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Solution: nonlinear (shock-capturing) methods

Nonlinear system : Find $\mathrm{U} \in \mathbb{R}^N$ such that

$$\sum_{j=1}^{N} \Big(a_{ij} u_h(\boldsymbol{x}_j) + \boldsymbol{n}(u_h)_{ij} u_h(\boldsymbol{x}_j) \Big) = (g, \phi_i)_\Omega \qquad \forall\, i = 1, \ldots, N\,,$$

where $(\boldsymbol{n}(u_h)_{ij})_{i,j=1}^N$ is a matrix that depends on the solution of the system. Ideally, this matrix should satisfy:

- $\boldsymbol{n}(u_h)_{ij} \neq 0$ only in neighbourhoods of extrema (and layers);
- $\boldsymbol{n}(u_h)_{ij} \approx 0$ in flat regions.

Theorem

Consider any $u_h \in \mathbb{P}_1(\Omega)$. Let us suppose that each time $u_h(\boldsymbol{x}_i)$ is a strict local extremum of u_h on S_i we have

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Then, the nonlinear method satisfies the discrete maximum principle. [2]

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The finite element version

Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$a(u_h, v_h) + d_h(u_h; u_h, v_h) = (g, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

Main features :

- d_h is a continuous form, may depend on the residual, or not.
- In some cases (not that many!), the maximum principle can be proved:
    1. Mizukami & Hughes, CMAME, (1985)
    2. Burman & Ern CMAME (2002), Math. Comp. (2005);
    3. Badia & Hierro CMAME (2015, dG);
    4. ...
- Optimal convergence can seldomly be proved.

Example I: Blending stabilised methods

The method : Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$a(u_h, v_h) + \underbrace{\sum_{E \in \mathscr{E}_h} \delta_0 h_E \left(\nabla u_h - \alpha_E(u_h)\Pi_E(\nabla u_h), \nabla v_h\right)_{\omega_E}}_{=d_h(u_h;u_h,,v_h)} = (g, v_h)_\Omega \,,$$

for all $v_h \in \mathbb{P}_1(\Omega)$, where:

- $\omega_E = \{K \in \mathscr{T}_h : K \cap E = E\}$;
- $\Pi_E : L^2(\omega_E)^2 \to \mathbb{P}_0^2$ is the orthogonal $L^2(\omega_E)$ projection;

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for all $v_h \in \mathbb{P}_1(\Omega)$, where:

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Example I: Blending stabilised methods

Discrete maximum principle : Let us suppose the mesh is Delaunay.

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$$a_{ij} + \boldsymbol{n}(u_h)_{ij} = (\varepsilon + \delta_0 h)\ell_{ij} + c_{ij}\,,$$

and the proof is similar to the case of linear diffusion.[3]

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Example I: Blending stabilised methods - Numerics

Data : $g = 0$, $\varepsilon = 10^{-5}$. The mesh used is a $2 \times 80 \times 80$ structured mesh.

Figure 5: Present method; 110 iterations for convergence.

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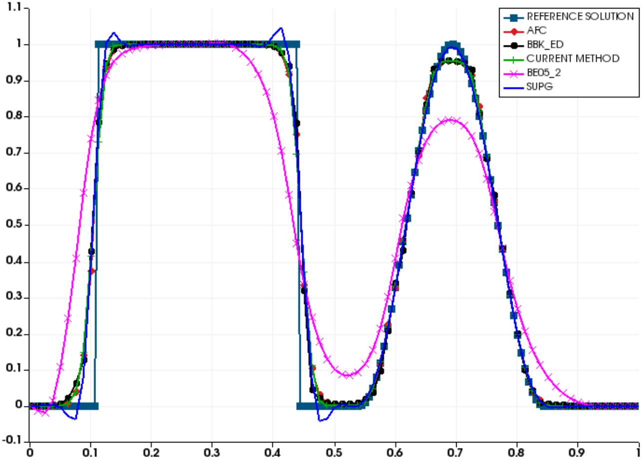

Figure 5: Cross-section along the line $x = 0.1$.

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Example II: Algebraic Flux Correction schemes

Starting point : the linear system:

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From the properties of $\mathbb{D}$ it follows that

$$\big(\mathbb{D}\mathrm{U}\big)_i = \sum_{j\neq i} f_{ij} \quad \text{where } f_{ij} = d_{ij}(u_j - u_i) \text{ are the fluxes}\,.$$

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$$(\mathbb{A}\mathrm{U})_i + \sum_{j \neq i} f_{ij} = g_i$$

Goal : To localise the artificial diffusion. In other words, to limit the fluxes f_{ij}.

The limiters α_{ij} should satisfy the following:

- $\alpha_{ij} \in [0,1]$;
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Let us suppose that $u_h(\boldsymbol{x}_i)$ is a strict local extremum in S_i. Then, $\alpha_{ij} = 1$ for all $j \in S_i$

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Example II: Algebraic Flux Correction schemes

A weak formulation : Find $u_h \in \mathbb{P}_1(\Omega)$ such that

$$a(u_h, v_h) + d_h(u_h; u_h, v_h) = (g, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

The stabilisation term $d_h(\cdot;\cdot,\cdot)$ is given by

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Remark : Then, AFC schemes achieve a stable result by adding edge-based diffusion to the formulation.[4]

[4] B., Burman, Karakatsani, Numer. Math. (2017); and B., John, Knobloch, Rankin, SeMA Journal, (2018).

Example II: Algebraic Flux Correction schemes

Possible definitions of the limiter α_{ij}:

- Boris-Book limiter : Boris, Book 1973 (time-dependent);
- Zalesak's algorithm : Zalesak 1979 (unsteady); Kuzmin 2007 (steady));
- (upwind) Kuzmin algorithm : Kuzmin 2007, + ..., time-dependent, steady state, transport, etc...
- Smootheness-based viscosity (and variants): Jameson, Schmidt, Turkel (1981, Euler); Jameson (2017); Guermond, Popov, et al (2014,15,etc..., transport mostly); Badia et al (2017, etc... transport mostly); B., Burman, Karakatsani 2017.
- Linearity-preserving indicators : Kuzmin 2012 (time-dependent); B., John, Knobloch 2017 (steady convection-diffusion);
- Differentiable limiters : Badia et.al. (2016,...; transport mostly, and Euler);
- ...

Example II: Algebraic Flux Correction schemes

Results in the analysis of the AFC schemes (steady-state):

- Kuzmin's upwind limiter (analysed in BJK16):
  - DMP in Delaunay meshes;
  - Convergence in Delaunay meshes;
- Smoothness indicator (BBK17):
  - DMP in Delaunay meshes;
  - Convergence in all regular meshes;
- Linearity preserving indicators (Kuzmin 12; BJK17):
  - DMP in general meshes;
  - Convergence in Delaunay meshes.

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Algebraic Flux Correction schemes: A $3D$ numerical comparison

Data: $\varepsilon = 10^{-5}$, $g = 0$.

Figure 6: The approximations obtained using an SUPG method on an adaptively refined mesh containing 135,408,953 elements.

Algebraic Flux Correction schemes: A $3D$ numerical comparison

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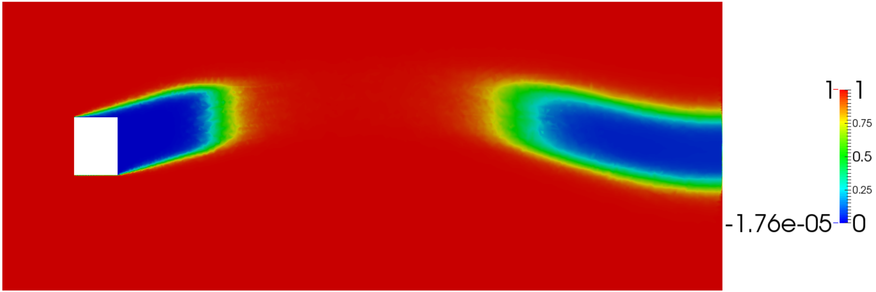

Figure 6: The slice at $z = 1$ of the approximation obtained by the Zalesak-Kuzmin limiters. 70 fixed-point iterations. Adapted mesh consisting of 1,308,237 elements.

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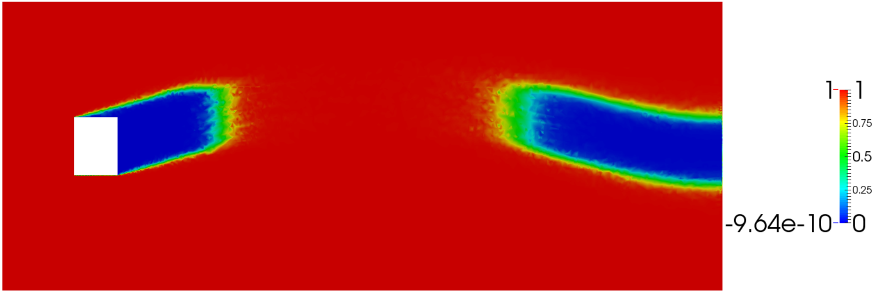

Figure 6: The slice at $z = 1$ of the approximation obtained using the new liminer. 166 fixed-point iterations. Adapted mesh consisting of 1,308,237 elements.

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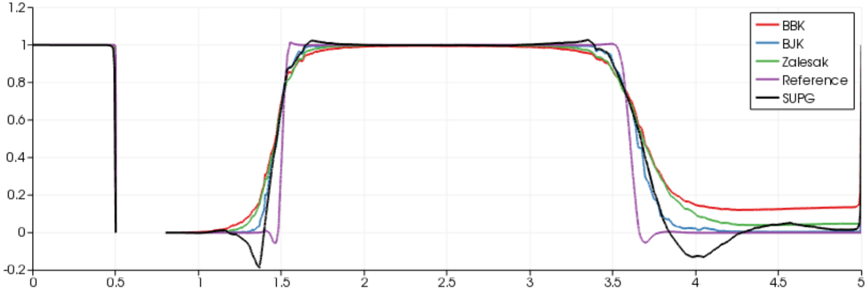

Figure 6: A comparison of the solution with all the limiters, and the reference, for the line $y = z = 1$.

Conclusions and open questions

Conclusions (so far) :

1. nonlinear schemes modify (primarily) just a few lines of the system of equations;
2. LPS methods can be blended to impose the satisfaction of the DMP;
3. AFC schemes can be rewritten as a nonlinear edge diffusion scheme;
4. the above has led to a stability/convergence analysis that was lacking for convection-diffusion equations.

Open questions:

- General meshes.
- The efficient solution of the nonlinear system.
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