Some recent results on algebraic flux correction schemes

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The continuous maximum principle :

Theorem

Let u be the solution of the problem

$$-\Delta u = f \quad \text{in}\, \Omega\,,$$

and $u = 0$ on $\partial\Omega$. Then, if $f \geq 0$ in Ω, then $u \geq 0$ in Ω, and attains its minimum at the boundary.

The discrete version :

Theorem

Let $u_h \in \mathbb{P}_1(\Omega)$ be the solution of the problem

$$(\nabla u_h, \nabla v_h)_\Omega = (f, v_h)_\Omega \quad \forall\, v_h \in \mathbb{P}_1(\Omega)\,.$$

Then, if $f \geq 0$ in Ω and the mesh is acute, then $u_h \geq 0$ in Ω, and attains its minimum at the boundary.

Remark : Under these hypothesis, the matrix $[(\nabla\lambda_j, \nabla\lambda_i)_\Omega]$ is an M-matrix. This is, it is invertible, all the diagonal elements are positive, and the off-diagonal ones are non-positive.

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The convection-diffusion equation

The DMP :

Theorem

Let $u_h \in \mathbb{P}_1(\Omega)$ be the solution of the problem

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

Then, if $f \geq 0$ in Ω, the mesh is acute, and $\frac{|\boldsymbol{b}|h}{2\varepsilon} < 1$, then $u_h \geq 0$ in Ω, and attains its minimum at the boundary.

Some early solutions

Artificial diffusion :

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

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

Bad news : The linear schemes, such as the artificial diffusion, have two main drawbacks:

- their consistency error leads to a convergence of $O(\sqrt{h})$;
- they produce results which are extremely diffusive.

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A representative numerical result

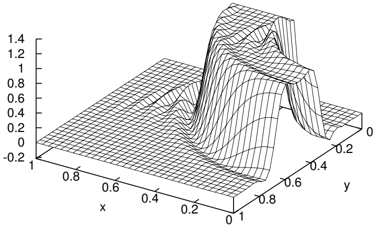

Figure 1 : Solution using a standard LPS method

A representative numerical result - II

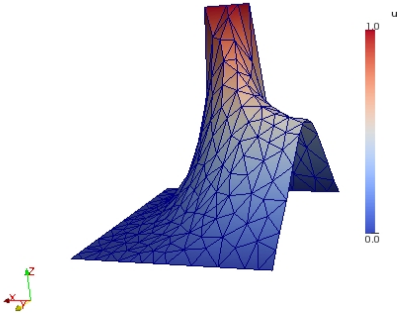

Figure 2 : Solution using the first order artificial diffusion method

Solution: nonlinear schemes

Idea :

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

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

Main features :

- N is a continuous form, may depend on the residual, or not.
- In some cases (not that many!), the maximum principle can be proved (cf. Burman & Ern).
- Optimal convergence can be proved in most cases.

A more recent alternative (D. Kuzmin) : Algebraic Flux Correction schemes. These work at the matrix level, and have provided very convincing numerical results.

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Goals and Outline

1. Goals:
   - Understand the method, and its main features.
   - Give the first steps towards a numerical analysis of it.
   - Study its numerical behaviour.
2. The method for the 1D problem.
3. The discrete maximum principle.
4. Solvability of the linear problems, and the nonlinear one.
5. Concluding remarks.

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Algebraic flux correction schemes

Starting point : A finite element discretisation of our problem of the form:

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

Define:

$$\mathbb{D} := (d_{ij}) \quad \text{where} \quad d_{ij} := -\max\{a_{ij}, 0, a_{ji}\} \text{ for } i \neq j\,, \quad d_{ii} = -\sum_{j \neq i} d_{ij}\,.$$

Remark: The matrix $\tilde{\mathbb{A}}$ is an M-matrix. Then, it preserves positivity.

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Algebraic flux correction schemes

Equivalent system :

$$\tilde{\mathbb{A}}\,\mathrm{U} = \mathrm{G} + \mathbb{D}\mathrm{U}\,.$$

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

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

Goal : To limit the fluxes f_{ij} which are responsible for spurious oscillations.

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Goal : To limit the fluxes f_{ij} which are responsible for spurious oscillations.
The limiters α_{ij} should satisfy the following:

- $\alpha_{ij} \in [0, 1]$;
- α_{ij} should be as close to 1 as possible;
- $\alpha_{ij} \approx 1$ where the Galerkin solution is smooth.

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Equivalent system :

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

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Definition of the limiters

1. Compute $P_i^+, P_i^-, Q_i^+, Q_i^-$ in such a way that, for each pair of neighbouring nodes x_i, x_j with indices such that $a_{ji} \leq a_{ij}$ one performs the updates

$$\begin{aligned} P_i^+ &:= P_i^+ + \max\{0, f_{ij}\}\,, & P_i^- &:= P_i^- - \max\{0, f_{ji}\}\,,\\ Q_i^+ &:= Q_i^+ + \max\{0, f_{ji}\}\,, & Q_i^- &:= Q_i^- - \max\{0, f_{ij}\}\,,\\ Q_j^+ &:= Q_j^+ + \max\{0, f_{ij}\}\,, & Q_j^- &:= Q_j^- - \max\{0, f_{ji}\}\,, \end{aligned}$$

2. Set

$$R_i^+ := \min\left\{1, \frac{Q_i^+}{P_i^+}\right\} \quad , \quad R_i^- := \min\left\{1, \frac{Q_i^-}{P_i^-}\right\}.$$

3. Finally,

$$\alpha_{ij} = \begin{cases} R_i^+ & \text{if } f_{ij} > 0\,,\\ R_i^- & \text{if } f_{ij} < 0\,, \end{cases} \qquad\qquad i,j = 1,\ldots,N\,.$$

The 1D convection-diffusion equation

Model problem :

$$-\varepsilon\, u'' + bu' = g \quad \text{in } (0,1) \quad u(0) = u(1) = 0\,,$$

with positive constants ε and b.

Galerkin FEM : Equidistant nodes $x_i = ih$, with $h = 1/N$. Find $u_h \in \mathbb{P}_1(0,1)$ such that $u_h(0) = u_h(1) = 0$ and

$$\varepsilon(u_h', v_h') + (bu_h', v_h) = (g, v_h) \qquad \forall\, v_h \in \mathbb{P}_1(0,1)\,.$$

Difference equation form : Setting $u_i = u_h(x_i)$, this problem is rewritten as

$$-\varepsilon\,\frac{u_{i-1} - 2\,u_i + u_{i+1}}{h^2} + b\,\frac{u_{i+1} - u_{i-1}}{2\,h} = g_i \quad i = 1, \ldots, N-1.$$

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Assume: $Pe := \frac{bh}{2\varepsilon} > 1$.

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The 1D convection-diffusion equation

Algebraic problem with limited fluxes:

$$\big(\mathbb{A}\mathrm{U}\big)_i + \sum_{j\neq i}(1-\alpha_{ij})f_{ij} = g_i \quad \text{with} \quad f_{ij} = d_{ij}(u_j - u_i)\,.$$

For the 1D problem: the system reduces to $u_0 = u_N = 0$, and

$$-(\varepsilon + \beta_i\,\tilde{\varepsilon})\,\frac{u_{i-1} - 2\,u_i + u_{i+1}}{h^2} + b\,\frac{u_{i+1} - u_{i-1}}{2\,h} = g_i\,, \qquad i = 1,\ldots,N-1\,,$$

where

$$\beta_i = \begin{cases} 1 & \text{if } u_{i+1} \neq u_i \quad \text{and} \quad \dfrac{u_i - u_{i-1}}{u_{i+1} - u_i} < 1\,, \\ 0 & \text{otherwise}\,, \end{cases}$$

and $\tilde{\varepsilon} = \frac{b\,h}{2} - \varepsilon = \varepsilon\,(Pe - 1)$.

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The Discrete Maximum Principle

Theorem

Consider any $\tilde{\varepsilon} \geq b\,h/2 - \varepsilon$. Then any solution of the nonlinear problem satisfies the discrete maximum principle, i.e., for any $i \in \{1, \ldots, N\}$, one has

$$g_i \geq 0 \qquad \Rightarrow \qquad u_i \geq \min\{u_{i-1}, u_{i+1}\}\,.$$

Moreover, for any $k, l \in \{0, 1, \ldots, N+1\}$ with $k + 1 < l$, one has

$$g_i \geq 0\,, \quad i = k+1, \ldots, l-1 \qquad \Rightarrow \qquad u_i \geq \min\{u_k, u_l\}\,, \quad i = k, \ldots, l\,.$$

Some numerics and the choice of $\tilde{\varepsilon}$

Other possible choices: The artificial diffusion matrix $\mathbb{D}$ can be defined using different combinations of the diffusion and convection matrices. For example:

(F) $\tilde{\varepsilon} = \frac{b\,h}{2} - \varepsilon = \varepsilon(Pe - 1)$.

(C) $\tilde{\varepsilon} = \frac{b\,h}{2}$.

(P) $\tilde{\varepsilon} = \frac{b\,h}{2}\left(\coth Pe - \frac{1}{Pe}\right)$.

Data: $b = f = 1$, $N = 16, \varepsilon = 0.03$, i.e., we solve

$$-0.03u'' + u' = 1 \quad \text{in } (0,1)\,,$$

and $u(0) = u(1) = 0$.

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Some numerics and the choice of $\tilde{\varepsilon}$

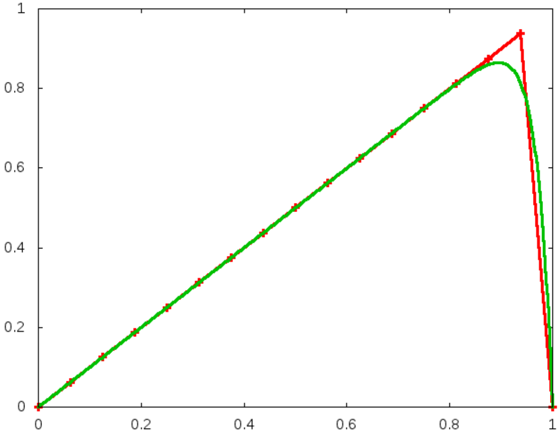

Figure 3 : Comparison of the exact solution (green) and discrete solution with $\tilde{\varepsilon}$ from (F).

Some numerics and the choice of $\tilde{\varepsilon}$

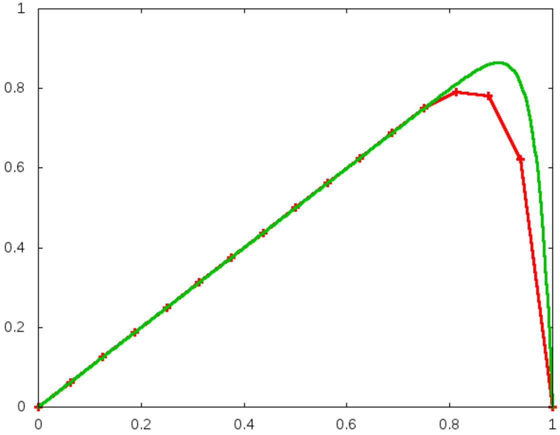

Figure 4 : Comparison of the exact solution (green) and discrete solution with $\tilde{\varepsilon}$ from (C).

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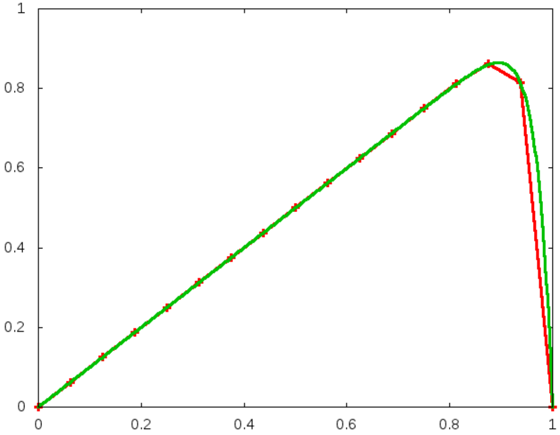

Figure 5 : Comparison of the exact solution (green) and discrete solution with $\tilde{\varepsilon}$ from (P).

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Bad news from the numerics

- Computations very sensitive to rounding errors.

Idea : replace the condition $u_i < \min\{u_{i-1}, u_{i+1}\}$ by $u_i < \min\{u_{i-1}, u_{i+1}\} - \tau$.

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Example: $N = 4$, $\varepsilon = 0.03$, $b = 1$, $f_1 = 6$, $f_2 = -6$, $f_3 = 3$, $f_4 = -2$, and $\tilde{\varepsilon}$ from (F).

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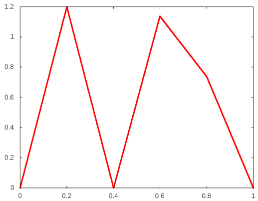
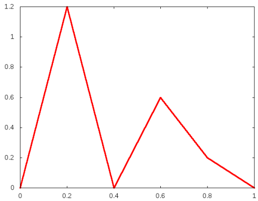
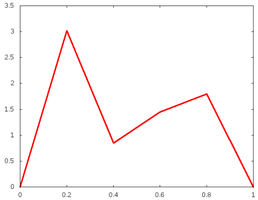


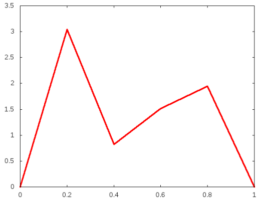
$1\ 1\ 0\ 1 \rightarrow 1\ 1\ 1\ 1$



$1\ 1\ 1\ 1 \rightarrow 1\ 1\ 1\ 0$



$0\ 0\ 1\ 0 \rightarrow 1\ 1\ 0\ 1$



$0\ 0\ 0\ 0 \rightarrow 1\ 1\ 0\ 1$

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Solvability of the linear subproblems

Theorem

For every choice of $\tilde{\varepsilon} \in \left[\frac{b\,h}{2} - \varepsilon, \frac{b\,h}{2}\right]$ *and every possible* $\beta_i \in [0,1]$, *the problem*

$$-(\varepsilon + \beta_i\,\tilde{\varepsilon})\,\frac{u_{i-1} - 2\,u_i + u_{i+1}}{h^2} + b\,\frac{u_{i+1} - u_{i-1}}{2\,h} = g_i\,,$$

has a unique solution.

Solvability of the nonlinear problem

Main remark : The lack of solvability is due to the discontinuity of the coefficients β_i

Theorem

Let us suppose that the functions $\beta_i : \mathbb{R}^{N+1} \to [0,1]$, $i = 1, ..., N-1$, are continuous, and let $\tilde{\varepsilon}$ be any of the previous choices. Then, the nonlinear FCT scheme has a solution.

Proof: Write the method as the fixed point equation

$$\mathbb{M}(\boldsymbol{\beta}(\boldsymbol{u}))\,\boldsymbol{u} = \boldsymbol{g}\,,$$

apply the fact that the determinant is a continuous function of the entries of a matrix, and Brouwer's fixed point Theorem. □

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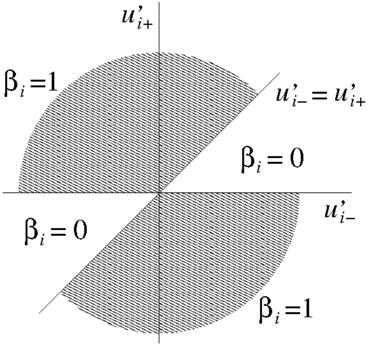
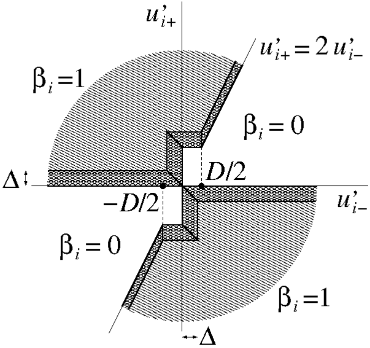
Graphical representation of the regularisation





The price to pay: A weak version of the DMP

Theorem

Let $u_0, \ldots, u_{N+1}$ *be a solution of the modified FCT scheme with any functions* $\beta_1, \ldots, \beta_N \in [0,1]$ *as described before. Then*

$$g_i \geq 0 \qquad \Rightarrow \qquad u_i \geq \min\{u_{i-1}, u_{i+1}\} \qquad \text{or} \qquad u_i \geq \max\{u_{i-1}, u_{i+1}\} - \delta\, h\,,$$

for $i = 1, \ldots, N$.

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Numerical evidence on the violation of the DMP

The problem : $-\varepsilon u'' + u' = 0$ subject to $u(0) = 1$ and $u(1) = 0$. We measured

- $MAX := u_h^{\max} - 1$;
- $RMAX := \max\{(u_h^{\max} - 1)/h\}$;
- Pe_{RMAX} the value of Pe for which the maximum $RMAX$ is attained.

Table 1 : Violation of the discrete maximum principle for the continuous β_i.

	$Pe \in [1, 20)$			$Pe \in [20, \infty)$		
ε	MAX	$RMAX$	Pe_{RMAX}	MAX	$RMAX$	Pe_{RMAX}
10^{-1}	6.62−3	2.65−2	1.25	no $Pe \geq 20$		
10^{-2}	3.55−3	9.27−2	1.85	no $Pe \geq 20$		
10^{-3}	7.14−4	1.28−1	2.79	4.88−15	4.88−14	25.0
10^{-4}	1.06−4	1.40−1	3.77	5.60−14	9.23−13	21.6
10^{-5}	1.41−5	1.47−1	4.80	4.81−13	5.59−10	21.6
10^{-6}	1.77−6	1.51−1	5.84	6.06−12	6.92−8	22.9

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Some preliminary numerics in 2D: The Hemker problem

Data: $\varepsilon = 10^{-4}$, $\approx 12,000$ $\mathbb{Q}_1$ elements, discontinuous α_{ij} as before, continuous as follows

$$R_i^+ = R_i^- = \min\left\{1, \frac{\min\{Q_i^+, -Q_i^-\}}{\max\{P_i^+, -P_i^-, \tau\}}\right\}.$$

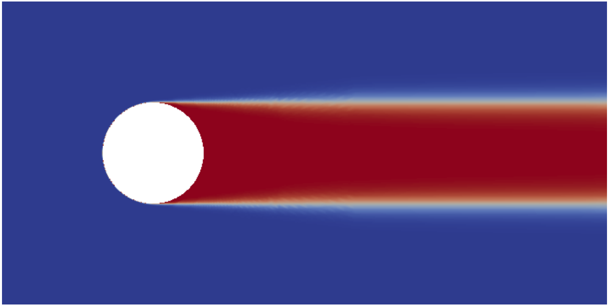

Figure 6 : Discontinuous α_{ij}, non-symmetric

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Some preliminary numerics in 2D: The Hemker problem

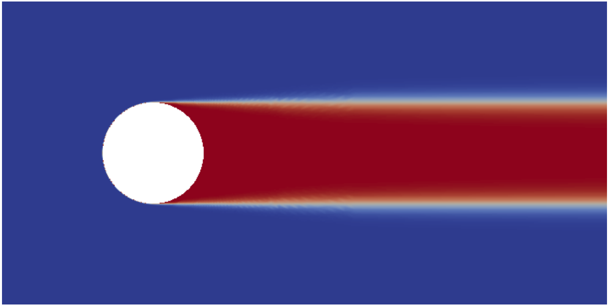

Figure 7 : Continuous α_{ij}, non-symmetric

Conclusions and perspectives

1. Some further insight on FCT schemes.
2. Analysis of a wider class of schemes.
3. Counter-examples of existence of solutions for the original method.
4. A modification that is proved to possess solutions, but satisfies only a weak version of the DMP.

Future extensions:

- Deeper study of the symmetric version in higher dimensions.
- Maximum principle on general meshes.
- (Order of) convergence.
- Time-dependent problems.
- Coupled nonlinear problems in chemical reactions.

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