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Numerical Analysis / *Analyse numérique*

A second order in space combination of methods verifying a maximum principle for the discretization of diffusion operators

Une combinaison d'ordre 2 de méthodes vérifiant un principe du maximum pour la discrétisation d'opérateurs de diffusion

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Abstract. We describe a second order in space combination of methods suppressing oscillations appearing for diffusion operator discretization with cell-centered finite volume schemes.

Résumé. Nous décrivons une combinaison d'ordre 2 de méthodes supprimant les oscillations apparaissant pour la discrétisation d'opérateur de diffusion avec des schémas volumes finis centrés sur les mailles.

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Il est bien connu que les schémas classiques discrétisant des opérateurs de diffusion ne satisfont pas toujours le principe du maximum pour des mailles très déformées ou des rapports d'anisotropie très élevés [11, 14, 16]. Nous proposons une nouvelle correction non linéaire qui donne des solutions non oscillantes pour des schémas volumes finis centrés sur les mailles. Elle se généralise aux schémas hybrides [13] ou aux schémas DDFV [4, 10] en suivant la méthode décrite dans [18]. En comparaison aux méthodes proposées dans [15, 17], elle est très simple à mettre en œuvre et s'avère également d'ordre 2. Comme les algorithmes décrits dans [5], le schéma est convergent avec des hypothèses spécifiques mais il peut être appliqué à des mailles de forme générale. C'est un point de vue différent des méthodes décrites dans [9, 17] (en dimension 1 ou en différences finies), où des preuves complètes de convergence sont proposées sans hypothèse sur la solution calculée.

Nous considérons le problème (1) et un schéma centré sur les mailles défini dans (3) avec des hypothèses de consistence et coercivité décrites dans les paragraphes 2.2.2 and 2.2.3 de la publication [5]. Ici, $\mathscr{M}$ et $\mathscr{E}$ désignent les mailles et les faces du maillage. Nous notons $|K|$ le volume d'une maille et $F_{K,\sigma}$ une approximation consistante de $\int_\sigma D\vec{\nabla}u.\vec{n}_{K,\sigma}\mathrm{d}\sigma$. Pour $\eta \geq 0$, nous proposons la correction non linéaire décrite dans (5). Il s'agit de la combinaison de deux méthodes proposées dans [5] et [6, 7].

Dans la proposition 1, nous montrons que le schéma modifié reste coercif. Dans la proposition 2, nous expliquons pourquoi il existe au moins une solution au système (5). Dans la proposition 3, nous établissons que le nouveau schéma vérifie le principe du maximum. Dans la proposition 7, nous prouvons qu'avec une hypothèse spécifique sur la solution calculée, la méthode converge vers l'unique solution de (1).

Nous donnons finalement quelques résultats numériques en cherchant la solution du problème (12). Le paramètre ϵ est égal à 10^{-3} ce qui donne un rapport d'anisotropie égal à 10^3. Nous vérifions que $f \geq 0$. Nous utilisons les maillages de triangles issus du test 1 dans le benchmark [14]. Nous calculons la solution du problème à l'aide d'un algorithme de point fixe. Notons u^i la valeur de la solution à l'itéré i et $A(u^i)$ la matrice discrétisant l'opérateur de diffusion. Le schéma itératif s'écrit $B(u^i)(u^{i+1} - u^i) = A(u^i)u^i - f$. Nous choisissons pour B la matrice obtenue pour $N = 1$ (voir remarque 4).

Nous montrons tout d'abord les résultats obtenus dans le tableau 1 avec le schéma développé dans [19] (Schéma 1) (Erreurs L^2 de u par rapport à la solution analytique, ordre, pourcentage de valeurs négatives, valeur minimum). Dans tous les calculs, nous choisissons $\eta = 0$. Nous présentons également les résultats obtenus avec le schéma décrit dans le paragraphe 3 (Schéma 2), le schéma 3 (avec $N = 2$ dans la remarque 4) et la méthode développée dans [5] (Schéma 4).

Nous vérifions que les schémas 2, 3 et 4 n'oscillent plus. Nous observons que les schémas 2 et 3 tendent vers l'ordre 2 alors que le schéma 4 reste d'ordre 1 comme déjà montré dans [5]. Pour les méthodes 2 et 4, le nombre d'itérations *nit* dans l'algorithme du point fixe reste inférieur à 20. Le schéma 3 semble encore plus rapide.

1. Introduction

We are interested in the discretization of an elliptic equation. It is well known that classical schemes discretizing diffusion operators do not always satisfy a maximum principle for highly distorted meshes or high anisotropy ratios [11, 14, 16]. We propose a new nonlinear maximum preserving correction for cell-centered finite volume schemes. It can be applied, for example, to the cell-centered finite volume schemes developed in [1, 3, 2, 8, 12, 19]. It can also be generalized to hybrid schemes [13] or DDFV [4, 10] following the method described in [18]. Compared to the methods proposed in [15], it is very simple to implement and we observe it is second order in space in the numerical results. Similar to the algorithms described in [5], this scheme is convergent under a specific assumption. Nervertheless, it can be applied to linear schemes using general meshes. It is a different point of view of methods described in [9, 17] (which can be only applied in 1 dimension in space or with finite difference schemes), where a complete proof of convergence is proposed (without specific assumptions).

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2. Presentation

Let be Ω a polygonal domain of $\mathscr{R}^2$ (or $\mathscr{R}^3$). We consider the following elliptic problem: find $u : \Omega \to \mathscr{R}$ such that

$$\begin{cases} -\operatorname{div} \overline{\overline{D}} \vec{\nabla} u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{1}$$

with

- $f \in L^2(\Omega)$;
- D, a symmetric tensor-valued function such that:
  - (a) D is piecewise Lipschitz-continuous on Ω; and
  - (b) the set of the eigenvalues is included in $[\lambda_{\min}, \lambda_{\max}]$ with $\lambda_{\min} > 0$ for all $x \in \Omega$.

3. A non linear correction

Here, we use the same notations and assumptions on the discretization of Ω as those presented in ([5, Section 2]). We recall that $\mathscr{M}$ is a family of non-empty open polygonal disjoint subsets of Ω (the *control volumes*) such that $\overline{\Omega} = \cup_{K\in\mathscr{M}} \overline{K}$. To study the convergence of the schemes, we will use the following quantities: the size of the mesh

$$h_{\mathscr{M}} = \sup_{K\in\mathscr{M}} \operatorname{diam}(K)$$

and the regularity of the mesh

$$\operatorname{reg}_{\mathscr{M}} = \sup_{\substack{K\in\mathscr{M}\\ \sigma\in\mathscr{E}_K}} \left\{ \frac{\operatorname{diam}(K)}{d_{K,\sigma}} \right\} + \sup_{\substack{K,L\in\mathscr{M}\\ \sigma\in\mathscr{E}_K\cap\mathscr{E}_L}} \left\{ \frac{d_{L,\sigma}}{d_{K,\sigma}} \right\}.$$

We recall that we consider cell-centered schemes consisting in finding :

$$\forall\, K \in \mathscr{M}, \quad \mathscr{S}_K(u) = |K|\, f_K, \tag{2}$$

where f_K denotes the mean value of f on the cell K, and $(\mathscr{S}_K(u), K \in \mathscr{M})$ is a system of Card($\mathscr{M}$) equations on some unknowns $(u_K)_{K\in\mathscr{M}}$. On the other hand, we denote by $\mathscr{H}_{\mathscr{M}}$ the set of functions which are constant on each control volume of $\mathscr{M}$.

We consider the discrete linear cell-centered operator $\mathscr{A}_K(u)$, with a stencil denoted $V(K)$ consisting of cells in the neighborhood of K and having cell faces on the edges of $\partial\Omega$. We assume that the operator $\mathscr{A}_K(u)$ can be written in the following form : $\mathscr{A}_K(u) = \sum_{Z\in V(K)} \alpha_{Z,K}(u_Z - u_K)$, where $\alpha_{Z,K}$ do not depend on u (with the convention $u_Z = u_\sigma$ if $Z = \sigma \in \mathscr{E}_{ext}$, where u_σ is given by the boundary conditions). We assume that the number of elements of $V(K)_{K\ in \mathscr{M}}$ is bounded independently of the mesh. The scheme $\mathscr{A}_K(u)$ is defined by:

$$\begin{cases} \forall\, K \in \mathscr{M}, & -\mathscr{A}_K(u) = |K| f_K, \\ \forall\, \sigma \in \mathscr{E}_{\text{ext}}, & u_\sigma = 0. \end{cases} \tag{3}$$

We also assume that the scheme is symmetric and satisfies the assumptions of coercivity and consistency described in 2.2.2 and 2.2.3 in [5]. For all $K \in \mathscr{M}$ and for all $Z \in V(K) \cap \mathscr{M}$, in the spirit of the formula (25) in [7] or the formula (20) in [6], $\Theta_{K,Z}(u)$ is defined as :

$$\Theta_{K,Z}(u) = \begin{cases} 1 - \frac{\min(\max(u_K,0),\max(u_Z,0))}{\max(|u_K|,|u_Z|)} & \text{if } \max(|u_K|,|u_Z|) \neq 0, \\ 1 & \text{if } \max(|u_K|,|u_Z|) = 0. \end{cases} \tag{4}$$

We propose to modify the previous scheme as follows:

$$\begin{cases} \forall\, K \in \mathscr{M}, & -\mathscr{A}_K(u) + \sum_{Z\in V(K)} \beta_{K,Z}(u)\Theta_{K,Z}(u)(u_K - u_Z) = -\mathscr{A}_K(u) + \mathscr{R}_K(u) = |K| f_K, \\ \forall\, \sigma \in \mathscr{E}_{ext}, & u_\sigma = 0 \end{cases} \tag{5}$$

where $\beta_{K,Z}(u)$ (which depends on $\eta \geq 0$), is defined by :

$$\beta_{K,Z}(u) = \max\left\{\frac{|\mathscr{A}_K(u)|}{\sum_{Y\in V(K)}|u_Y - u_K|}, \frac{|\mathscr{A}_Z(u)|}{\sum_{Y\in V(Z)}|u_Y - u_Z|}\right\} + \eta \min\left(|K|, |Z|, \frac{|K|^2}{\sum_{Y\in V(K)}|u_Y - u_K|} + \frac{|Z|^2}{\sum_{Y\in V(Z)}|u_Y - u_Z|}\right) \quad (6)$$

with the convention $\mathscr{A}_Z(u) = 0$ if $Z \in \mathscr{E}_{ext}$.

4. Properties of the algorithm

Proposition 1. *The modified scheme is coercive.*

Proof. We can immediately check that $\forall\, K \in \mathscr{M}$, $\forall\, Z \in V(K)\cap\mathscr{M}$, $\Theta_{Z,K} = \Theta_{K,Z}$ and $0 \leq \Theta_{Z,K} \leq 1$. Since $\forall\, K \in \mathscr{M}$, $\forall\, Z \in V(K)\cap\mathscr{M}$, $\beta_{K,Z}(u) = \beta_{Z,K}(u)$ and $\beta_{K,Z}(u) \geq 0$, we deduce that

$$\sum_{K\in\mathscr{M}}\sum_{Z\in V(K)} \beta_{K,Z}(u)\Theta_{Z,K}(u_K - u_Z) \geq 0.$$

We conclude using the coercivity of the original scheme. □

Proposition 2. *With the admissible meshes defined in* [5]*, there exists at least one solution to the system* (5).

Proof. For all $K \in \mathscr{M}$ and for all $Z \in V(K)\cap\mathscr{M}$, we remark that $\Theta_{K,Z}(u)(u_K - u_Z) \to 0$ as $\max(|u_K|, |u_Z|) \to 0$. On the other hand, for all $K \in \mathscr{M}$, for all $Z \in V(K)\cap\mathscr{M}$, we obtain the inequalities:

$$|\beta_{K,Z}(u)\Theta_{K,Z}(u)(u_K - u_Z)| \leq |\beta_{K,Z}(u)||(u_K - u_Z)|.$$

As the terms $|\beta_{K,Z}(u)|$ are bounded as shown in [5], we deduce the continuity of $\mathscr{R}_K(u)$ from $\mathscr{H}_{\mathscr{M}}$ into $\mathscr{H}_{\mathscr{M}}$. We conclude using Proposition 1, and applying Proposition 6 in [5]. □

Proposition 3. *If, for all $K \in \mathscr{M}$, $f_K > 0$ and if $\eta > 0$, the modified scheme satisfies :*

$$\forall\, K \in \mathscr{M},\ u_K > 0.$$

Proof. We use a proof by contradiction. Let be $u_{K^*} = \min_{K\in\mathscr{M}} u_K$. Let us assume that $u_{K^*} \leq 0$. We deduce that $\forall\, Z \in V(K^*), \Theta_{K^*,Z}(u) = 1$ and we can write:

$$\mathscr{A}_{K^*}(u) = \sum_{Z\in V(K^*)} \frac{1}{\sum_{L\in V(K^*)}|u_L - u_K^*|}\mathscr{A}_{K^*}(u)|u_K^* - u_Z| = \sum_{Z\in V(K^*)} \Delta_K^* sgn(u_K^* - u_Z)\mathscr{A}_{K^*}(u)(u_K^* - u_Z)$$

with $\Delta_K^* = \frac{1}{\sum_{L\in V(K^*)}|u_L - u_K^*|}$. We deduce that the modified scheme can be written:

$$\mathscr{S}_{K^*}(u) = \sum_{Z\in V(K^*)} \tau_{K^*,Z}(u)(u_K^* - u_Z) = |K^*|f_K^* \quad (7)$$

with $\tau_{K^*,Z}(u) = \Delta_K^* sgn(u_K^* - u_Z)\mathscr{A}_K^*(u) + \beta_{K^*,Z}(u)$. According to the definition of $\beta_{K^*,Z}(u)$, we check that $\tau_{K^*,Z}(u) > 0$. As $\sum_{Z\in V(K^*)} \tau_{K^*,Z}(u)(u_K^* - u_Z) \leq 0$ and $f_K^* > 0$, we deduce it is impossible. □

Remark 4. A variant of the method consists in modifying $\Theta_{K,Z}(u)$ as follows:

$$\Theta_{K,Z}(u) = \begin{cases} 1 - \left\{\frac{\min(\max(u_K,0),\max(u_Z,0))}{\max(|u_K|,|u_Z|)}\right\}^N & \text{if } \max(|u_K|,|u_Z|) \neq 0 \\ 1 & \text{if } \max(|u_K|,|u_Z|) = 0 \end{cases} \quad (8)$$

where N is an integer. Of course, by similar reasoning, Propositions 1, 2 and 3 remain true.

Remark 5. Consider the following problem : find $u : \Omega \to \mathscr{R}$ such that

$$\begin{cases} -\operatorname{div} \overline{\overline{D}} \vec{\nabla} u = 0 & \text{in } \Omega, \\ u = u_b & \text{on } \partial\Omega \end{cases} \tag{9}$$

with $0 \le u_b \le 1$. It is clear that the solution of the equation (9) satisfies: $0 \le u \le 1$. To satisfy these inequalities, we modify $\Theta_{K,Z}(u)$ as follows:

$$\Theta_{K,Z}(u) = \begin{cases} 1 - \frac{\min(\max(u_K,0),\max(u_Z,0)) \min(\max(1-u_K,0),\max(1-u_Z,0))}{\max(|u_K|,|u_Z|) \max(|1-u_K|,|1-u_Z|)} \\ \quad \text{if } \max(|u_K|, |u_Z|) \neq 0 \text{ and } \max(|1-u_K|, |1-u_Z|) \neq 0 \\ 1 \quad \text{if } \max(|u_K|, |u_Z|) = 0 \text{ or } \max(|1-u_K|, |1-u_Z|) = 0. \end{cases} \tag{10}$$

We show in a similar way that Propositions 1 and 2 are also satisfied and that $\forall\, K \in \mathscr{M}$, $0 \le u_K \le 1$.

Assumption 6. *We assume there exists a constant C independent of $h_{\mathscr{M}}$ such that*

$$\sum_{K\in\mathscr{M}} |\mathscr{A}_K(u)| \le \frac{C}{h_{\mathscr{M}}^{\tau}} \sum_{K\in\mathscr{M}} |K| f_K \textit{ with } 0 \le \tau < 1.$$

Proposition 7. *With admissible meshes $\mathscr{M}$ defined in* [5] *such that* $\operatorname{reg}_{\mathscr{M}}$ *is bounded and with Assumption 6, the solutions of the system 5 converge to the unique solution of* (1) *as $h_{\mathscr{M}}$ tends toward zero.*

Proof. We recall that for all $K \in \mathscr{M}$ and for all $J \in V(K) \cap \mathscr{M}$, $0 \le \Theta_{K,J}(u) \le 1$. As the number of elements of $V(K)_{K\in\mathscr{M}}$ is bounded, with Assumption 6, we deduce there exists constant C_2 not depending on $h_{\mathscr{M}}$ such that:

$$\begin{aligned} h_{\mathscr{M}} \sum_{K\in\mathscr{M}} \sum_{J\in V(K)} \beta_{K,J}(u)\Theta_{K,J}(u)|u_K - u_J| &\le h_{\mathscr{M}} \sum_{K\in\mathscr{M}} \sum_{J\in V(K)} \beta_{K,J}(u)|u_K - u_J| \\ &\le \frac{C_2}{h_{\mathscr{M}}^{\tau}} h_{\mathscr{M}} \sum_{K\in\mathscr{M}} |K|(f_K + 1). \end{aligned} \tag{11}$$

As $f \in L^2(\Omega)$, we deduce that:

$$\sum_{K\in\mathscr{M}} h_{\mathscr{M}} \sum_{J\in V(K)} \beta_{K,J}(u)|u_K - u_J| \to 0 \text{ as } h_{\mathscr{M}} \to 0,$$

which gives:

$$\sum_{K\in\mathscr{M}} h_K \sum_{J\in V(K)} \beta_{K,J}(u)|u_K - u_J| \to 0 \text{ as } h_{\mathscr{M}} \to 0.$$

We conclude using Proposition 7 described in [5]. □

Remark 8. In the future, we will try to suppress the Assumption 6 to prove the convergence of the modified scheme.

5. Numerical results

In order to numerically estimate the convergence of the scheme, let us consider the following elliptic problem:

$$\begin{cases} -\operatorname{div}(\overline{\overline{D}} \vec{\nabla} u) = f & \text{on } \Omega =]0, 0.5[\times]0, 0.5[\\ u = \sin(\pi x)\sin(\pi y) & \text{pour } (x, y) \in \partial\Omega \end{cases} \quad \text{with } \overline{\overline{D}} = \frac{1}{(x^2+y^2)} \begin{pmatrix} y^2 + \epsilon x^2 & -(1-\epsilon)xy \\ -(1-\epsilon)xy & x^2 + \epsilon y^2 \end{pmatrix} \tag{12}$$

and

$$\begin{cases} u_{\text{ana}} = \sin(\pi x)\sin(\pi y) \\ f = -\operatorname{div} \overline{\overline{D}} u_{\text{ana}}. \end{cases} \tag{13}$$

The parameter ϵ is equal to 10^{-3} and the anisotropy ratio is equal to 10^3. We shall check that $f \ge 0$. We use triangular meshes of test 1 in the benchmark [14]. To deal with the nonlinear terms, we perform an iterative algorithm. Let us denote u^i the value of the solution where i is a fixed point iteration index, $A(u^i)$ the matrix for the discretization of the diffusion operator and $B(u^i)$, the matrix for the discretization of the diffusion operator for $N = 1$ (see Remark 4). The iterative scheme can be written: $B(u^i)(u^{i+1} - u^i) = A(u^i)u^i - f$.

We show the results in the Table 1 obtained using the linear scheme developed in [19] (scheme 1) (L^2 error of the computed solution u with respect to the analytical solution, order of convergence, percentage of negative values, minimum value).

We also present the results obtained with the scheme described in Section 4 ($N = 1$: scheme 2, $N = 2$: scheme 3) and the method developed in [5] (scheme 4 : $\forall\ K \in \mathscr{M}$, $\forall\ Z \in V(K) \cap \mathscr{M}$, $\Theta_{K,Z}(u) = 1$). In all the numerical results, we choose $\eta = 0$. Concerning the schemes 2, 3 and 4, we check that they are non oscillating. We observe that the scheme 2 and 3 are second order in space whereas scheme 4 remains first order in space as described in [5]. For the method 2 and 4, the number of iterations (*nit*) in the fixed point algorithm is less than 20. The scheme 3 seems to converge faster.

Remark 9. It could be interesting to use ideas developed in [9] to theoretically prove that the method is second order in space for the heat equation.

Table 1. Numerical results with scheme 1, 2, 3 and 4 as a function of the discretization step

h	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$
L^2 error (scheme 1)	8.15×10^{-1}	1.32×10^{-1}	2.06×10^{-2}	3.46×10^{-3}	6.88×10^{-4}
Order in space (scheme 1)		2.64	2.66	2.58	2.33
Negative values (scheme 1)	23	6.7	1.45	0.37	0.1
Mininum value (scheme 1)	-5.84×10^{-1}	-1.55×10^{-1}	-3.94×10^{-2}	-9.90×10^{-3}	-2.48×10^{-3}
L^2 error (scheme 2)	5.73×10^{-2}	2.12×10^{-2}	6.92×10^{-3}	2.05×10^{-3}	5.79×10^{-4}
Order in space (scheme 2)		1.44	1.61	1.75	1.82
nit (scheme 2)	16	17	16	13	11
L^2 error (scheme 3)	9.81×10^{-2}	3.64×10^{-2}	9.84×10^{-3}	2.39×10^{-3}	5.96×10^{-4}
Order in space (scheme 3)		1.43	1.89	2.04	2.00
nit (scheme 3)	9	9	8	7	7
L^2 error (scheme 4)	6.77×10^{-2}	3.53×10^{-2}	1.82×10^{-2}	9.46×10^{-3}	4.89×10^{-3}
Order in space (scheme 4)		0.94	0.96	0.94	0.95
nit (scheme 4)	13	15	14	14	13

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