

Numerical Analysis

A nine-point finite volume scheme for the simulation of diffusion in heterogeneous media [☆]

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Received 6 January 2009; accepted 6 February 2009

Available online 25 April 2009

Presented by Philippe G. Ciarlet

Abstract

We propose a cell-centered symmetric scheme which combines the advantages of MPFA (multipoint flux approximation) schemes such as the L or the O scheme and of hybrid schemes: it may be used on general non-conforming meshes, it yields a 9-point stencil on two-dimensional quadrangular meshes, it takes into account the heterogeneous diffusion matrix, it is coercive and it can be shown to converge. The scheme relies on the use of special points, called harmonic averaging points, located at the interfaces of heterogeneity. *To cite this article: L. Agelas et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).*

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Résumé

Un schéma à neuf points pour la diffusion en milieu hétérogène. Nous proposons un schéma ayant ses inconnues aux centres des mailles, combinant les avantages des schémas à flux multi-points et des schémas hybrides : il possède un stencil à 9 points en 2D, respecte les hétérogénéités de la matrice de diffusion, et il est coercif ; de plus, on peut montrer qu'il converge. Le schéma est basé sur l'utilisation de points situés aux interfaces d'hétérogénéité, en lesquels la formule de la moyenne harmonique est utilisable. *Pour citer cet article : L. Agelas et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).*

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1. Introduction

The aim of this Note is to provide an approximation of the unique weak solution to the diffusion problem $-\operatorname{div}(\Lambda(\mathbf{x})\nabla u) = f$ in Ω with boundary condition $u = 0$ on $\partial\Omega$, where we denote by $\partial\Omega = \overline{\Omega} \setminus \Omega$ the boundary of the domain Ω . Hence we wish to find an approximation of the solution to the problem:

$$\text{find } u \in H_0^1(\Omega) \text{ such that } \forall v \in H_0^1(\Omega), \quad \int_{\Omega} \Lambda(\mathbf{x})\nabla u(\mathbf{x}) \cdot \nabla v(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega} f(\mathbf{x})v(\mathbf{x}) \, d\mathbf{x}. \quad (1)$$

[☆] Work supported by Groupement de Recherche MOMAS, PACEN/CNRS.

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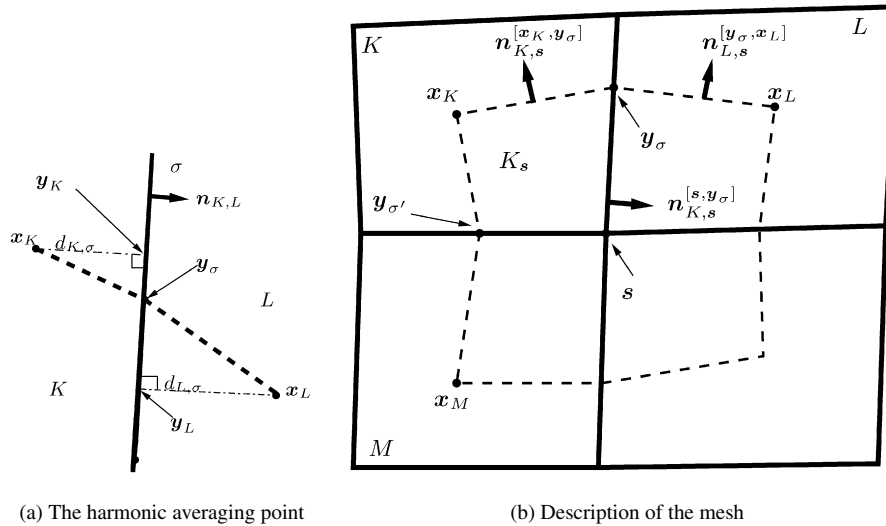


Fig. 1.

We assume that Ω is an open bounded connected polygonal subset of \mathbb{R}^2 (the adaptation of the present paper to the three-dimensional case will be the subject of future work), Λ is a measurable function from Ω to $\mathcal{M}_d(\mathbb{R})$ with $d = 2$, where we denote by $\mathcal{M}_d(\mathbb{R})$ the set of $d \times d$ matrices, such that for a.e. $\mathbf{x} \in \Omega$, $\Lambda(\mathbf{x})$ is symmetric, and such that the set of its eigenvalues is included in $[\underline{\lambda}, \bar{\lambda}]$, with $\underline{\lambda}$ and $\bar{\lambda} \in \mathbb{R}$ satisfying $0 < \underline{\lambda} \leq \bar{\lambda}$, and $f \in L^2(\Omega)$. Our quest is motivated in particular by the numerical simulation of complex flows in porous media, which includes coupling with thermodynamics and/or chemistry; because of these complex couplings, the discretization method is often chosen to be cell-centered in industrial codes. Although several schemes were recently proposed see e.g. [7] and references therein, there is yet no “ultimate” scheme, *i.e.* a centered scheme with small stencil, which respects the physical bounds and yields good approximations even on non-conforming distorted meshes and with a sharp contrast in the permeabilities (or diffusion coefficients).

The new scheme which we introduce here is designed in the framework of this quest, and has the following characteristics:

- (i) it may be used on any polygonal non-conforming mesh;
- (ii) it provides the exact solution if Λ is piecewise constant in polygonal subdomains and u is affine in each of these subdomains (this property is sought in the multipoint flux approximation schemes given for instance in [1]);
- (iii) it leads to a nine-point scheme in the case of quadrilateral meshes which are not too distorted (in a sense involving the diffusion matrix Λ);
- (iv) it is symmetric and coercive with respect to an adequate discrete norm, and therefore a convergence proof holds.

2. Harmonic averaging points

Consider two domains K and L of \mathbb{R}^2 with different diffusion matrices (or permeabilities) Λ_K and Λ_L , separated by a planar interface σ , and let $\mathbf{x}_K \in K$ and $\mathbf{x}_L \in L$. In order to obtain a scheme with smallest possible stencil, we seek some point in σ where the value of any piecewise affine solution u to (1) can be expressed as a linear combination of $u(\mathbf{x}_K)$ and $u(\mathbf{x}_L)$ only. We show in the next lemma that such a point always exists in the hyperplane containing σ :

Lemma 2.1. *Let σ be a hyperplane of \mathbb{R}^d , with $d \in \mathbb{N}^*$ and let K, L be the two open half-spaces with the common boundary σ . Let $\Lambda_K \in \mathcal{M}_d(\mathbb{R})$ and $\Lambda_L \in \mathcal{M}_d(\mathbb{R})$ be two given symmetric definite positive matrices, let \mathbf{n}_{KL} be the unit vector normal to σ oriented from K to L , $\mathbf{x}_K \in K$ and $\mathbf{x}_L \in L$ be given and $d_{K,\sigma}$ (resp. $d_{L,\sigma}$) the distance from*

x_K (resp. x_L) to σ (see Fig. 1(a)). Let \mathbf{y}_K and $\mathbf{y}_L \in \sigma$ such that $\mathbf{x}_K = -d_{K,\sigma}\mathbf{n}_{KL} + \mathbf{y}_K$ and $\mathbf{x}_L = d_{L,\sigma}\mathbf{n}_{KL} + \mathbf{y}_L$. Let $\mathbf{y}_\sigma \in \sigma$ (called the harmonic averaging point) be defined by

$$\mathbf{y}_\sigma = \frac{\lambda_L d_{K,\sigma} \mathbf{y}_L + \lambda_K d_{L,\sigma} \mathbf{y}_K}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}} + \frac{d_{K,\sigma} d_{L,\sigma}}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}} (\boldsymbol{\lambda}_K^\sigma - \boldsymbol{\lambda}_L^\sigma), \quad (2)$$

denoting by $\lambda_K = \mathbf{n}_{KL} \cdot \Lambda_K \mathbf{n}_{KL}$, $\boldsymbol{\lambda}_K^\sigma = (\Lambda_K - \lambda_K \text{Id}) \mathbf{n}_{KL}$, $\lambda_L = \mathbf{n}_{KL} \cdot \Lambda_L \mathbf{n}_{KL}$ and $\boldsymbol{\lambda}_L^\sigma = (\Lambda_L - \lambda_L \text{Id}) \mathbf{n}_{KL}$. Then the following averaging formula holds, for all functions u defined on \mathbb{R}^d , affine in K and L , such that u is continuous on σ , and such that $\Lambda_K \nabla u|_K \cdot \mathbf{n}_{KL} = \Lambda_L \nabla u|_L \cdot \mathbf{n}_{KL}$:

$$u(\mathbf{y}_\sigma) = \frac{\lambda_L d_{K,\sigma} u(\mathbf{x}_L) + \lambda_K d_{L,\sigma} u(\mathbf{x}_K)}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}}. \quad (3)$$

Let us sketch the proof of the lemma. We denote by \mathbf{G}_K the gradient of u in K , with $\mathbf{G}_K = g_K \mathbf{n}_{KL} + \mathbf{G}_K^\sigma$, $\mathbf{G}_K^\sigma \cdot \mathbf{n}_{KL} = 0$ and by $\mathbf{G}_L = g_L \mathbf{n}_{KL} + \mathbf{G}_L^\sigma$, $\mathbf{G}_L^\sigma \cdot \mathbf{n}_{KL} = 0$ the gradient of u in L . The continuity property of u on σ first leads to $\mathbf{G}_K^\sigma = \mathbf{G}_L^\sigma = \mathbf{g}^\sigma$ and then to $d_{K,\sigma} g_K + d_{L,\sigma} g_L = u(\mathbf{x}_L) - u(\mathbf{x}_K) + (\mathbf{y}_K - \mathbf{y}_L) \cdot \mathbf{g}^\sigma$, and the condition $\Lambda_K \mathbf{G}_K \cdot \mathbf{n}_{KL} = \Lambda_L \mathbf{G}_L \cdot \mathbf{n}_{KL}$ can be written $g_K \lambda_K - g_L \lambda_L = \mathbf{g}^\sigma \cdot (\boldsymbol{\lambda}_L^\sigma - \boldsymbol{\lambda}_K^\sigma)$. Expressing g_K with respect to \mathbf{g}^σ and using $u(\mathbf{y}) = u(\mathbf{x}_K) + \mathbf{G}_K \cdot (\mathbf{y} - \mathbf{x}_K)$, for all $\mathbf{y} \in \sigma$, allows us to write that $u(\mathbf{y}) = u(\mathbf{x}_K) + d_{K,\sigma} \frac{\lambda_L(u(\mathbf{x}_L) - u(\mathbf{x}_K)) + (\mathbf{y}_K - \mathbf{y}_L) \cdot \mathbf{g}^\sigma + d_{L,\sigma} \mathbf{g}^\sigma \cdot (\boldsymbol{\lambda}_L^\sigma - \boldsymbol{\lambda}_K^\sigma)}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}} + (\mathbf{y} - \mathbf{y}_K) \cdot \mathbf{g}^\sigma$. The point \mathbf{y}_σ is then defined as the unique point $\mathbf{y} \in \sigma$ such that the preceding expression no longer depends on \mathbf{g}^σ , and the resulting expression for $u(\mathbf{y}_\sigma)$ follows.

3. Definition of the scheme

We consider general polygonal, possibly non-conforming, meshes of Ω (as in [4]). Let \mathcal{T} be the set of control volumes, that are disjoint open polygonal subsets of Ω such that $\bigcup_{K \in \mathcal{T}} \bar{K} = \bar{\Omega}$. We denote by Λ_K the mean value of Λ in $K \in \mathcal{T}$. Let \mathcal{E} be the set of edges of the mesh; we denote by \mathcal{E}_K the set of the edges of any $K \in \mathcal{T}$. Let $\mathcal{P} = \{\mathbf{x}_K, K \in \mathcal{T}\}$ be the set of the so-called ‘‘centers’’ of the control volumes, which are the approximation points. We assume that, for all $K \in \mathcal{T}$, K is star-shaped with respect to \mathbf{x}_K . Let \mathcal{V} be the set of the vertices of the mesh, and let \mathcal{V}_σ (resp. \mathcal{V}_K) be the set of the vertices of any $\sigma \in \mathcal{E}$ (resp. $K \in \mathcal{T}$). For any edge $\sigma \subset \partial\Omega$, we denote by \mathbf{y}_σ its center point. For any interior edge σ , we denote by \mathbf{y}_σ the harmonic averaging point defined by (2) if this point is interior to σ (we then denote by \mathcal{E}_\sharp the set of such edges), and by the center of σ otherwise.

Remark 1 (Harmonic averaging points and meshes). The condition $\sigma \in \mathcal{E}_\sharp$ generally holds for meshes which are not ‘‘too distorted’’. It holds in particular if $[\mathbf{x}_K, \mathbf{x}_L] \cap \sigma$ is an interior point to σ in the case of identical diffusion matrices Λ_K and Λ_L . It also holds if the orthogonal projections of \mathbf{x}_K and \mathbf{x}_L on σ are interior points to σ in the case of isotropic diffusion matrices Λ_K and Λ_L .

Let $X_{\mathcal{T}}$ be the set of all families $u = \{u_K, u_\sigma, u_{\sigma,s}, K \in \mathcal{T}, \sigma \in \mathcal{E}, s \in \mathcal{V}_\sigma, \text{ with } u_\sigma = u_{\sigma,s} = 0 \text{ for } \sigma \subset \partial\Omega\}$. Let $X_{\mathcal{T}}^\sharp$ be the subset of all $u \in X_{\mathcal{T}}$ such that, for any $\sigma \in \mathcal{E}_\sharp$, u_σ is defined by:

$$u_\sigma = \frac{\lambda_L d_{K,\sigma} u_L + \lambda_K d_{L,\sigma} u_K}{\lambda_L d_{K,\sigma} + \lambda_K d_{L,\sigma}}. \quad (4)$$

For $u \in X_{\mathcal{T}}$, we define by $\Pi_{\mathcal{T}} u$ the piecewise constant function defined on Ω , with the constant value u_K in $K \in \mathcal{T}$. For all $K \in \mathcal{T}$ and $s \in \mathcal{V}_K$, we denote by K_s the open quadrilateral domain, the boundary of which is composed of the line segments belonging to the set: $\mathcal{E}_{K,s} = \{[\mathbf{x}_K, \mathbf{y}_\sigma], [\mathbf{x}_K, \mathbf{y}_{\sigma'}], [s, \mathbf{y}_\sigma], [s, \mathbf{y}_{\sigma'}]\}$, where $\sigma, \sigma' \in \mathcal{E}_K$ are the two edges of K with vertex s (see Fig. 1(b)). For all $\epsilon \in \mathcal{E}_{K,s}$, we denote by $\mathbf{n}_{K,s}^\epsilon$ the normal vector to ϵ outward to K_s . For any $u \in X_{\mathcal{T}}$, we denote by $u_{K,s}^\epsilon$, for any $\epsilon \in \mathcal{E}_{K,s}$, the values defined by:

$$u_{K,s}^\epsilon = \frac{u_K + u_\tau}{2} \quad \text{if } \epsilon = [\mathbf{x}_K, \mathbf{y}_\tau] \quad \text{and} \quad u_{K,s}^\epsilon = u_{\tau,s} \quad \text{if } \epsilon = [s, \mathbf{y}_\tau] \quad \text{for } \tau = \sigma \text{ or } \sigma'. \quad (5)$$

We then define a piecewise discrete gradient $\nabla_{\mathcal{T}} u$ by its constant values $\nabla_{K,s} u \in \mathbb{R}^2$ on the subcells K_s :

$$|K_s| \nabla_{K,s} u = \sum_{\epsilon \in \mathcal{E}_{K,s}} |\epsilon| (u_{K,s}^\epsilon - u_K) \mathbf{n}_{K,s}^\epsilon. \quad (6)$$

This discrete gradient satisfies the following two fundamental properties, which are also those of the cell piecewise constant gradient used in [6]:

- (i) consistency of $\nabla_{\mathcal{T}}\varphi_{\mathcal{T}}$ with $\nabla\varphi$ for a class of regular functions φ and their interpolation $\varphi_{\mathcal{T}}$ in $X_{\mathcal{T}}$;
- (ii) weak convergence, as the size of the mesh tends to 0, of $\nabla_{\mathcal{T}}u$ to $\nabla\bar{u}$ such that $u \rightarrow \bar{u}$ under suitable estimates on $u \in X_{\mathcal{T}}$.

Both properties follow from the choice (6) and the fact that, for any $\mathbf{w} \in \mathbb{R}^2$, one has: $|K_s|\mathbf{w} = \int_{\partial K_s} \mathbf{w} \cdot \mathbf{x} \mathbf{n}_{K,s}$; property (i) is also a consequence of the choice (4). For all $u, v \in X_{\mathcal{T}}$, we define a discrete inner product, expected to approximate the bilinear form $(u, v) \mapsto \int_{\Omega} \Lambda \nabla u \cdot \nabla v$. A natural choice would be $[u, v] = \sum_{K \in \mathcal{T}} \sum_{s \in \mathcal{V}_K} [u, v]_{K,s}$, where $[u, v]_{K,s} = |K_s| \Lambda_K \nabla_{K,s} u \cdot \nabla_{K,s} v$. However, this choice yields a non-coercive bilinear form, and therefore, as in [6], we stabilize it by choosing rather:

$$\langle u, v \rangle = \sum_{K \in \mathcal{T}} \sum_{s \in \mathcal{V}_K} \langle u, v \rangle_{K,s}, \quad \text{with } \langle u, v \rangle_{K,s} = |K_s| \Lambda_K \nabla_{K,s} u \cdot \nabla_{K,s} v + \sum_{\tau=\sigma, \sigma'} \alpha_{K\tau} R_{K,s}^{\tau} u R_{K,s}^{\tau} v, \quad (7)$$

where $\alpha_{K\tau} > 0$, $R_{K,s}^{\tau} u = u_{\tau} - u_K - \nabla_{K,s} u \cdot (\mathbf{y}_{\tau} - \mathbf{x}_K)$, for $\tau = \sigma$ and σ' . The scheme is then defined by

$$\text{find } u \in X_{\mathcal{T}}^{\sharp}, \text{ such that for any } v \in X_{\mathcal{T}}^{\sharp}, \quad \langle u, v \rangle = \int_{\Omega} f(\mathbf{x}) \Pi_{\mathcal{T}} v(\mathbf{x}) \, d\mathbf{x}. \quad (8)$$

This scheme is symmetric; its convergence can be proved under quite general hypotheses on the meshes. Moreover, in the case where all interior edges satisfy $\sigma \in \mathcal{E}_{\sharp}$, the edges unknowns $u_{\sigma,s}$ can be eliminated vertex by vertex, hence providing a symmetric cell-centered scheme which has the nine-point stencil on structured quadrilateral meshes (note that this elimination is also a feature of the O-scheme [2]).

4. Numerical results

We tested the scheme for some of the cases described in the benchmark [5], in particular those with anisotropy and heterogeneity such as test cases 5 and 6 (geological barrier and drain), and, as expected, the results are exact since the solution is piecewise affine in these cases. We have also run test case 5 (heterogeneous rotating anisotropy). An order 2 of convergence is then observed on the L^2 -norm of the unknown. The finest mesh that we used for this test has 640×640 grid blocks, computed in a few minutes on a PC. A direct solver could be used, numbering the unknowns using classical methods holding for 9-point stencils [3]. The convergence order 2 has also been observed on test cases, using a mesh inspired from geological studies.

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