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A linear and accurate diffusion scheme respecting the maximum principle on distorted meshes

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Abstract

This Note is devoted to the presentation of a linear diffusion scheme that respects the maximum principle on very distorted meshes. The main idea is to use a classical Finite Volumes scheme and to perform a first integration on the Voronoï mesh based on the centers of the cells. A second integration on the primary mesh is then performed. By construction the scheme preserves the maximum principle. A numerical example is also given. ***To cite this article: V. Siess, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Un schéma de diffusion linéaire respectant le principe du maximum sur des maillages déformés. Cette Note est consacrée à la présentation d'un schéma de diffusion qui respecte le principe du maximum sur des maillages très déformés. L'idée essentielle consiste à utiliser un schéma de Volumes Finis classique sur le maillage de Voronoï basé sur les barycentres des mailles primales. On procède alors à une deuxième intégration sur les mailles primales. Par construction, le schéma respecte le principe du maximum. Un exemple numérique est fourni. ***Pour citer cet article : V. Siess, C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

1. Introduction

In this Note, we are interested with the numerical resolution of the following diffusion equation:

$$\begin{cases} -\operatorname{div}\big(D(x)\vec{\nabla}\phi\big) + A(x)\phi = S(x) & \text{in } \Omega \subset \mathbb{R}^N,\ N = 2 \text{ or } 3, \\ -D(x)\vec{\nabla}\phi\cdot\vec{n} = 0 & \text{on } \partial\Omega. \end{cases} \tag{1}$$

The data D, A, and S are non-negative L^∞ functions. Moreover, we want to solve this problem on very distorted unstructured meshes, such as the ones that arise in Lagrangian Hydrodynamics codes.

Diffusion schemes have been extensively studied for a long time. There exists a wide range of schemes devoted to the resolution of (1), Finite Differences, Finite Elements, Mixte and Mixte Hybrid Finite Elements, Finite Volumes, Discrete Duality Finite Volumes [2], etc. In summary, most of these schemes are accurate on a lot of meshes, including

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very distorted unstructured meshes. However, they do not always preserve the maximum principle on very distorted meshes. It follows that non-positive and non-physical values of the solution can be obtained after resolution of (1).

Numerous remedies have been tried to overcome this difficulty. Most of them are empirical [4]. Recently nonlinear schemes were also developed [1,3,6]. They give good results and ensure positivity of the solution, but at the cost of a nonlinearity. However, other solutions, which have the advantage to be linear, are already known for a long time. For instance, one could decide to use a classical Finite Volumes scheme on a Voronoï mesh. Even if one wants or needs to work on the primary distorted mesh, this idea remains possible as is explained in what follows.

2. Description of the scheme

Let I_i denote the center of the cell i of the primary mesh, $\mathcal{C}_i$ the cell centered on I_i, $\mathcal{V}_i$ the Voronoï cell centered on I_i. Let I_j denote a neighbour of I_i, and S_{ij} the interface between the two Voronoï cells $\mathcal{V}_i$ and $\mathcal{V}_j$. Using a classical Finite Volumes scheme, we obtain the following approximated value of $-\Delta\phi$ around the point I_i.

$$-\overline{\Delta\phi}_i \approx \frac{1}{|\mathcal{V}_i|}\int_{\mathcal{V}_i} -\Delta\phi = \frac{1}{|\mathcal{V}_i|}\int_{\partial\mathcal{V}_i} -\vec{\nabla}\phi\cdot\vec{n} = \frac{1}{|\mathcal{V}_i|}\sum_j\int_{\mathcal{S}_{ij}} -\vec{\nabla}\phi\cdot\vec{n} \approx \frac{1}{|\mathcal{V}_i|}\sum_j|\mathcal{S}_{ij}|\frac{\phi(I_i)-\phi(I_j)}{I_iI_j}. \tag{2}$$

Let $\mathcal{A}(\phi) = -\operatorname{div}(D\vec{\nabla}\phi)$ be an isotropic elliptic operator. It can be linked to the Laplace operator Δ through the following formula.

$$\begin{aligned}
\mathcal{A}(\phi) &= -\operatorname{div}(D\vec{\nabla}\phi) = -D\Delta\phi - \vec{\nabla}D\cdot\vec{\nabla}\phi,\\
\mathcal{A}(\phi) &= \frac{1}{2}\big(\mathcal{A}(\phi)+\mathcal{A}^*(\phi)\big) = -\frac{1}{2}\big(D\Delta\phi+\Delta(D\phi)\big) - \frac{1}{2}\big(\vec{\nabla}D\cdot\vec{\nabla}\phi - \operatorname{div}(\phi\vec{\nabla}D)\big)\\
&= -\frac{1}{2}\big(D\Delta\phi+\Delta(D\phi)\big) + \frac{1}{2}\phi\Delta D\\
&= \mathcal{A}_1(\phi)+\mathcal{A}_2(\phi).
\end{aligned} \tag{3}$$

Now comes the algorithm to follow:

(i) Forget the primary mesh. Just keep in memory the positions of the centers of the cells and compute the Voronoï mesh based on these points.
(ii) Compute with (2) the matrix of the Laplace operator using a classical Finite Volumes scheme on the Voronoï mesh.
(iii) Multiply line i of this matrix by $D_i|\mathcal{C}_i|$ and symmetrize the matrix. This gives the matrix corresponding to the integration of $\mathcal{A}_1$ on the primary cells.
(iv) Modify the diagonal of this matrix so that the sum of each line or column of the matrix be zero. This gives the matrix corresponding to the integration of $\mathcal{A}$ on the primary cells. By construction, it is an M-matrix and the discrete maximum principle will be verified.
(v) The other terms in (1) are classically integrated on each primary cell, like in a classical Finite Volumes scheme.

Remark 1. In this paper, for the sake of simplicity, I do not deal with the question of the boundary conditions. It is an important one, but many efficient answers can easily be imagined, so I prefer focusing on the diffusion operator.

Remark 2. It is well known that the classical Finite Volumes scheme respects the discrete maximum principle and is very accurate on Voronoï meshes. Here was described a way to modify this scheme so as to respect the primary distorted mesh. Intuition as well as the various computations performed by the author lead to the conclusion that the convergence order of the modified Finite Volumes scheme (for the solution in L^2-norm) lies between 1 and 2. In fact, the convergence order depends on the distance between the centers of the primary cells and the centers of the Voronoï cells. The closer they are, the higher the convergence order is. As refinement processes usually regularize the meshes, one expects a convergence order close to 2. Notice also that step (iii) leads to a weighted arithmetic mean $\frac{1}{2}(\frac{D_i|\mathcal{C}_i|}{|\mathcal{V}_i|}+\frac{D_j|\mathcal{C}_j|}{|\mathcal{V}_j|})$ for the diffusion coefficient at the interface S_{ij}. But for discontinuous diffusion coefficient D, a harmonic mean $\frac{2}{\frac{1}{D_i}+\frac{1}{D_j}}$ is known to give better results. So it is a point that has to be more precisely studied.

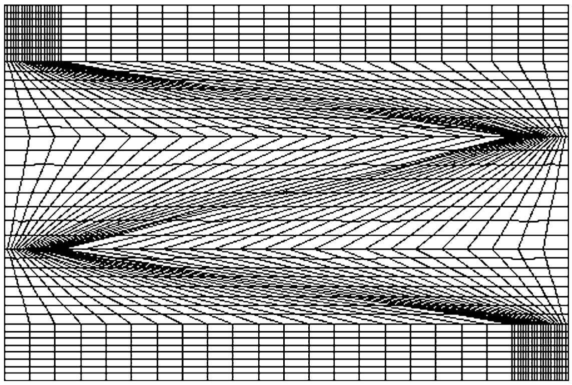

Fig. 1. A Kershaw mesh . . .

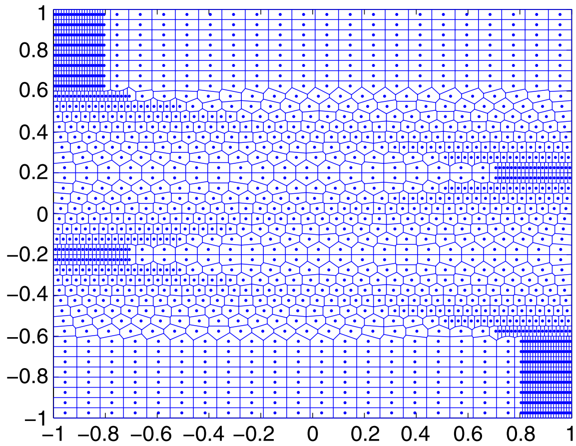

Fig. 2. . . . and its Voronoï mesh.

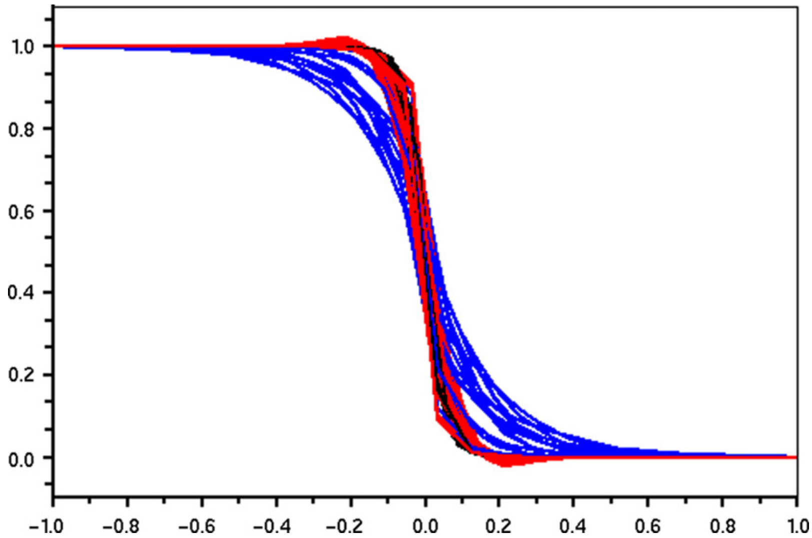

Fig. 3. Finite Volumes (blue) and DDFV scheme (red).

3. A numerical result

Here is a numerical example which shows that the scheme is accurate and does preserve the maximum principle on distorted meshes. The mesh used in this example is very distorted and is known under the name of Kershaw mesh. Figs. 1 and 2 represent a 40 × 40 Kershaw mesh and its Voronoï diagram.

Let us consider the following equation:

$$\begin{cases} -\Delta\phi + \omega^2\phi = \omega^2\chi_{\{x\leqslant 0\}} & \text{in } \Omega =]-1,1[^2, \\ \vec{\nabla}\phi\cdot\vec{n} = 0 & \text{on } \partial\Omega. \end{cases} \tag{4}$$

In fact, this problem is one-dimensional. The analytical solution is given by

$$\phi(x,y) = 1 - \frac{\cosh(\omega(x+1))}{2\cosh\omega} \quad \text{if } x \leqslant 0, \qquad \phi(x,y) = \frac{\cosh(\omega(x-1))}{2\cosh\omega} \quad \text{if } x \geqslant 0. \tag{5}$$

For large values of the parameter ω, here $\omega = 100$, we have a strong gradient around zero. This can lead to negative values depending on the scheme used to solve (4). We use here 3 different schemes, a classical Finite Volumes scheme (FV), a Discrete Duality Finite Volumes scheme (DDFV), and the modified Finite Volumes scheme. The FV scheme respects the maximum principle, but gives a very unaccurate solution, as can be seen in Fig. 3. On the other

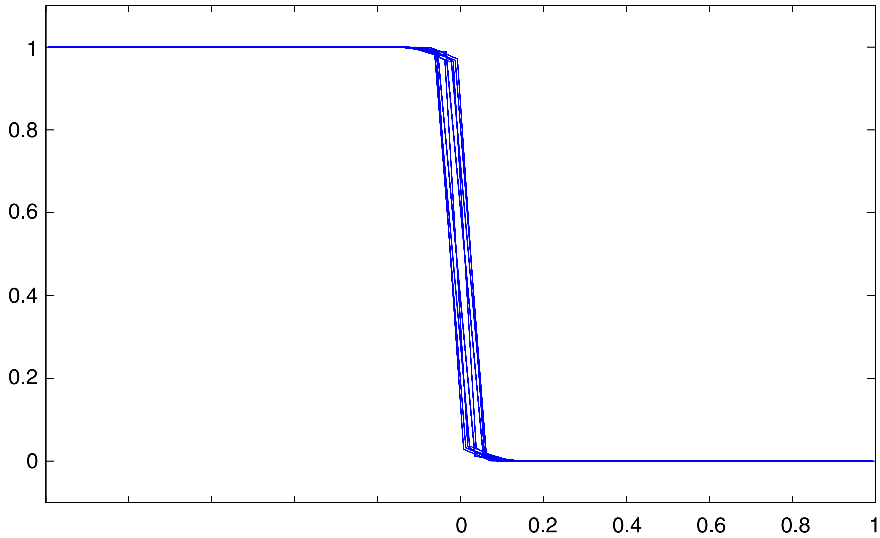

Fig. 4. Modified FV.

hand, the DDFV scheme gives an accurate solution but does not respect the maximum principle (Fig. 3). Finally, the solution given by the modified FV scheme presents the same accuracy as the DDFV scheme but respects the maximum principle (Fig. 4).

4. Final remarks and conclusion

The diffusion scheme described in this Note is a modified Finite Volumes scheme. By construction it respects the maximum principle. It requires the computation of a Voronoï mesh based on the centers of the primary cells. However, this cost is in $n\log(n)$ and is low compared with the one of nonlinear schemes. Moreover, it presents a good accuracy.

A question that naturally arises is to know whether this approach can be extended to generic anisotropic diffusion operators. The answer is probably yes, again at the cost of the computation of a Voronoï mesh, but this time on a Riemann space, whose metrics depends on the diffusion operators [5].

Other approaches using Voronoï mesh are possible and should also give good results. Of course, the idea of using a Voronoï mesh is not new, but this modified Finite Volumes scheme is a simple and efficient answer to the difficult problem of respecting the maximum principle on distorted meshes, that could be very useful particularly for industrial production codes.

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