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Perfectly matched layers for the heat and advection–diffusion equations

Couches parfaitement adaptées pour les équations de la chaleur et d'advection–diffusion

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A R T I C L E   I N F O

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A B S T R A C T

We design a perfectly matched layer for the advection–diffusion equation. We show that the reflection coefficient is exponentially small with respect to the damping parameter and the width of the PML and independently of the advection and of the viscosity parameters. Numerical tests assess the efficiency of the approach.

R É S U M É

Nous avons construit des Couches Parfaitement Adaptées (CPA) aux équations d'advection diffusion. Nous montrons que le coefficient de réflexion est exponentiellement petit par rapport au paramètre d'amortissement et de la largeur des CPA et ce, indépendamment des coefficients d'advection ou de viscosité. Les tests numériques présentés prouvent l'efficacité de la méthode.

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Version française abrégée

On s'intéresse ici au problème de troncature de domaine pour calculer la solution numérique de problème défini sur un domaine non borné de telle sorte que la solution sur le domaine réduit soit une bonne approximation de la solution sur le domaine initial.

Dans leur papier fondateur, Engquist et Majda [3] ont introduit, pour l'équation des ondes, une technique générale de construction de conditions aux limites artificielles (CLA). En ce qui concerne l'équation de la chaleur, cette méthode a pu être construite au niveau continu dans [6,4] et [5] et au niveau discret dans [2]. Dans tous ces travaux, la difficulté réside dans l'approximation de la racine carrée d'un opérateur aux dérivées partielles par un opérateur aux dérivées partielles.

Pour des équations hyperboliques, J.P. Bérenger a introduit dans [1] une technique alternative qui consiste à entourer le domaine de calcul par un milieu artificiel dissipatif et surtout non refléxif à l'interface entre le milieu physique et le milieu artificiel : les Couches Parfaitement Adaptées (CPA) (voir [7] et les références contenues). La nécessité d'utiliser les CPA vient des modes propagatifs de la solution que les CPA transforment en modes évanescents.

Nous allons quant à nous considérer une équation de type parabolique pour laquelle il n'y a pas de mode propagatif. Néamoins, l'application des CPA aux équations de convection diffusion (voir Éq. (1)), permet de transformer un mode évanescent lent en un mode évanescent rapide. La racine carrée de l'opérateur n'a pas besoin d'être approché par un opérateur aux dérivées partielles.

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L'opérateur $\mathcal{L}$ (voir (1)) est originelement défini sur l'ensemble du plan $\mathbb{R}^2$, mais on souhaite tronquer le domaine $x > 0$ par une CPA. L'étude de l'opérateur $\mathcal{L}$ par l'utilisation de la transformée de Fourier permet de déterminer le changement de variable nécessaire à la définition du modèle de CPA associé par le remplacement de la dérivée en x par une dérivée « CPA » en x définie en (3). Le modèle CPA est ainsi donné par

$$\mathcal{L}_{pml} := \partial_t + a\partial_x^{pml} + b\partial_y - \nu\partial_{xx}^{pml} - \nu\partial_{yy}.$$

L'interface ($x = 0$) définit maintenant deux milieux : celui de convection–diffusion ($x < 0$) avec la solution u_{cd} et la CPA avec la solution u_{pml}. On impose à cette interface la condition présentée en (4). On peut montrer que le coefficient de réflexion pour une CPA de largeur $\delta > 0$ est exponentiellement petit par rapport au coefficient d'amortissement σ et à la largeur δ et ceci, indépendamment des coefficients d'advection (a, b) ou de viscosité ν (formule (6)). Pour cela, on reproduit la démarche de calcul du coefficient de réflexion dans le cadre de l'équation des ondes. Le même type de changement de variable peut s'appliquer sans difficultés à la direction y. Pour les coins on décide de simplement superposer les modèles CPA-x et CPA-y en ne tenant pas compte des coefficients de convection a et b dans les changements de variable CPA en x et en y.

Nous présentons différents résultats numériques pour l'équation de la chaleur puis de convection–diffusion pour une condition initiale particulière (voir Éq. (7)). On voit Fig. 1-gauche et Fig. 2-gauche que, en utilisant des CPA, l'erreur est, dans les deux cas, concentrée au centre du domaine de calcul. L'erreur provient donc seulement du schéma de discrétisation et les Fig. 1-droit et Fig. 2-droit, confirment la pertinence des CPA. Les schémas numériques présentés sont stables en temps longs.

1. Introduction

We are concerned here with the problem of truncating domains to compute numerical solutions of problems in unbounded domains so that the solution of the problem in the reduced domain is a good approximation to the solution of the original problem. In their seminal work on the wave equation, Engquist and Majda [3] introduced a quite general technique to address this problem by designing absorbing boundary conditions (ABC). As far as the heat equation is concerned, in [6,4] and [5], ABCs are designed at the continuous level and in [2] at the discrete level. In all these works, the difficulty lies in the approximation of the square root of a partial differential operator by a partial differential operator.

For hyperbolic equations a different way to handle artificial boundaries was introduced by Berenger [1]. In this method, the computational domain is surrounded by a dissipative and non-reflexive artificial media: Perfectly Matched Layer (PML) (see, for example, [7] and the references therein). For the hyperbolic equations the need for a PML comes from the propagative modes that exist in the solution. The purpose of a PML is then to turn a propagative mode into a vanishing one. In this Note, we consider a parabolic equation for which there are only vanishing modes. We show that it is nevertheless possible to design and test a PML for the convection–diffusion equation:

$$\mathcal{L}(u) := \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} - \nu\,\Delta u. \tag{1}$$

The purpose of the PML is now to turn a slowly vanishing mode into a rapidly vanishing one and there is no need to approximate the square root of an operator by a partial differential operator.

The Note is organized as follows. In the first part, we analyze the operator (1) in the Fourier space and introduce the perfectly matched layers to the convection–diffusion equation. In the second part, we present numerical results.

2. Perfectly matched layers

In order to study the operator $\mathcal{L}$, we look for solutions of the equation $\mathcal{L}(u) = 0$. Let $u(t, x, y)$ be a function and $\hat{\hat{u}}(\omega, x, k)$ be its Fourier transform w.r.t. the variables t and y and let $\mathcal{F}^{-1}$ denote the inverse Fourier transform. We have:

$$\left(i\,\omega + a\partial_x + bik - \nu\partial_{xx} + \nu k^2\right)\left(\hat{\hat{u}}(\omega, x, k)\right) = 0.$$

For fixed ω and k, this is an ordinary differential equation in the variable x whose solutions are of the form $\hat{\hat{u}}(\omega, x, k) = \alpha(\omega, k)\exp(\lambda^+(\omega, k)x) + \beta(\omega, k)\exp(\lambda^-(\omega, k)x)$ where α and β are fixed by the boundary conditions and

$$\lambda^{\pm}(\omega, k) := \frac{\frac{a}{\nu} \pm \sqrt{\frac{a^2}{\nu^2} + \frac{4}{\nu}(i\omega + ikb + \nu k^2)}}{2}. \tag{2}$$

The operator $\mathcal{L}$ is originally defined in the whole plane $\mathbb{R}^2$ and we want to truncate the domain $x > 0$ by a PML. The PML model for this operator $\mathcal{L}$ is defined by replacing the x-derivative by a "pml" x-derivative whose definition is: let σ be a positive damping parameter, we define

$$\partial_x^{pml}(u) := \mathcal{F}^{-1}\left(\frac{i\omega + ikb}{i\omega + ikb + \frac{\nu}{4}\sigma}\partial_x\hat{\hat{u}}(\omega, x, k)\right) \tag{3}$$

and

$$\mathcal{L}_{pml} := \partial_t + a\partial_x^{pml} + b\partial_y - \nu\partial_{xx}^{pml} - \nu\partial_{yy}$$

is the PML equation with the following interface conditions at $x=0$ between the solution u_{cd} in the convection–diffusion media and u_{pml} the solution in the PML media:

$$u_{cd} = u_{pml} \quad \text{and} \quad \partial_x(u_{cd}) = \partial_x^{pml}(u_{pml}). \tag{4}$$

The function $u_{inc} := \mathcal{F}^{-1}(\exp(\lambda^-(\omega,k)x))$ satisfies $\mathcal{L}(u_{inc}) = 0$ and u_{inc} tends to zero as x tends to infinity. We approach this special solution by the following problem where the domain is truncated on the right by the PML:

$$\text{Find } (u_{cd}, u_{pml}) \text{ such that:} \quad \begin{aligned} &\mathcal{L}(u_{cd}) = 0,\ t>0,\ x<0,\ y\in\mathbb{R},\\ &\mathcal{L}_{pml}(u_{pml}) = 0,\ t>0,\ \delta > x > 0,\ y\in\mathbb{R},\\ &u_{pml}(t,\delta,y) = 0,\ t>0,\ y\in\mathbb{R},\\ &u_{cd} - u_{inc} \text{ tends to 0 as } x \text{ to } -\infty,\\ &\text{and the interface conditions (4) are satisfied.}\end{aligned}$$

If we take the Fourier transform of the above system, easy computations show that we have $u_{cd} := \exp(\lambda^- x) + R\exp(\lambda^+ x)$ and $u_{pml} := \alpha\exp(\lambda_{pml}^- x) + \beta\exp(\lambda_{pml}^+ x)$ with

$$\lambda_{pml}^{\pm} := \frac{i\omega + ikb + \frac{\nu}{4}\sigma}{i\omega + ikb}\lambda^{\pm} \tag{5}$$

and coefficients R, α and β that will be determined in the sequel. If R were equal to zero, the solution in the left-plane would be equal to u_{inc} and the PML would be an exact way to truncate the computational domain. Thus, the smallness of R is a measure of the quality of the PML procedure and defines a reflection coefficient. By using (5), the Fourier transform of the interface conditions (4) and the Dirichlet boundary condition at the end of the PML ($x=\delta$), we can prove that we have a uniform bound on the reflection coefficient R independent of the physical parameters (a, b, ν) and of the Fourier variables (ω, k):

$$|R| \leqslant \exp\left(-\sqrt{2\sigma}\,\delta\right). \tag{6}$$

It is easy to check that the same reflection coefficient is obtained if the PML is used to truncate the computational domain on the left. The same technique can be applied in the y direction without any difficulties. For the corner regions, we simply place side by side PML-x and PML-y regions, where convection coefficients a and b are chosen null in the PML' changes of variable (3).

3. Numerical results

We now present the numerical application of the method defined previously. We are interesting in solving this convection–diffusion problem:

$$\begin{cases} \dfrac{\partial u}{\partial t} + a\dfrac{\partial u}{\partial x} + b\dfrac{\partial u}{\partial y} - \nu\,\Delta u = 0 \quad \text{with } (x,y)\in\mathbb{R}^2,\ 0\leqslant t\leqslant T,\\ u(x,y,0) = \dfrac{1}{\gamma}e^{-\frac{x^2+y^2}{\nu\gamma}}, \end{cases} \tag{7}$$

where ν is the viscosity, (a,b) is the velocity field and T is the final time. Problem (7) admits the analytical solution

$$u^{Ex}(x,y,t) = \frac{1}{4t+\gamma}e^{-\frac{(x+at)^2+(y+bt)^2}{\nu(4t+\gamma)}}.$$

We approximate our problem with a P1-triangular Finite Element Method (FEM) on a truncated domain $\Omega_L = [-L\times stdv, +L\times stdv]^2$ where $stdv = \sqrt{2\nu T}$ is the standard deviation and L is a positive parameter. The associated approximated solution of the FEM is denoted as u_h, where h stands for the space step. We discretize the time derivative with an implicit Euler scheme. In the PML zone, in order to discretize (3) without using a Fourier transform, we proceed classically by adding two extra fields, see [7] and references therein. To study the numerical results, we define with a parameter $0<\eta<L$ an arbitrary domain $\Omega_\eta = [-\eta\times stdv, +\eta\times stdv]^2$ nested in Ω_L where errors will be computed. We also introduce u_h^∞, a reference numerical solution of (7) on a computational domain Ω_L sufficiently large ($L=5$) to avoid any boundary conditions issue. Finally, let $\epsilon_h^\infty(x,y,t) = |u_h(x,y,t) - u_h^\infty(x,y,t)|$ and $\epsilon^{Ex}(x,y,t) = |u_h(x,y,t) - u^{Ex}(x,y,t)|$ be two absolute errors

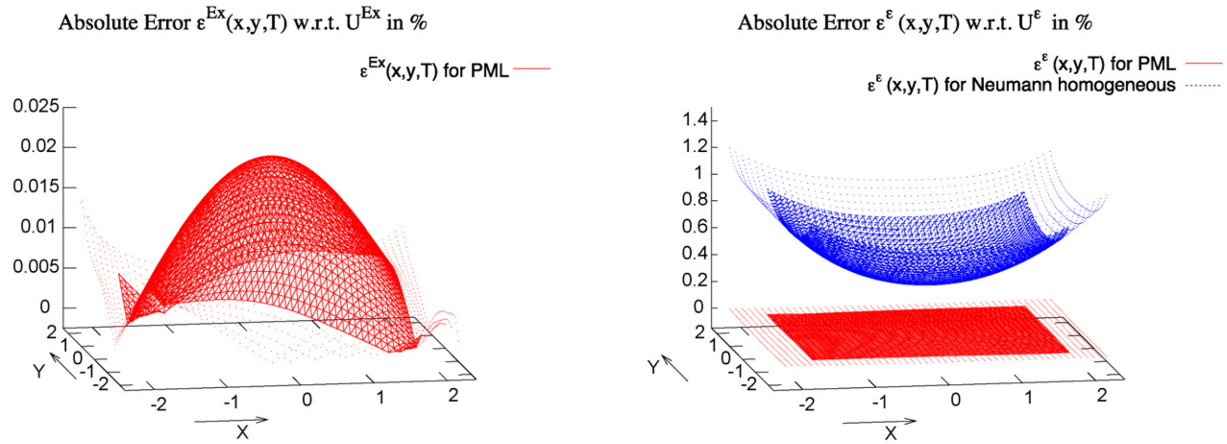

Fig. 1. Left: the error $\epsilon^{Ex}(x,y,T)$ w.r.t. U^{Ex} (in %) for the PML. Right: the error $\epsilon_h^{\infty}(x,y,T)$ w.r.t. U^{∞} (in %) for Neumann homogeneous boundary condition (N) and the PML.

Fig. 1. Gauche : erreur $\epsilon^{Ex}(x,y,T)$ calculé à partir de U^{Ex} (en %) pour des CPA. Droite : erreur $\epsilon_h^{\infty}(x,y,T)$ calculée à partir de U^{∞} (en %) pour une condition aux bords de type Neumann homogène (N) et des CPA.

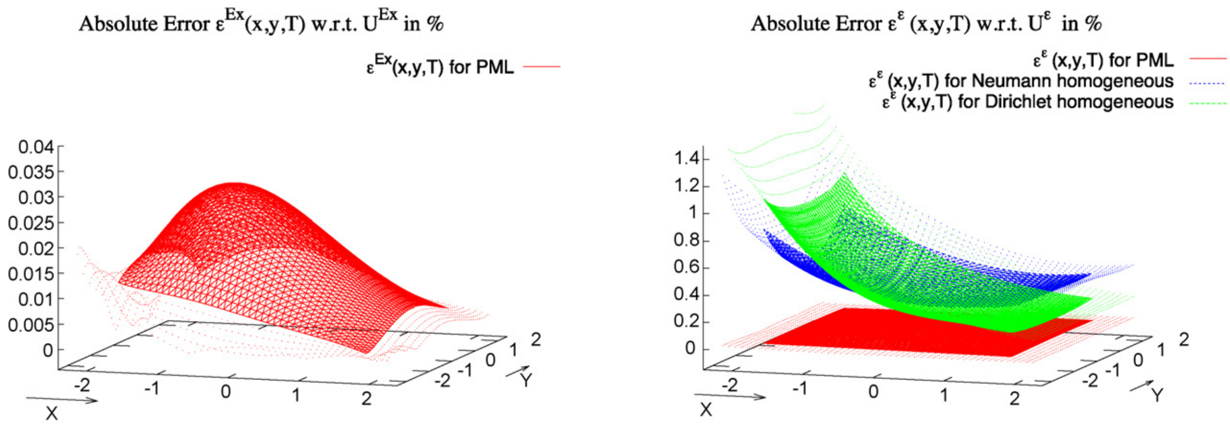

Fig. 2. Left: the error $\epsilon^{Ex}(x,y,T)$ w.r.t. U^{Ex} (in %) for the PML boundary condition with positive advection coefficient in the x-direction. Right: the error $\epsilon_h^{\infty}(x,y,T)$ w.r.t. U^{∞} (in %) for Neumann homogeneous, Dirichlet homogeneous and PML boundary condition.

Fig. 2. Gauche : erreur $\epsilon^{Ex}(x,y,T)$ calculée selon U^{Ex} (en %) pour des CPA avec un coefficient de convection positif dans la direction x. Droit : erreur $\epsilon_h^{\infty}(x,y,T)$ calculée selon U^{∞} (en %) pour des conditions aux bords de Neumann homogène, Dirichlet homogène et CPA.

expressed in percentage. We introduced the error ϵ_h^{∞} to only highlight the truncation error and on the other hand, the ϵ^{Ex} error is composed of the discretization error of the FEM and the truncation error of the domain.

We use for σ the following profile $\sigma(z) = 10(\frac{z}{\delta})^2$ where z is the distance to the interface in the normal direction to the interface ($z \in [0,\delta]$). We took the following parameters for the discretization scheme $L = 1$ and the number of discretization nodes in the PML is 11. The viscosity ν is 0.5, the final time $T = 5$, the time step $\Delta t = 0.025$ and $\gamma = 0.2$. Errors in the L^2 and L^{∞} norm are always computed on Ω_η with $\eta = 0.8$. The space step h is the ratio $2stdv/51$ and remains constant between the physical and the PML domain.

To highlight the accuracy of the PML method we will compare our numerical application to Dirichlet and Neumann homogeneous. In order to have a fair comparison, when Neumann or Dirichlet boundary conditions are used the computational domain includes the PML zone. In Figs. 1 and 2, the meshed surface of the curves in the middle represents the domain Ω_η where the error is computed, the dotted part stands for the rest of the physical domain ($\Omega_L \setminus \Omega_\eta$).

First numerical results on a pure heat equation are presented in Fig. 1 and Table 1. Diffusion with non-null convection coefficient in the x-direction ($a = 0.5$ and $b = 0$) is shown in Fig. 2 and Table 1. In this case, the PML change of variable introduces a convection dominated problem in the associated partial differential equations system: we use SUPG to improve the resolution. For larger velocity coefficients, we are going to deal with a convection dominated equation and a simple Neumann boundary condition will surely have a better efficiency.

We see in Fig. 1-left and Fig. 2-left, that with PML, the most important part of the error is in the center of the computational domain far from the artificial boundary: the remaining error only comes from the discretization scheme. As shown in Fig. 1-right and Fig. 2-right the PML outperforms the other classical boundary conditions. The table confirms that the error

Table 1
Left: numerical results obtained for the heat equation ($a = 0$, $b = 0$). Right: numerical results obtained under a convection–diffusion model ($a = 0.5$, $b = 0$).

Tableau 1
Gauche : résultats numériques obtenus pour l'équation de la chaleur ($a = 0$, $b = 0$). Droit : résultats numériques obtenus pour l'équation de convection–diffusion ($a = 0{,}5$, $b = 0$).

	$\|\epsilon_h^\infty\|_2$	$\|\epsilon_h^\infty\|_\infty$	$\|\epsilon^{Ex}\|_2$	$\|\epsilon^{Ex}\|_\infty$		$\|\epsilon_h^\infty\|_2$	$\|\epsilon_h^\infty\|_\infty$	$\|\epsilon^{Ex}\|_2$	$\|\epsilon^{Ex}\|_\infty$
u_h^∞	0	0	0.0154 %	0.0263 %	u_h^∞	0	0	0.0199 %	0.0340 %
u_h^N	0.5915 %	1.0194 %	0.6038 %	1.0188 %	u_h^N	0.3467 %	0.8491 %	0.3636 %	0.8564 %
u_h^D	0.5363 %	0.8545 %	0.5363 %	0.8545 %	u_h^D	0.3809 %	1.0785 %	0.3809 %	1.0785 %
u_h^{PML}	0.0030 %	0.0075 %	0.0131 %	0.0221 %	u_h^{PML}	0.0035 %	0.0129 %	0.0173 %	0.0288 %

for Dirichlet and Neumann boundary conditions w.r.t. the exact solution comes mainly from the truncation error and not from the discretization of the equation.

The numerical scheme is stable for long time applications in all cases.

4. Conclusion and perspectives

In this article, we designed a perfectly matched layer for the heat and/or advection–diffusion equation. After its definition, we prove that the reflection coefficient is exponentially small with respect to the damping parameter and the width of the PML. It is worth noticing that the reflection coefficient is independent of the equation parameters such as velocity or viscosity. We have implemented this method with a P1-finite element method and its efficiency is highlighted by numerical results.

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