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Numerical Analysis

An exact bounded PML for the Helmholtz equation

Alfredo Bermúdez^a, L. Hervella-Nieto^b, A. Prieto^a, R. Rodríguez^c

^a *Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, 15706 Santiago de Compostela, Spain*

^b *Departamento de Matemáticas, Universidade da Coruña, 15707 A Coruña, Spain*

^c *GP²MA, Departamento de Ingeniería Matemática, Universidad de Concepción, Chile*

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Abstract

We study the Helmholtz equation with a Sommerfeld radiation condition in an unbounded domain. We prove the existence of an exact bounded perfectly matched layer (PML) for this problem, in the sense that we recover the exact solution in the physical domain by choosing a singular PML function in a bounded domain. We approximate the solution for the PML problem using a standard finite element method and assess its performance through numerical tests. **To cite this article:** *A. Bermúdez et al., C. R. Acad. Sci. Paris, Ser. I 339 (2004).*

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Résumé

Une PML exacte et bornée pour l'équation de Helmholtz. Nous étudions l'équation de Helmholtz avec une condition de radiation de Sommerfeld dans un domaine non borné. Pour ce problème nous démontrons l'existence d'une couche bornée parfaitement adaptée et exacte, au sens où nous retrouvons la solution exacte dans le domaine physique. Nous approchons la solution du problème PML avec une méthode standard d'éléments finis et nous montrons ses bonnes propriétés sur des exemples test. **Pour citer cet article :** *A. Bermúdez et al., C. R. Acad. Sci. Paris, Ser. I 339 (2004).*

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Version française abrégée

Dans cette Note, nous étudions le problème de Helmholtz avec une condition de radiation de Sommerfeld dans un domaine non borné (voir (1)). Dans cette équation nous utilisons la notation $k := \omega/c$ pour le nombre d'onde, avec ω la fréquence et c la vitesse de propagation. La fonction u_D est supposée appartenir à $H^{1/2}(\Gamma)$ et le domaine

E-mail addresses: mabermud@usc.es (A. Bermúdez), luisher@udc.es (L. Hervella-Nieto), maprieto@usc.es (A. Prieto), rodolfo@ing-mat.udc.cl (R. Rodríguez).

$\Omega_E := \mathbb{R}^2 \setminus \overline{\Omega_I}$, où Ω_I est un domaine borné dans \mathbb{R}^2 avec une frontière régulière, Γ . Nous supposons que l'origine est contenu dans Ω_I et nous choisissons $R > 0$ tel que $\Omega_I \subset B_R$, B_R étant le cercle de rayon R centré à l'origine, qui a pour frontière la circonférence S_R (voir Fig. 1).

Le problème (1) est un problème classique de *scattering*, pour lequel on connaît l'existence et l'unicité de solution pour toute valeur de la fréquence ω .

Nous définissons l'opérateur *Dirichlet-to-Neumann* (DtN), \tilde{G} , qui à une fonction $g \in H^{1/2}(S_R)$ fait correspondre $\tilde{G}(g) := (\partial \tilde{u} / \partial r)|_{S_R} \in H^{-1/2}(S_R)$, où \tilde{u} est la solution du problème (2). Alors (1) peut s'écrire comme (3) dans $\Omega_E \cap B_R$. Le lemme qui suit caractérise $\tilde{G}(g)$:

Lemme 0.1. Soit $g = \sum_{n=-\infty}^{\infty} g_n e^{in\theta}$ une fonction quelconque de $H^{1/2}(S_R)$. Alors on a : $\tilde{G}(g) = \sum_{n=-\infty}^{\infty} k g_n \frac{[H_n^{(1)}]'(kR)}{H_n^{(1)}(kR)} e^{in\theta}$, où $H_n^{(1)}$ est la n -ème fonction de première espèce de Hankel.

Le problème (1) n'est pas adéquat pour une résolution par éléments ou différences finies, car il est défini dans un domaine non borné. Nous utiliserons la méthode PML (couche absorbante parfaitement adaptée), introduite par Bérenger dans [1], pour le réduire à un domaine borné. Pour ceci nous considérons une boule B_{R^*} avec rayon $R^* > R$ (voir Fig. 2).

En coordonnées polaires, le problème PML s'écrit comme (4) (voir [4]). Dans ces équations $\gamma(r) := [\omega + i\sigma(r)]/\omega$ et $\hat{\gamma}(r) := 1 + [i/(r\omega)] \int_R^r \sigma(s) ds$, avec $\sigma(r)$ fonction croissante dans $[0, R^*]$, qui s'annule dans $[0, R]$. On remarque que, formellement, le problème (4) peut être obtenu avec le changement complexe de variables (5) (voir [4]).

La méthode PML dépend du choix de σ dans $[R, R^*]$. Face au choix classique d'une fonction σ linéaire ou quadratique (voir [2] ou [4]), nous proposons une fonction σ telle que $\int_R^{R^*} \sigma(s) ds = +\infty$; par exemple, $\sigma(r) := 0$, $r \in [0, R]$, et $\sigma(r) := 1/(R^* - r)$, $r \in [R, R^*]$.

Nous considérons l'opérateur associé à cette PML qui transforme une fonction $g \in H^{1/2}(S_R)$ dans $\hat{G}(g) := \gamma^{-1}(\partial \hat{v} / \partial r)|_{S_R} \in H^{-1/2}(S_R)$, \hat{v} étant la solution de (7)–(9). Le résultat fondamental est que les opérateurs \tilde{G} et \hat{G} sont égaux et, par conséquent, si l'on restreint la solution de l'Éq. (4) à $\Omega_E \cap B_R$, on récupère exactement la restriction de la solution du problème de Helmholtz à ce domaine. Plus précisément, on a les résultats suivants :

Théorème 0.2. Soit σ une fonction croissante dans $[0, R^*]$, nulle dans $[0, R]$, régulière dans (R, R^*) et telle que $\int_R^{R^*} \sigma(s) ds = +\infty$. Alors le problème (7)–(9) a une solution unique donnée par (10).

Corollaire 0.3. L'opérateur \hat{G} est bien défini et $\hat{G}(g) = \tilde{G}(g) \forall g \in H^{1/2}(S_R)$.

Corollaire 0.4. On a $u = v$ dans $\Omega_E \cap B_R$, où u et v sont les solutions des problèmes (1) et (4), respectivement.

Bien que nous ayons introduit le problème de Helmholtz en coordonnées polaires, dans la pratique il est plus intéressant d'utiliser des couches PML qui forment un rectangle (voir Fig. 3). Nous résolvons numériquement (12) par une méthode d'éléments finis utilisant des éléments rectangulaires Q_1 de Lagrange, avec intégration exacte des matrices élémentaires.

Pour tester la méthode nous choisissons f mesure de Dirac, pour laquelle on connaît la solution exacte. Dans la Fig. 4 on trace la courbe de l'erreur relative face à la taille de la discretisation. On peut voir la convergence quadratique de la solution du problème PML discretisé vers la solution exacte du problème dans le domaine non borné, en dehors d'un petit voisinage du point où la mesure de Dirac est concentrée.

Finalement, dans le Tableau 1, on montre une comparaison entre les méthodes PML avec fonction σ quadratique (PML classique) et fonction σ non bornée. On peut voir que, même pour un choix optimal des paramètres dans le cas quadratique, notre méthode PML semble plus performante.

1. The Helmholtz problem in an unbounded domain

We consider the following Helmholtz problem which models the propagation of a wave of frequency $\omega > 0$ and velocity of propagation $c > 0$ in an unbounded homogeneous medium:

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega_E, \\ u = u_D & \text{on } \Gamma, \\ \lim_{r \rightarrow \infty} \sqrt{r} \left(\frac{\partial u}{\partial r} - iku \right) = 0, \end{cases} \tag{1}$$

where $k := \omega/c$ is the wave number, $\Omega_E := \mathbb{R}^2 \setminus \overline{\Omega_I}$, with Ω_I being a bounded domain in \mathbb{R}^2 with regular boundary Γ , and $u_D \in H^{1/2}(\Gamma)$ a given function. Throughout the paper, Sommerfeld-like conditions as the third equation in (1) are assumed to hold uniformly in all directions.

Problem (1) is a classical scattering problem, whose existence and uniqueness of solution is well known (see for instance [5]).

We assume that the origin is in Ω_I and we choose $R > 0$ such that $\Omega_I \subset B_R$, where B_R is the ball of radius R centered at the origin and whose boundary is the circumference S_R (see Fig. 1).

We define the exterior Dirichlet-to-Neumann (DtN) operator, \tilde{G} , that maps any function $g \in H^{1/2}(S_R)$ to $\tilde{G}(g) := (\partial \tilde{u} / \partial r)|_{S_R} \in H^{-1/2}(S_R)$, with \tilde{u} being the solution of:

$$\begin{cases} \Delta \tilde{u} + k^2 \tilde{u} = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B_R}, \\ \tilde{u} = g & \text{on } S_R, \\ \lim_{r \rightarrow \infty} \sqrt{r} \left(\frac{\partial \tilde{u}}{\partial r} - ik\tilde{u} \right) = 0. \end{cases} \tag{2}$$

Then the solution of problem (1) satisfies:

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega_E \cap B_R, \\ u = u_D & \text{on } \Gamma, \\ \frac{\partial u}{\partial r} = \tilde{G}(u|_{S_R}) & \text{on } S_R. \end{cases} \tag{3}$$

The DtN mapping has the explicit form given in the following lemma (see for instance [6]).

Lemma 1.1. For all $g = \sum_{n=-\infty}^{\infty} g_n e^{in\theta} \in H^{1/2}(S_R)$, there holds: $\tilde{G}(g) = \sum_{n=-\infty}^{\infty} k g_n \frac{[H_n^{(1)}]'(kR)}{H_n^{(1)}(kR)} e^{in\theta}$, where $H_n^{(1)}$ is the n -th Hankel function of first class.

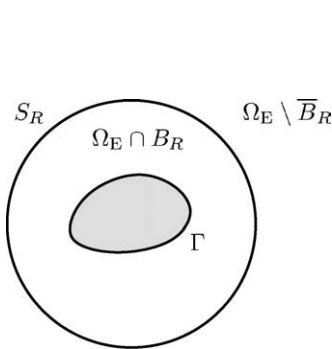


Fig. 1. Scatterer and artificial circular boundary.

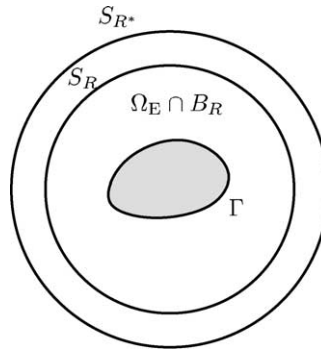


Fig. 2. Domains for the PML problem.

2. PML problem in a bounded domain

The numerical solution of problem (1) by finite elements or finite differences is not straightforward because the domain is unbounded. Thus, as a first step, we reduce it to a bounded domain by using a PML (*Perfectly Matched Layer*) method introduced by Bérenger in [1] in the context of electromagnetic waves. To this aim, we consider a ball B_{R^*} centered at the origin and with radius $R^* > R$ (see Fig. 2). Then, the PML problem associated with (1) can be written in polar coordinates as follows (see [4]):

$$\begin{cases} \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left[\frac{\hat{\gamma}(r)r}{\gamma(r)} \frac{\partial v}{\partial r} \right] + \frac{\gamma(r)}{\hat{\gamma}(r)r} \frac{\partial^2 v}{\partial \theta^2} \right\} + k^2 \gamma(r) \hat{\gamma}(r) v = 0 & \text{in } \Omega_E \cap B_{R^*}, \\ v = u_D & \text{on } \Gamma, \\ \lim_{r \rightarrow R^*} \sqrt{r \hat{\gamma}(r)} \left[\frac{1}{\gamma(r)} \frac{\partial v}{\partial r} - ikv \right] = 0, \end{cases} \tag{4}$$

where $\gamma(r) := [\omega + i\sigma(r)]/\omega$ and $\hat{\gamma}(r) := 1 + [i/(r\omega)] \int_R^r \sigma(s) ds$, with σ being an increasing function defined in $[0, R^*)$ and vanishing in $[0, R)$.

The PML equations (4) can be formally obtained by performing in the Helmholtz equations the complex change of variables given by (see [4]):

$$\hat{r} = \hat{r}(r) := r + \frac{i}{\omega} \int_0^r \sigma(s) ds \quad \forall r \in [0, R^*). \tag{5}$$

Notice that $\hat{r} = r$ for $r \in [0, R)$, because σ vanishes in this interval.

The PML method depends on the choice of σ in $[R, R^*)$. The classical choice is a linear or quadratic function taking a finite value σ^* at R^* (see [2,4]). Also, the boundary condition on S_{R^*} in the third equation of (4) is typically replaced by a homogeneous Dirichlet or Neumann condition. According to the literature, the value σ^* should be large enough as to minimize the reflections due to the fictitious boundary S_{R^*} , but not too large in order to avoid numerical errors arising from the discretization.

Instead, we propose to choose a function σ such that $\int_R^{R^*} \sigma(s) ds = +\infty$ as, for instance, $\sigma(r) := 0, r \in [0, R)$, and $\sigma(r) := 1/(R^* - r), r \in [R, R^*)$. We will show that, in this case, the solution of the PML problem (4) coincides in $\Omega_E \cap B_R$ with the solution of the original problem (1).

If we restrict the first equation in problem (4) to $\Omega_E \cap B_R$, since σ vanishes in $[0, R)$, we recover the Helmholtz equation. More precisely, any solution of problem (4) satisfies:

$$\begin{cases} \Delta v + k^2 v = 0 & \text{in } \Omega_E \cap B_R, \\ v = u_D & \text{on } \Gamma, \\ \frac{\partial v}{\partial r} = \widehat{G}(v|_{S_R}) & \text{on } S_R, \end{cases} \tag{6}$$

where \widehat{G} is the operator mapping any function $g \in H^{1/2}(S_R)$ to $\widehat{G}(g) := [(1/\gamma)(\partial \hat{v}/\partial r)]|_{S_R} \in H^{-1/2}(S_R)$, with \hat{v} being the solution of:

$$\begin{cases} \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left[\frac{\hat{\gamma}(r)r}{\gamma(r)} \frac{\partial \hat{v}}{\partial r} \right] + \frac{\gamma(r)}{\hat{\gamma}(r)r} \frac{\partial^2 \hat{v}}{\partial \theta^2} \right\} + k^2 \gamma(r) \hat{\gamma}(r) \hat{v} = 0 & \text{in } B_{R^*} \setminus \overline{B}_R, \\ \hat{v} = g & \text{on } S_R, \\ \lim_{r \rightarrow R^*} \sqrt{r \hat{\gamma}(r)} \left[\frac{1}{\gamma(r)} \frac{\partial \hat{v}}{\partial r} - ik\hat{v} \right] = 0. \end{cases} \tag{7}$$

In the next theorem we prove that this operator \widehat{G} is well defined.

Let us denote by \mathcal{V} the space of measurable functions u defined in $B_{R^*} \setminus \overline{B}_R$ and such that

$$\int_0^{2\pi} \int_R^{R^*} \left[\left| \frac{\hat{\gamma}(r)r}{\gamma(r)} \frac{\partial u}{\partial r}(r, \theta) \right|^2 + \left| \frac{\gamma(r)}{\hat{\gamma}(r)r} \frac{\partial u}{\partial \theta}(r, \theta) \right|^2 + |r\gamma(r)\hat{\gamma}(r)| |u(r, \theta)|^2 \right] dr d\theta < \infty.$$

Theorem 2.1. *Let σ be an increasing function defined in $[0, R^*)$, vanishing in $[0, R)$, smooth in (R, R^*) , and such that $\int_R^{R^*} \sigma(s) ds = +\infty$. Then problem (7)–(9) has a unique solution in \mathcal{V} given by:*

$$\hat{v}(r, \theta) = \sum_{n=-\infty}^{\infty} \frac{g_n}{H_n^{(1)}(k\hat{r})} H_n^{(1)}(k\hat{r}(r)) e^{in\theta} \quad \forall r \in (R, R^*). \tag{10}$$

Proof. We give a sketch of the proof, which can be found in [3]. It consists of the following steps:

- (i) We prove the existence of an outgoing fundamental solution Φ of problem (7).
- (ii) We prove that $\hat{v} \in \mathcal{V}$ satisfies (7) and (9) if and only if the following Green’s formula holds:

$$\hat{v}(x) = \int_{S_R} \frac{1}{\gamma(R)} \left[\hat{v}(y) \frac{\partial \Phi(x, y)}{\partial r(y)} - \frac{\partial \hat{v}}{\partial r}(y) \Phi(x, y) \right] ds(y) \quad \forall x \in B_{R^*} \setminus \bar{B}_R. \tag{11}$$

(iii) Following the techniques in [5], we prove that \hat{v} is a solution of (11) verifying $\hat{v} = g$ on S_R if and only if \hat{v} is given by (10). Furthermore, one can prove that the series is uniformly convergent on compact subsets of $B_{R^*} \setminus \bar{B}_R$ and that \hat{v} belongs to \mathcal{V} .

Corollary 2.2. *The operator \widehat{G} is well defined and $\widehat{G}(g) = \widetilde{G}(g) \forall g \in H^{1/2}(S_R)$.*

Corollary 2.3. *If u and v are the solutions of problems (1) and (4), respectively, then $u = v$ in $\Omega_E \cap B_R$.*

Remark 1. By using the Green’s formula and the behaviour of Φ as $|x| \rightarrow R^*$, we deduce that the above solution \hat{v} also satisfies $\hat{v} = 0$ on S_{R^*} . Thus, in practice, we can use this Dirichlet boundary condition rather than (9) when solving the PML problem.

3. Numerical results

Numerical experiments showing the efficiency of this approach can be found in [3]. Now, although the previous analysis has been made for the Helmholtz problem in polar coordinates, in practice it is more interesting to solve numerically the problem with a rectangular PML layer as that shown in Fig. 3.

We denote $\Omega_P := [-X_1, X_1] \times [-X_2, X_2]$ and $\Omega := [-X_1^*, X_1^*] \times [-X_2^*, X_2^*]$. Instead of a prescribed Dirichlet data, we consider a harmonic source with support contained in Ω_P . The equations of the corresponding PML problem are the following (see [4]):

$$\begin{cases} \frac{\partial}{\partial x_1} \left(\frac{\gamma_2}{\gamma_1} \frac{\partial u}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\frac{\gamma_1}{\gamma_2} \frac{\partial u}{\partial x_2} \right) + k^2 \gamma_1 \gamma_2 u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{12}$$

Here $\gamma_1 = \gamma_1(x_1) := [\omega + i\sigma_1(x_1)]/\omega$, with σ_1 being the even function vanishing for $|x_1| < X_1$ and such that $\sigma_1(x_1) := c/(X_1^* - |x_1|)$ for $X_1 \leq |x_1| < X_1^*$. We recall that c is the velocity of propagation of the wave. The definition of $\gamma_2 = \gamma_2(x_2)$ is analogous.

We solve the above problem with a finite element method based on Q_1 -Lagrange rectangular elements on uniform partitions of mesh-size h . We use exact integration to compute the element stiffness and mass matrices.

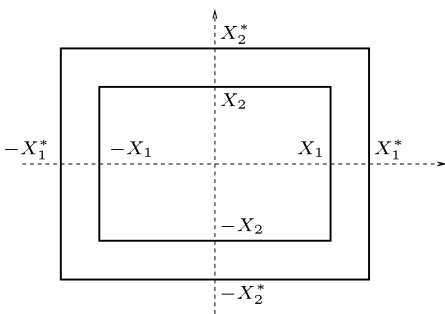


Fig. 3. PML layers in Cartesian coordinates.

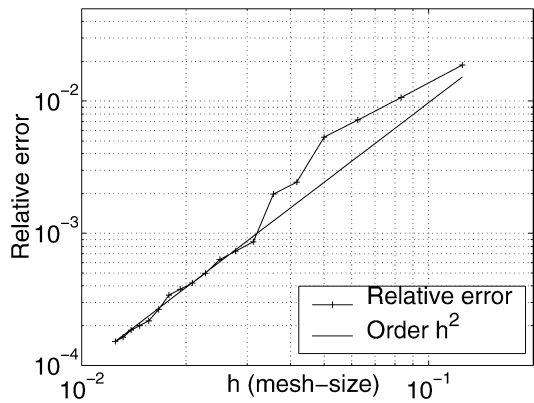


Fig. 4. Error curve for the exact PML method.

Table 1
Performance comparison: PML with singular σ versus PML with quadratic σ

Number of d.o.f.	σ type	Relative error (%)	CPU time (s)	Condition number
2401	singular	0.086	46.16	1.673e+04
2401	quadratic ($\sigma^* = 39.36$)	1.047	44.35	1.522e+04
5329	singular	0.042	106.99	5.872e+04
5329	quadratic ($\sigma^* = 44.37$)	0.506	102.45	4.249e+04

Let us remark that all the entries of these matrices are finite in spite of the fact that γ_1 and γ_2 go to infinity as the variable x goes to $\partial\Omega$. In fact, the finite element basis functions vanish on $\partial\Omega$ and, hence, it is simple to show that all the integrals are finite (see [3]).

To test the method we take as f the Dirac delta measure supported at the origin, $k = \omega/c = 750/340$, $X_1 = X_2 = 0.5$, and $X_1^* = X_2^* = 0.75$. In this case, the exact solution for the unbounded domain is explicitly known: $u^{\text{ex}}(x_1, x_2) := (i/4)H_0^{(1)}(k\sqrt{x_1^2 + x_2^2})$. Fig. 4 shows a plot of the relative error versus the mesh-size h . We measure the error in the L^2 -norm in Ω_P excluding a small neighborhood of the origin: $\|u_h - u^{\text{ex}}\|_{0, \tilde{\Omega}_P} / \|u^{\text{ex}}\|_{0, \tilde{\Omega}_P}$, with $\tilde{\Omega}_P := \{x \in \Omega_P: |x| > 0.05\}$ and where u_h is the discrete solution. It can be clearly seen that a quadratic order of convergence is achieved.

Finally, Table 1 shows a comparison between the performance of our PML method with singular σ_1 and σ_2 versus the classical PML method with σ_i being the quadratic function defined by $\sigma_i(x_i) := c\sigma^*(|x_i| - X_i)^2 / (X_i^* - X_i)^2$, for $X_i \leq |x_i| < X_i^*$, $i = 1, 2$. The value of σ^* is chosen as to keep the error as small as possible. The systems of equations have been solved by a standard direct method.

Table 1 shows that our PML method has essentially the same computational cost than the classical one, but it is much more efficient, even though an optimal value of σ^* has been used for the latter. We remark that the reported CPU time for the classical PML method is somehow fictitious, in that the time necessary to find the optimal value of σ^* has not been included. Moreover, such optimal value of σ^* can only be found when the exact solution of the problem is known. Table 1 also shows the condition numbers of the corresponding matrices. It can be seen that they are similar for both methods, in spite of the choice of a singular function on the boundary.

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