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ON THE LOCALLY-CONFORMAL PERFECTLY MATCHED LAYER IMPLEMENTATION FOR HELMHOLTZ EQUATION

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ABSTRACT

This paper deals with a new implementation of the perfectly matched layers (PML) for Helmholtz equation. Our approach is based on the “locally-conformal” technique introduced for Maxwell equations by Ozgun et al. [1]. This method greatly extends the flexibility of the classical Cartesian, cylindrical or spherical based layer definition, allowing to cope with any general convex domain. As a result, the “white space” between the scatterer and the PML region can often be reduced, yielding substantial time and memory savings for some applications. However, its practical implementation requires special attention. On unstructured grids, numerical experiments prove that slight deflections of the absorption axis can spoil the entire solution at certain frequencies. To alleviate that issue, an original calculation of the locally defined absorption axes is proposed, based on the fluxes obtained from a Laplace problem performed in the PML region. This approach guarantees a “smooth” behavior of the absorption properties in the layer which improves the PML efficiency. Numerical examples are presented showing the potentialities of the method.

1 INTRODUCTION

For many industrial applications, like exterior acoustics or guided wave applications, the numerical finite element (FE) domain must be truncated by a reflection-less artificial boundary. Originally introduced by Berenger [2] for electromagnetics, the perfectly matched layers (PML) is a very powerful technique which consists in appending to the FE domain a surrounding artificial layer in which the waves are absorbed. This layer has the specific property to only absorb along a certain direction. From a mechanical point of view, it can be interpreted as an “anisotropic absorbing medium”.

The standard PML derivation needs to rely on a global separable coordinate system to define properly the absorption direction. Using Cartesian, spherical or cylindrical based PML definitions and combining them, a wide range of geometries can be covered [3]. Still, in many applications an unnecessarily large free-space region must be discretized between the PML and the object under investigation.

Consequently, many researchers tried to extend the flexibility of the method by implementing more general formulations. Lassas *et al.* [4] introduced a normal tangential coordinate system based on a parametrization of the boundary. Later on, Zschiedrich *et al.* [5] developed a specific coordinate system able to cope with any polygonal domains. Recently, a new PML realization was proposed by Ozgun *et al.* called “locally-conformal PML” [1, 6], which allows to design a PML

layer enclosing any arbitrarily-shaped convex spatial domain. The originality of the method lies in the fact that the formulation is solved directly in the layer complex space, using elements with complex nodal coordinates.

Though this approach is very promising, its practical implementation must be carefully handled, especially the design of the locally defined absorption vectors. We propose in this paper an original way of computing them by solving an artificial boundary value problem inside the layer. We prove that enhanced results are obtained for certain applications which even enhances the flexibility and robustness of the locally conformal PML concept.

2 PRESENTATION OF THE METHOD

The locally-conformal PML method is based on a locally-defined complex coordinate transformation as originally introduced by Chew *et al.* [7]. It starts by the construction of a PML region Ω_{pml} conformally surrounding a domain Ω_{phy} , which represents the “physical domain”. Note that Ω_{phy} can be chosen as the smallest convex volume that encloses all scatterers and sources, in order to minimize the computational domain $\Omega = \Omega_{pml} \cup \Omega_{phy}$. A cross section of the layer is illustrated in Figure 1(a), we denote Γ_{in} and Γ_{out} the PML internal and external boundaries.

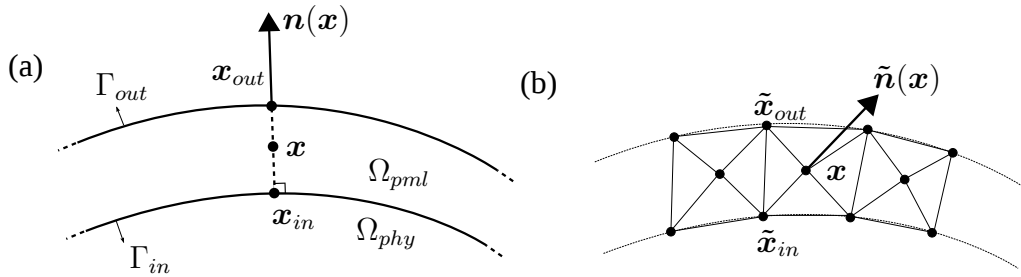


Figure 1: Illustration of the locally-conformal PML implementation. (a) Optimal design, (b) Node based approach

In the locally-conformal PML realization, the layer properties do not depend on a global coordinate system and must be defined for each point. The transformation is the following, assuming an implicit harmonic time dependence of the form $e^{i\omega t}$, each point of coordinates $\mathbf{x} \in \mathbb{R}^3$ in the layer is mapped to $\hat{\mathbf{x}} \in \mathbb{C}^3$ through:

$$\hat{\mathbf{x}} = \mathbf{x} + \frac{1}{i\kappa} f(\mathbf{x}) \mathbf{n}(\mathbf{x}), \quad (1)$$

where κ denotes the wave number. The unit vector $\mathbf{n}(\mathbf{x})$ represents the absorption vector, it indicates along which direction the wave will be absorbed and writes:

$$\mathbf{n}(\mathbf{x}) = \frac{\mathbf{x} - \mathbf{x}_{in}}{\|\mathbf{x} - \mathbf{x}_{in}\|}, \quad (2)$$

where $\mathbf{x}_{in}$ is the solution to the minimization problem:

$$\min_{\mathbf{x}_{in} \in \Gamma_{in}} \|\mathbf{x} - \mathbf{x}_{in}\|. \quad (3)$$

Obviously, this solution is unique if Γ_{in} is the boundary of a convex set. Function $f(\mathbf{x})$ is the absorption amplitude function which writes [1]:

$$f(\mathbf{x}) = \frac{\alpha \|\mathbf{x} - \mathbf{x}_{in}\|^m}{m \|\mathbf{x}_{out} - \mathbf{x}_{in}\|^{m-1}}, \quad (4)$$

where α and m are positive parameters and the quantity $\|\mathbf{x}_{out} - \mathbf{x}_{in}\|$ represents the local PML width (denoted d_{pml}).

To illustrate the effect of the complex coordinate transformation (1), simply consider a x -propagating wave ersatz of the form $e^{-i\kappa x}$. While penetrating a PML region with absorption vector $\mathbf{n} = (1, 0, 0)$, the transmitted wave will become exponentially decaying:

$$e^{-i\kappa\hat{x}} = e^{-i\kappa x} e^{-f(x)x}. \quad (5)$$

The PML is said to be “perfectly matched” because it produces no reflection at interface between domains Ω_{phy} and Ω_{pml} , irrespectively of the frequency and angle of incidence of the incoming wave [8]. However, since the PML region has to be truncated (i.e d_{pml} is finite), spurious reflections still occur on the external boundary Γ_{out} . Theoretically, these reflections are of minor importance due to the exponential decay of the wave in the layer. In fact, for a given PML width, they can be made arbitrarily small by taking f sufficiently large. Unfortunately, this conclusion does not hold when the problem is discretized: the finite element layer is no more “perfectly matched” and taking big values of absorption coefficients can lead to bad representations and ill-conditioning [9].

Consequently, for a given mesh and layer width, the values of the absorption coefficients have to be optimized to take the most of the discrete layer. To cope with that issue, different approaches were proposed, notably one by Bermudez *et al.* [8], which uses an unbounded absorption function. However, as demonstrated numerically in Section 3, satisfying results can be obtained if the set of coefficient values is carefully chosen.

2.1 Formulation

To account for the complex PML space, the Helmholtz equation which governs the evolution of the harmonic linear pressure perturbations p , is modified as follows:

$$\hat{\nabla}^2 p(\hat{\mathbf{x}}) + \kappa^2 p(\hat{\mathbf{x}}) = -g(\hat{\mathbf{x}}), \quad (6)$$

where $\hat{\nabla}$ is the transformed nabla operator which reads:

$$\hat{\nabla} = [J^{-1}]^T \cdot \nabla, \quad (7)$$

where J is the Jacobian matrix of transformation (1):

$$J = \begin{bmatrix} \partial\hat{x}/\partial x & \partial\hat{x}/\partial y & \partial\hat{x}/\partial z \\ \partial\hat{y}/\partial x & \partial\hat{y}/\partial y & \partial\hat{y}/\partial z \\ \partial\hat{z}/\partial x & \partial\hat{z}/\partial y & \partial\hat{z}/\partial z \end{bmatrix}, \quad \forall \mathbf{x} \in \Omega_{pml} \quad \text{and} \quad J = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \forall \mathbf{x} \in \Omega_{phy}. \quad (8)$$

Thus, solving (6) is strictly equivalent to solving:

$$([J^{-1}]^T \cdot \nabla) \cdot ([J^{-1}]^T \cdot \nabla p(\mathbf{x})) + \kappa^2 p(\mathbf{x}) = -g(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega. \quad (9)$$

In standard PML realization, the weighted residual approach is applied to Equation (9), yielding modified operators in the PML region. One remarkable aspect of the method proposed by Ozgun *et al.*[1] is that the variational approach is directly applied to the original Equation (6). Since all algebraic relations are evaluated in terms of the nodal coordinates, one can use a standard FEM implementation and just replace the real coordinates by their complex counterparts given by (1). Apart from that, all FEM machinery (i.e shape functions operations and Jacobian derivations) remains unchanged. The weak form of Equation (9) simply consists in finding $p^h \in H^1(\Omega)$ such that, $\forall q^h \in H^1(\Omega)$:

$$\begin{aligned} \int_{\Omega_{pml}} \hat{\nabla} p^h(\hat{\mathbf{x}}) \cdot \hat{\nabla} q^h(\hat{\mathbf{x}}) - \kappa^2 q^h(\hat{\mathbf{x}}) p^h(\hat{\mathbf{x}}) d\Omega_{pml} \\ + \int_{\Omega_{phy}} \nabla q^h(\mathbf{x}) \cdot \nabla p^h(\mathbf{x}) - \kappa^2 q^h(\mathbf{x}) p^h(\mathbf{x}) d\Omega_{phy} = \int_{\Omega_{phy}} q^h(\mathbf{x}) g(\mathbf{x}) d\Omega_{phy}. \end{aligned} \quad (10)$$

Though Robin-like boundary conditions could also be considered, homogeneous Neumann conditions are applied on external boundary Γ_{out} , making all surface integrals vanish.

2.2 Practical implementation

The localization of $\mathbf{x}_{in}$ on boundary Ω_{in} is of utmost importance, knowing that it fully determines the computation of the absorption axis $\mathbf{n}(\mathbf{x})$. The most straightforward discrete interpretation of minimization problem (3) would consist in finding for each PML node, the closest node on interface, denoted $\tilde{\mathbf{x}}_{in}$. As illustrated in Figure 1 (b), this “node based” approach may yield a poor estimation on a coarse unstructured grid. Though in many applications it has very little effect on the performance, it is demonstrated numerically in Section 3.2 that a slight deflection of the absorption axis can yield local instabilities. To cope with that issue, one could choose to increase the nodal density of Γ_{in} by, for example, defining virtual nodes in the middle of each interface element. Another possible approach, which can be called “element based”, would consist in applying a projection based operator, by solving:

$$\text{find } \tilde{\mathbf{x}}_{in} \in \Gamma_{in} / (\mathbf{x} \cdot \tilde{\mathbf{x}}_{in}) = 0, \quad (11)$$

using the FE based geometric description of the interface. In most cases, this approach will yield an optimal estimation of $\tilde{\mathbf{x}}_{in}$. Unfortunately, any curvature discontinuity at inter-element connection yields a indefinite zone which is gray-shaded in Figure 2, where Equation (11) has no solution.

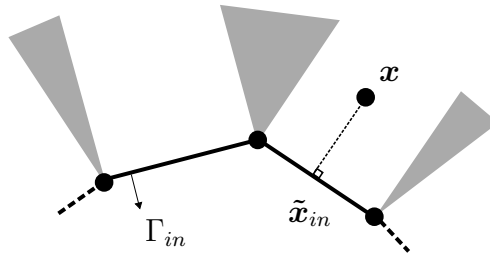


Figure 2. Projection based procedure to find $\tilde{\mathbf{x}}_{in}$.

Though a robust algorithm could be derived through the combination of the “nodal based” and the “element based” procedures, we explore here a very different approach. Instead, we propose to derive the absorption vectors by solving the following boundary value problem in the PML region:

$$\nabla^2 \phi(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in \Omega_{pml}, \quad (12)$$

where ϕ is a real valued potential field, subject to the following Dirichlet boundary conditions:

$$\phi(\mathbf{x}) = -1 \quad \text{on } \Gamma_{in} \quad \text{and} \quad \phi(\mathbf{x}) = 0 \quad \text{on } \Gamma_{out}. \quad (13)$$

Once problem (12) is solved, one can derive the following vector field:

$$\mathbf{v}(\mathbf{x}) = \nabla \phi(\mathbf{x}) \quad (14)$$

which, once normalized, will represent an excellent estimation of the local absorption vector:

$$\tilde{\mathbf{n}}(\mathbf{x}) = \frac{\mathbf{v}(\mathbf{x})}{\|\mathbf{v}(\mathbf{x})\|}. \quad (15)$$

In this approach, internal and external boundaries define potential isovalues, which by definition are locally normal to the gradient field $\mathbf{v}$. In practice, this Laplace problem is solved using a finite element method on the existing PML mesh part. The weak form of Equation (12) consists in finding $\{\phi^h \in H^1(\Omega_{pml}) / \phi^h = -1 \text{ on } \Gamma_{in}; \phi^h = 0 \text{ on } \Gamma_{out}\}$ such that :

$$\int_{\Omega_{pml}} \nabla \varphi^h(\mathbf{x}) \cdot \nabla \phi^h(\mathbf{x}) d\Omega_{pml} = 0, \quad \forall \varphi^h \in H^1(\Omega_{pml}) / \varphi^h = 0 \text{ on } \Gamma_{in} \cup \Gamma_{out}. \quad (16)$$

Using a standard finite element post-processing procedure, the discrete counterpart of vector field $\mathbf{v}$ is obtained at each PML node. As demonstrated numerically in Section 3, using such a diffusion equation guarantees a “smooth” behavior of the absorption properties of the layer and ensures that the vector $\tilde{\mathbf{n}}$ always closely follows the normal to the inner surface.

It should be emphasized that formulation (16) is not frequency dependent and that it should be computed only once. Furthermore, the bandwidth of the associated system matrix is generally small due to the typical “strip-like” geometry pattern of the layer. As a consequence, compared to the expense of solving the global acoustic problem at multiple frequencies, the added computational cost of the PML preparation is relatively small.

3 NUMERICAL VALIDATION

In this section, we validate our approach on two bi-dimensional models. The geometries and associated meshes of isoparametric linear triangle elements are given in Figure 3. Their typical mesh size is respectively of $h = 0.03$ and $h = 0.05$. Neglecting any pollution effect [10] and using a low criterion of $n_\lambda = 2\pi/\kappa h = 6$ points per wavelength, the meshes are approximately valid up to respectively 1900 Hz and 1100 Hz. Note that a classic PML realization could not handle the second model, because inner and outer surfaces are not defined on any ‘constant coordinates’ of a given coordinate system.

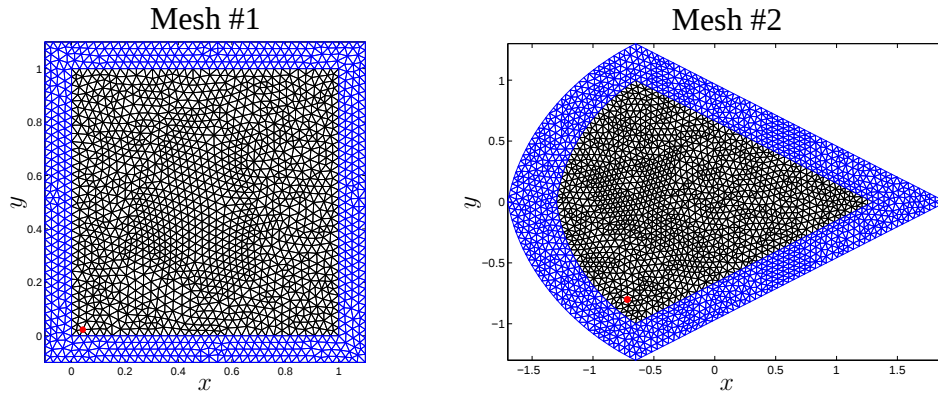


Figure 3: Two meshes used for the validation example: PML elements are plotted in blue and monopole source is indicated by a red spot.

The problem solved is the free radiation of a monopole source, which analytical solution writes:

$$G(\mathbf{x}, \mathbf{x}_s) = \frac{-i}{4} H_0^2(\kappa \|\mathbf{x} - \mathbf{x}_s\|), \quad (17)$$

where H_0^2 is the Hankel function of the second kind and $\mathbf{x}_s$ is the source coordinates. The influence of the source position on the locally defined PML was thoroughly studied in [1] at a fixed frequency, using Monte Carlo analysis. Therefore, we will use only one source position (indicated in Figure 3) and focus on the spectrum analysis by carefully covering the whole frequency range.

3.1 Parameter study

The values of the PML parameters α and m must be carefully chosen to ensure a good behavior of the PML. In general, a quadratic ($m = 2$) or a cubic ($m = 3$) absorption function is preferred,

since it guarantees a smooth transition at interface Γ_{in} . If the transition is too sharp, the discrete layer can be far from “perfectly matched” and yield very important reflections [9]. Regarding the value of parameter α , Ozgun *et al.* recommend the use of $\alpha = \gamma\kappa$, with ($5 < \gamma < 15$) if the PML thickness is between $\lambda/4$ and $\lambda/2$. Note that the absorption amplitude is taken linearly dependent on κ in order to make the transformation (1) frequency independent.

In practice, a single mesh is often used to cover the whole frequency range. In standard FEM, the stiffness and mass operators can be pre-assembled before the frequency loop, sparing a lot of computational effort. For this approach to hold with the PML formulation (10), some fixed parameter values for m and γ must be determined.

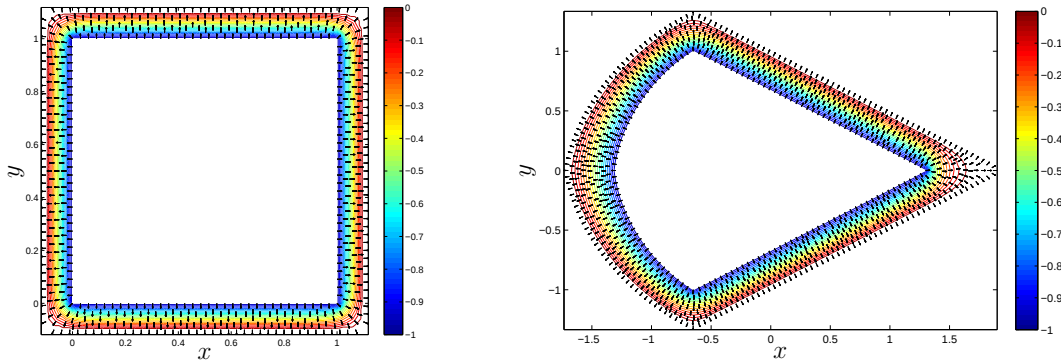


Figure 4: Solution of the Laplace problem in the PML region. Contour plots of ϕ^h (color lines) and post-processed values of $\tilde{n}$ (arrows).

We first solve the Laplace problem (12) in the layer region. Results are presented in Figure 4. For the two models the absorption vectors obtained seem of excellent quality. They closely follow the normal and vary smoothly at curvature discontinuities of the inner PML surface. We now solve the source radiation problem for 100 frequencies on interval $[20, 2000]$ Hz for mesh #1 and $[20, 1400]$ Hz for mesh #2 for different values of m and γ . Taking the analytical solution (17) as reference, the mean numerical error on the physical domain Ω_{phy} is computed and plotted in Figure 5 for mesh #1 and in Figure 6 for mesh #2.

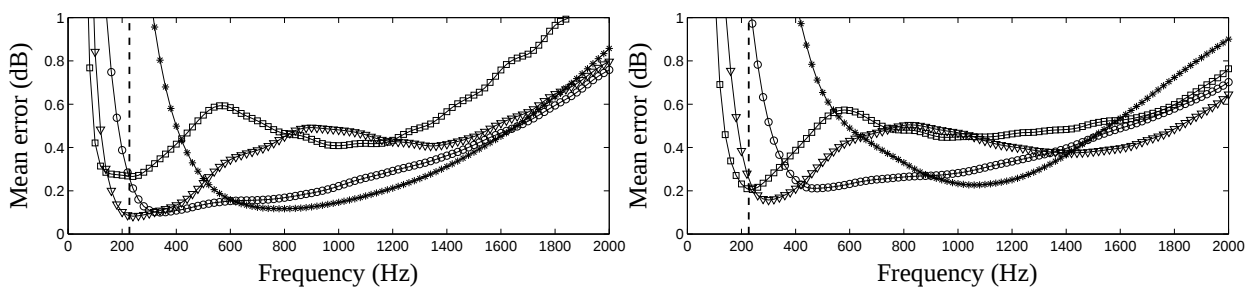


Figure 5: Numerical error as a function of frequency on mesh # 1 for quadratic (left) and cubic (right) absorption functions. $\star(\gamma = 5)$; $\circ(\gamma = 10)$; $\square(\gamma = 15)$; $\nabla(\gamma = 20)$.

The conclusions for both models are similar, the best compromise is obtained with the quadratic shape function ($m = 2$) with amplitude $\gamma = 10$. In the low frequency range, good accuracy is reached as long as the layer width verifies:

$$d_{pml} > \lambda/15, \quad (18)$$

(represented by a dashed vertical line). Following (5), the wave decays proportionally to $\gamma\kappa$ in the layer. For small values of κ , the incoming wave is not damped enough and enters back with important magnitude into the physical domain after reflecting on the outer surface. Increasing the

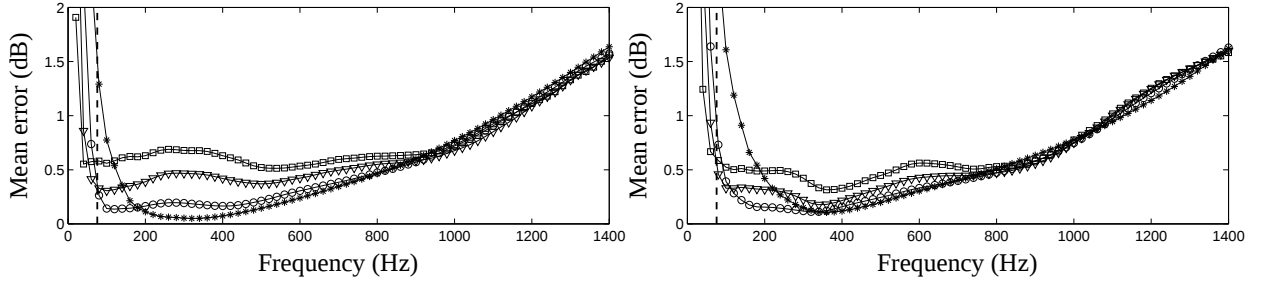


Figure 6: Numerical error as a function of frequency on mesh # 2 for quadratic (left) and cubic (right) absorption functions. $\star(\gamma = 5)$; $\circ(\gamma = 10)$; $\square(\gamma = 15)$; $\nabla(\gamma = 20)$.

value of γ slightly shifts this low frequency limit, approximately up to $\lambda/20$ but no further, and this is to the price of a deterioration in the rest of the spectrum. With parameters ($m = 2, \gamma = 10$), provided that condition (18) is fulfilled, reasonable accuracy is obtained on the whole mesh validity spectrum.

3.2 Comparison of Laplace and node based approaches

To illustrate the importance of the PML absorption vector definition on the results, let us now perform computations with a node based approach, as described in Section 2.2. Choosing parameter values ($m = 2, \gamma = 10$), a comparison is plotted in Figure 7 for mesh # 1 and in Figure 8 for mesh # 2.

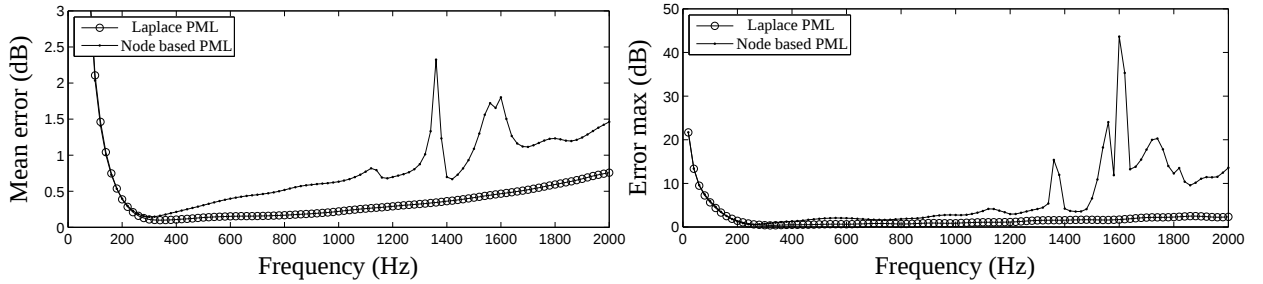


Figure 7: Comparison between the Laplace PML and the node based PML on mesh # 1 ($m = 2, \gamma = 10$). Mean (left) and maximum (right) numerical errors inside the physical domain.

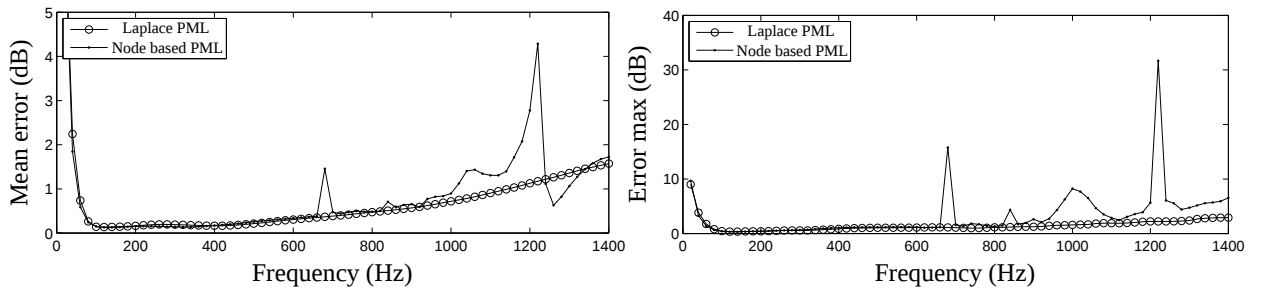


Figure 8: Comparison between the Laplace PML and the node based PML on mesh # 2 ($m = 2, \alpha = 10$). Mean (left) and maximum (right) numerical errors inside the physical domain.

The locally-conformal approach, using a node based definition of the absorption axes deteriorates significantly as the frequency increases and is obviously unstable at certain frequencies. On mesh #1, at frequency 1600 Hz, the maximum error is above 40 dB. The real part of the pressure is plotted for the two solutions at this frequency in Figure 9. In the solution computed with the node based approach, instabilities are clearly visible in the $x < 0$ and the $y < 0$ PML regions:

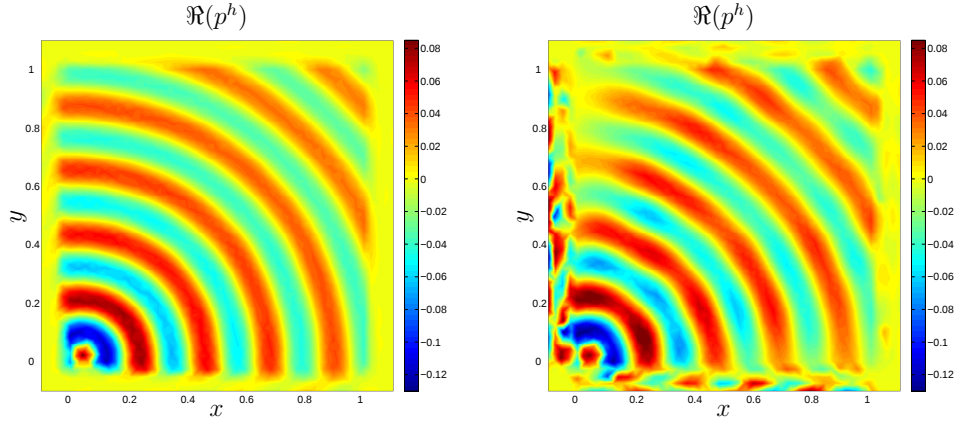


Figure 9: Real part of pressure on mesh # 1 at 1600 Hz using Laplace PML (left) and the node based PML (right).

pressure field is locally amplified inside the layer and it increases the spurious reflections. At this frequency the mean error is 1 dB superior to the solution obtained with a Laplace based computation of the absorption vectors. On mesh #2, this difference can reach up to 4dB at $f = 1220$ Hz. To analyze the origin of these instabilities, a detail of the absorption vectors obtained with the two methods in the $x < 0$ PML region is given in Figure 10.

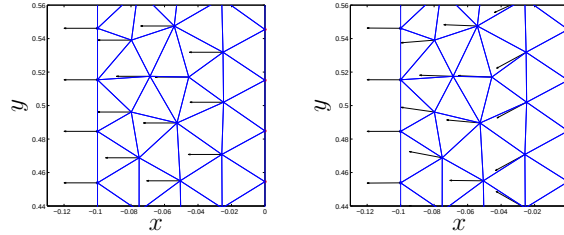


Figure 10: Detail of absorption vectors on mesh #1 using Laplace approach (left) and the node based approach (right).

Some absorption vectors computed with the node based approach exhibit a significant vertical component. If the incoming wave has a non negligible opposite vertical propagation component, it will undoubtedly yield locally exponentially growing pressure fields. This simple numerical example clearly highlights the benefits of our Laplace approach. To the cost of a preliminary finite element calculation inside the layer, the robustness and accuracy of the locally-conformal PML is clearly improved.

3.3 Radiation from a duct

As a last numerical example to illustrate the interest of the locally-conformal approach, we consider the problem of the free radiation of a 2D unbaffled open end duct. The FEM mesh and the preprocessed PML Laplace computation are shown in Figure 11. Mesh size is $h = 0.01$, which makes it valid up to approximately 5400 Hz (with low $n_\lambda \approx 6$ criterion). We apply a 0.1m s^{-1} velocity on the vertical panel at $x = 0$ and we compute the solution for 100 frequencies on interval $[20, 5400]\text{Hz}$. Let us now define $\theta \in [-\pi, \pi]$, the standard directivity angle at the duct outlet and the non dimensional frequency $\kappa d = 2\pi f d / c_0$, with d the duct diameter and c_0 the sound speed.

To plot the directivity patterns, we are interested in evaluating the solution at points located outside the computational domain. A post-processing tool was implemented that computes a Helmholtz Kirchhoff integral on the inner PML boundary to retrieve pressure at points outside the physical domain Ω_{phy} . It writes [11]:

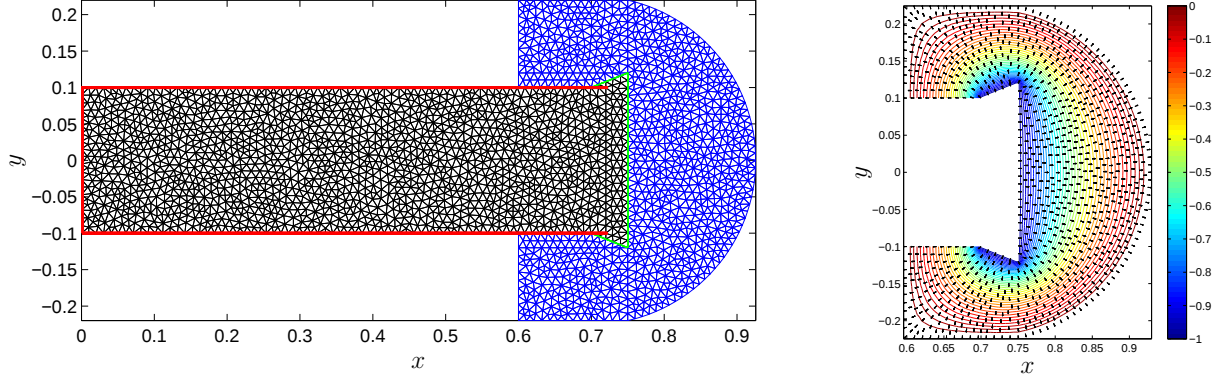


Figure 11: Unbaffled radiating duct mesh (left); PML elements are in blue, duct and inner PML boundaries are plotted respectively in red and green color. Solution of the Laplace problem in the PML region (right).

$$p(\mathbf{x}) = \int_{\Gamma_{phy}} G(\mathbf{x}, \mathbf{y}) \frac{\partial p^h(\mathbf{y})}{\partial \nu} - p^h(\mathbf{y}) \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial \nu} d\Gamma_{phy}(\mathbf{y}), \quad \forall \mathbf{x} \in \mathbb{R}^3 / \Omega_{phy}, \quad (19)$$

where ν is the unit normal pointing inside the physical domain. It should be noted that in that specific example, integral (19) only represents an approximation of the external problem. The inner PML boundary (plotted in green in Figure 11) does not form a closed surface and the solution is expected to perform poorly for $|\theta| > \pi/2$, as the boundary integral does not take into account most of the scattering on the duct rigid surfaces.

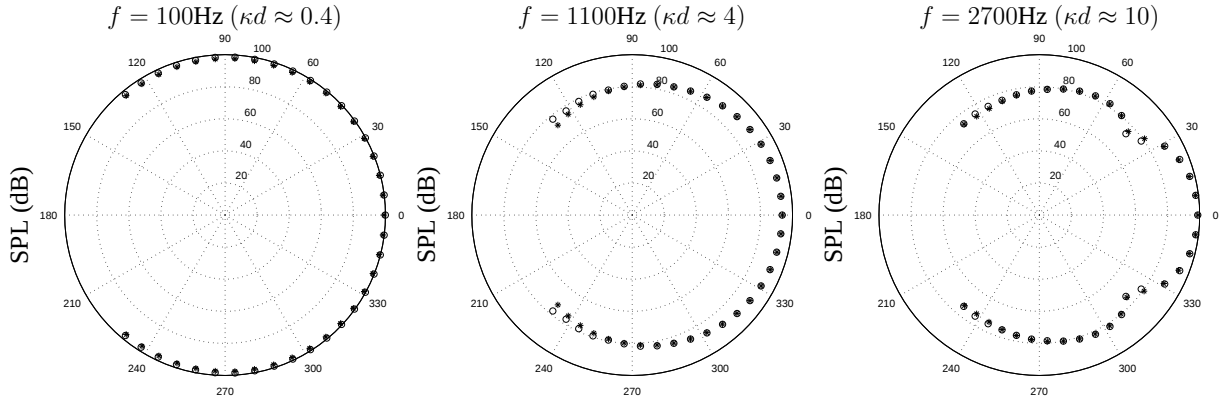


Figure 12: Sound pressure levels variations in θ for the IBEM model (circle) and the FEM model (stars) at a 1 meter distance from the duct outlet.

Though far field approximate solutions can be derived for such problems [12], we perform an indirect variational boundary element computation (IBEM) with acoustical software LMS.Sysnoise and take it as a reference. The IBEM mesh consists of the trace of the FEM mesh on the duct boundary represented in red in Figure 11. The sound pressure levels (SPL) are computed at different θ values at a distance of 1 meter from the duct outlet. The comparison between FEM-PML and IBEM models are plotted in Figure 12, for three frequencies. The two solutions are in good agreement, surprisingly enough even for $|\theta| > \pi/2$. Note that the maximum SPL does not evolve much as the frequency increases, but the directivity pattern is radically modified. Low frequencies radiate in all directions whereas at high frequency, most of the energy is radiated along the duct axis ($\theta = 0$).

To further illustrate the robustness of the locally-conformal PML for such applications, we present in figure 13 the error obtained at central point ($\theta = 0$) as a function of frequency. The layer

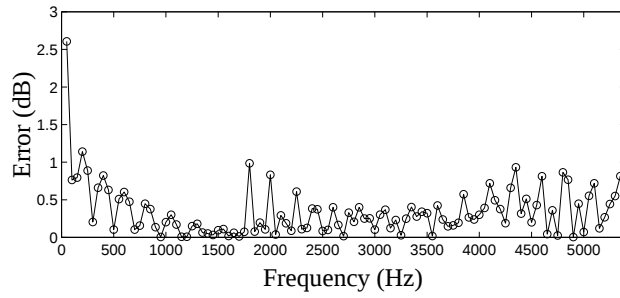


Figure 13. Error as a function of the frequency at a 1 meter distance from the duct outlet ($\theta = 0$).

is too narrow to be precise below 40 Hz (condition (18) would impose a layer of 0.5 meter width), but an accuracy of maximum 1dB is obtained on the rest of the spectrum without the need to adjust any parameter of the layer.

4 CONCLUSION

In this paper, a new PML realization for Helmholtz equation was explored. This method greatly extends the flexibility of the standard separable coordinate system based PML, being able to cope with any convex geometry. The practical implementation was discussed with a particular emphasis on the computation of the locally defined absorption vectors. Numerical evidence show that slight deflections of the absorption axis can spoil the entire solution at certain frequencies. To alleviate that issue, an original calculation of the locally defined absorption axes was proposed, based on the gradient fluxes obtained from a Laplace problem performed in the PML region. Provided that a layer width as low as $\lambda/15$ is fulfilled, fixed parameter values are proposed that offer a reasonable accuracy on the whole frequency range.

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