Abstract

Perfectly Matched Layer (PML) techniques are widely used for dealing with unbounded problems. However, their performance depends critically on both an absorption coefficient and the numerical method. The coefficient is generally tuned by using costly and case-dependent optimization procedures or set empirically. In this paper we present some efficient profiles of the coefficient that allow to avoid any tuning in discrete contexts. These profiles are compared by means of two benchmarks with different numerical methods.

Introduction

A major challenge for the numerical simulation of wave-like problems on unbounded domains is to truncate the computational domain without altering too much the original solution. Different techniques have been developed to simulate the open boundary produced by the truncation. The Perfectly Matched Layer (PML) technique is one of them. It has been introduced by Berenger [1] in the context of electromagnetics for time-dependent problems and is now developed and widely used in many physical and numerical contexts [2]-[6].

The idea is to surround the computational domain with a specific layer. Inside it, the physical medium is adapted in such a way that the outgoing waves are progressively damped and seem to leave the domain without reflection. To achieve this, the differential equations of the problem are transformed and an absorption coefficient $\sigma$ governing the damping is introduced.

This paper deals with the choice of the coefficient $\sigma$, which is still tricky in discrete contexts when numerical methods are used. After introducing the PML equations and the numerical methods in section 1, we present and analyse some unbounded absorption coefficient profiles [2] in section 2 and compare them in section 3 with the case-dependent-optimized polynomial profiles commonly used in the literature. Preliminary results on 1-D and 2-D benchmarks highlight the performance and ease of use of the unbounded profiles in different numerical methods.

1 Mathematical and numerical framework

To introduce the equations of the PML, we consider a time-dependent wave problem on a semi-infinite two-dimensional domain $\Omega = \{(x, y) : x < 0, y \in \mathbb{R}\}$ bounded on the right side ($x = 0$) by an open boundary. The domain $\Omega$ is extended with a PML $\Omega_{pml} = \{(x, y) : x \in [0, \delta], y \in \mathbb{R}\}$ to simulate as accurately as possible this open boundary.

Inside both the domain and the PML, we consider the dimensionless fields $\eta$, $u$, and $v$ that are governed by the cartesian equations:

\[
\frac{\partial \eta}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = -\sigma \eta + q \tag{1}
\]

\[
\frac{\partial u}{\partial t} + \frac{\partial \eta}{\partial x} = -\sigma u \tag{2}
\]

\[
\frac{\partial v}{\partial t} + \frac{\partial \eta}{\partial y} = 0 \tag{3}
\]

while the additional dimensionless field $q$ is governed by:

\[
\frac{\partial q}{\partial t} + \sigma \frac{\partial v}{\partial y} = 0 \tag{4}
\]

The absorption coefficient $\sigma(x)$ is assumed to be zero inside the domain $\Omega$ and positive inside the PML $\Omega_{pml}$. Therefore the equations of the wave problem are recovered in the domain $\Omega$. These equations are equivalent to those obtained by Hu in [4].

If the coefficient $\sigma(x)$ is singular at $x = \delta$, the solution must satisfy a homogeneous Dirichlet condition on one of the fields to have a well-posed problem. When a profile that does not present any singularity is used, a Neumann condition or even a radiation condition could be implemented to improve the efficiency of the layer. However, the exact nature of this boundary condition has little influence on the solution if outgoing waves are efficiently damped in the PML medium [7]. In this paper, outgoing waves are assumed to be fully damped when reaching the outer boundary of the PML. A homogeneous Dirichlet boundary condition on $u$ at $x = \delta$ is used in all cases.
To approximate the solution of this general problem we consider two popular numerical methods:

- A Finite Difference (FD) method with a structured grid. The fields $\eta$, $u$ and $v$ are discretized on an Arakawa C-grid. The equations (1) – (3) are solved using a forward-backward scheme in time and a centred scheme in space as in [6]. The additional field $q$ is discretized in the same way as $\eta$ and solved with a scheme similar to the one applied to (1).

- A Discontinuous Galerkin (DG) method with an unstructured grid of triangular cells. The weak forms of the governing equations (1) – (4) are integrated on each cell and numerical fluxes are defined between adjacent cells. For the three first equations the numerical fluxes are based on the Rankine-Hugoniot condition at the discontinuous lines as in [5], while the numerical flux of the additional equation (4) is computed using the meaning value of $v$ at the interface between the cells and is penalized with the jump of $q$. The integrals on each cell are computed using a full Gaussian quadrature procedure. Finally, all the results are obtained with linear basis functions and a Crank-Nicolson time stepping scheme.

## 2 Absorption coefficient profiles

The choice of the optimum absorption coefficient $\sigma$ is trivial in the continuous context. Using a plane wave analysis, it can be shown that any spurious reflection is avoided for outgoing waves of any frequency and incidence if and only if $\sigma$ is unbounded in the PML (see [2] or [3]), i.e. if

$$ \int_0^\delta \sigma(x) \, dx = +\infty \quad (5) $$

However this condition does not apply to the discrete context. Indeed the performance of the PML decreases dramatically when the damping of the solution induced by large values of $\sigma$ cannot be captured by the discretization grid [6]. Therefore $\sigma$ must be chosen in such a way to introduce enough damping of outgoing waves without inducing a too sharp decrease of the fields in the PML.

A polynomial profile of $\sigma$ allows such a progressive damping

$$ \sigma(x) = \sigma_{\text{max}} \left( \frac{x}{\delta} \right)^n \quad (6) $$

with $n > 0$ and where $\sigma_{\text{max}}$ is the value of the absorption coefficient at the outer side of the layer. This profile is widely used and can perform better with numerical schemes than some unbounded profiles. However no general rule exists to choose the parameters $\sigma_{\text{max}}$ and $n$. Therefore some expensive and case-dependent optimization procedures are used to tune them.

As an alternative, unbounded profiles have been proposed by Bermúdez et al. [2]

$$ \sigma(x) = \frac{\alpha}{(\delta - x)^n} \quad (7) $$

$$ \sigma(x) = \frac{\alpha}{(\delta - x)^n} - \frac{\alpha}{\delta^n} \quad (8) $$

with again two free dimensionless parameters: $\alpha$ and $n$. Fortunately these two profiles do not require any tuning with $n = 1$ in the context of the continuous finite element method [2]. With $\alpha = 1$ the solution is close to optimum.

## 3 Numerical results

In this section we present the results of two benchmarks to compare the different profiles of $\sigma$ and to show the influence of the numerical method on the optimum parameters.

### 3.1 One-dimensional benchmark with the FD method

Consider first the simplest case of a one-dimensional domain $\Omega = [-L, 0]$ extended on the right side with a PML $\Omega_{\text{pml}} = [0, \delta]$. Since the aim of the procedure is to compare optimum parameters for a wide range of frequencies, a Gaussian incident pulse is propagated near the open boundary. Initially, the Gaussian pulse is located in the second half of the domain $[-L/2, 0]$. As time goes by, this pulse propagates to the right and is partly reflected by the PML. The final time of the numerical experiment and the size of the computational domain are such that the reflected signal ends in $[-L/2, 0]$ and any influence from the left boundary ($x = -L$) is avoided in $[-L/2, 0]$ at the end of the simulation.

The accuracy of the PML is measured with the relative error $\xi_r$ of the numerical solution at the final time

$$ \xi_r = \sqrt{\frac{\int_\Omega (|\eta|^2 + |u|^2)}{\int_\Omega (|\eta|^2 + |u|^2) \, dx}} \quad (9) $$

where $\eta$ and $u$ are the initial discrete fields while $\eta$ and $u$ are the numerical solution. For a perfectly absorbing boundary, $\xi_r = 0$ while $\xi_r = 1$ with a perfectly reflective boundary. The aim is to minimize $\xi_r$ by adjusting $\sigma$.

The optimum parameters are shown in Figure 1 for different thicknesses of the PML (from 2 to 15 spatial steps $\Delta x$), and the corresponding relative errors are plotted in Figure 2. The optimum $\alpha$ of the unbounded profiles is nearly constant unlike the optimum $\sigma_{\text{max}}$ of the polynomial profiles. In particular the optimum $\alpha$ is close to 1.
as with continuous finite element methods. However the smallest relative error corresponds to the optimized polynomial profiles. The second unbounded profile performs better than the first one while the opposite was true in the context of continuous finite elements [2].

![Figure 1](image1.png)

**Figure 1:** Optimum parameters associated with the different profiles for different thickness of layer.

![Figure 2](image2.png)

**Figure 2:** Relative errors associated with the optimum parameters from Figure 1 (same legend as in Figure 1) and to the discrete optimum (bold red line).

By considering the discrete values of $\sigma$ in each cell of the PML as control parameters, a more complete optimization procedure can be developed using a similar benchmark [6]. The discrete profile obtained using this costly procedure outperforms the other ones (Figure 2).

Obviously this procedure is impractical for realistic cases, but it is informative. As shown in Figure 3 this discrete optimum profile corresponds to a spatially increasing smooth function, which gives rise to a progressive decrease of the fields in the PML. The optimized polynomial and unbounded profiles considered in this paper are close to the discrete optimum but not exactly identical.

![Figure 3](image3.png)

**Figure 3:** Profiles of $\sigma$ with optimum parameters and discrete optimum for a 5-cells PML.

### 3.2 Two-dimensional benchmark

In order to test the performance of the different profiles in a more realistic context, we consider the two-dimensional case of the collapse of a Gaussian-shaped mound of water in a rectangular domain $\Omega = \{(x, y) : x \in [-L_x, L_x], y \in [-L_y, L_y]\}$. Zero Dirichlet conditions are imposed at each boundary except one ($x = L_x$) where an open boundary is simulated with a PML $\Omega_{pml} = \{(x, y) : x \in [L_x, L_x + \delta], y \in [-L_y, L_y]\}$. The Gaussian-shaped mound of water is prescribed as initial condition

$$\eta(x, y, t = 0) = \eta_0 \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{R^2}\right)$$  \hspace{1cm} \text{(10)}$$

while zero values are prescribed for the other fields $u$, $v$ and $q_v$ everywhere at $t = 0$. During the collapse, circular waves appear and propagate outwards. The main wave front reaches the interface between the domain and the PML with a normal incidence. As time goes by, the wave front propagates along the boundaries and approaches the PML with a decreasing angle of incidence.
For both methods the performance of the polynomial and the second unbounded profiles with optimum parameters are comparable: the relative errors differ at most by one order of magnitude. The first unbounded profile is less efficient than the second one. Simulations with other numerical and geometrical parameters (not shown in this paper) lead to similar conclusions.

However a major advantage of the unbounded profiles is that the optimum parameter $\alpha$ is always close to 1 while the optimum $\sigma_{\text{max}}$ for polynomial profiles is case dependent. In practice, this means that the second efficient unbounded profile can be used as is, without any optimization procedure. A more detailed analysis as well a comparison with continuous finite elements will be provided in the extended paper.

References


