Introduction to Perfectly Matched Layers (PML) for the Wave and Helmholtz Equations

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Abstract

When one is trying to numerically solve the scattering problem for the wave equation or the Helmholtz equation, one often runs into problems because the computation domain is infinite. We would like to truncate the domain to facilitate computational solutions, however, we still need to make sure that (a) the solution still satisfies the desired radiation condition at infinity and (b) the truncation does not cause any extra reflections/affect the solution in the region of interest. Perfectly Matched Layers (PML) provide a method to do exactly this, by adding a specific layer of material to the outside of the region of interest that will absorb all of the radiation coming to it without causing any reflections. In this talk, I will present a basic introduction to and formulation of PML, as well as state some results by Lassas and Somersalo that prove that this method does not change the value of the solution in the region of interest.

1 Introduction/Motivation

One of the classical problems that people try to solve with the Wave or Helmholtz Equation is the external scattering problem. For a more complicated domain Ω, the problem must generally be solved numerically, which then becomes problematic because the computation region is infinite. In order to solve this problem, we need to truncate the computation region, which would normally be done with a Dirichlet or Neumann condition on the boundary. However, since we are dealing with wave-type equations, this type of simple solution is not possible. Imposing this kind of condition on the boundary of a large domain would result in reflections back into the region of interest, which will change the solution there. The solutions will decay at infinity, but not fast enough to make this kind of truncation viable. The infinite solution would not be the same as the solution from the finite, truncated domain, which is not what we want. We would like whatever solution we get to work for any radiation reaching the boundary, as well as cause minimal reflections back into the region of interest.

Perfectly Matched Layers (PML) provide a solution of this kind. It involves adding a special layer of material around the region of interest, where the material may be non-physical. The parameters of this material are chosen to convert oscillatory functions into exponentially decaying waves. These waves can then be truncated with a Dirichlet or Neumann condition, which will cause reflections, but since the waves have decayed exponentially in terms of the thickness of the layer, the amount of reflection is negligible. This type of formulation will work for both the wave equation and the Helmholtz equation, but the only error bounds that we have currently are from Lassas and Somersalo about the Helmholtz equation. The full wave equation poses some other interesting problems, which will be discussed over the course of the talk.

There will be two main parts to this talk. The first will discuss the formulation of PML in the case of Cartesian coordinates and the wave equation. In this, we will see how the frequency shows up in a way that causes problems for solving this equation for an arbitrary set of frequencies. In the second part of the talk, we will restrict to the Helmholtz equation in polar coordinates and look at the more rigorous development of this procedure. By being more careful about all of the choices we make in this process, we can prove that the solution will be exponentially close to the infinite solution as we expand the computation region.

2 Basic Formulation

We are trying to solve the scattering wave equation in an external domain, with the outgoing radiation condition. Restricting ourselves to $\mathbb{R}^2$, we have

$$\begin{aligned} \frac{\partial^2 p}{\partial t^2} - c^2 \Delta p &= 0 \qquad \text{in } \mathbb{R}^2 \setminus \Omega \\ p &= -p_{inc} \qquad \text{on } \partial\Omega \end{aligned} \tag{1}$$

We consider a plane-wave, time harmonic solution to this equation; namely, we take

$$p(x,t) = Ce^{i(\vec{k}\cdot\vec{x}-\omega t)}$$

and we will want any solution we have to work for all plane-waves and superpositions of them. Now, if we look at this equation and isolate the positive x direction, we see that we have

$$p(x,t) = Ce^{ik_x x}e^{ik_y y}e^{-i\omega t}.$$

So, if we were to somehow make the x-direction have a positive imaginary part, the exponential in the x-direction would have a decaying factor, so the oscillations would go to zero rapidly as x increased, possibly allowing us to truncate the region with minimal reflections. This is exactly what we do.

Firstly, in order to make all of this work, we assume that the space outside of the "region of interest" is homogeneous, linear, and time-invariant. The process for forming the PML consists of three main steps.

(a) Analytically continue the solutions to complex-valued x. We currently have a solution $p(x,y,t)$ that is valid for all real-valued x, and since it is a complex exponential, we can analytically continue it to the complex plane. Now, since the space outside of the region of interest was assumed to be x-invariant, the solution in the complex plane still solves the same differential equation. Since x only shows up in the equation as $\frac{\partial}{\partial x}$, this expression is still the same whether or not x is complex-valued. The derivative in any dx direction is the same. Our original solution can still be found on the real axis, where $Im\ x = 0$.

(b) Pick a complex contour on which to solve the differential equation/evaluate the function. We now pick a contour in the complex plane that will give us the desired exponential decay of the waves, but still leave the solution unchanged in the region of interest. If we denote the complex contour by $\tilde{x}$, we define

$$\tilde{x} = x + if(x) \qquad \partial\tilde{x} = (1 + i\frac{df}{dx})\partial x$$

where $f(x) = 0$ for small x (in the region of interest) and $f(x) > 0$ outside, then this will give us a desired contour. Since the equation is unchanged for any dx direction, we have that our original wave equation is now of the form

$$\frac{\partial^2 p}{\partial t^2} - c^2\frac{\partial^2 p}{\partial \tilde{x}^2} - c^2\frac{\partial^2 p}{\partial y^2} = 0$$

and the solutions to this equation will have the desired exponential decay outside of the region of interest. However, solving differential equations on complex contours is difficult so we...

(c) Coordinate Transform back to Real x. In this step, we simply invert the transformation to get back to an expression that only involves the real-valued x. For notational purposes, we denote

$$\frac{df}{dx} = \frac{\sigma_x(x)}{\omega}$$

so we then have that

$$\partial\tilde{x} = \left(1 + i\frac{\sigma_x(x)}{\omega}\right)\partial x$$

(the significance of the ω will be discussed later). Therefore, we have the transform

$$\frac{\partial}{\partial \tilde{x}} = \frac{1}{\left(1 + i\frac{\sigma_x(x)}{\omega}\right)} \frac{\partial}{\partial x}$$

which will convert the equation back to real-valued x. This gives a much more complicated equation to solve, which we will see explicitly for the radial case later, but it will have the desired decay outside of the region of interest.

(d) Truncate the computation domain. At this point, the step is fairly simple. Since the waves are all exponentially decaying, we can just put a Dirichlet Boundary a certain distance into the PML layer, and the reflections will be negligible. Thus, by adding this fictitious layer of material, we have been able to truncate the computation domain without adding any extra reflections and without changing the solution in the region of interest.

2.1 System Approach: ADE

In order to investigate how this change of variables affect the PDE that we are trying to solve, we will look at the wave equation in terms of a system. Namely, we write

$$\frac{\partial u}{\partial t} = b\nabla \cdot \vec{v} \qquad \frac{\partial \vec{v}}{\partial t} = a\vec{\nabla} u$$

We will also assume that all of our solutions are time-harmonic, that is, there is a time-dependence of the form $e^{-i\omega t}$. We will now try to implement the PML approach to the wave equation in 1 and 2 space dimensions.

2.1.1 One Space Dimension

The $1 - d$ system, adding in the time-harmonic dependence of the functions, now becomes

$$\frac{\partial u}{\partial t} = b\frac{\partial v}{\partial x} = -i\omega u \qquad \frac{\partial v}{\partial t} = a\frac{\partial u}{\partial x} = -i\omega v$$

If we now make the transform described before

$$\frac{\partial}{\partial x} \to \frac{1}{\left(1 + i\frac{\sigma_x(x)}{\omega}\right)} \frac{\partial}{\partial x}$$

and multiply both sides by $1 + i\frac{\sigma_x(x)}{\omega}$ gives

$$b\frac{\partial v}{\partial x} = -i\omega u + \sigma_x u \qquad a\frac{\partial u}{\partial x} = -i\omega v + \sigma_x v$$

which can easily be transformed back into time-domain to

$$\frac{\partial u}{\partial t} = b\frac{\partial v}{\partial x} - \sigma_x u \qquad \frac{\partial v}{\partial t} = a\frac{\partial u}{\partial x} - \sigma_x v$$

For $\sigma_x > 0$, we see that the solutions will decay in both space and time. Also, the point of choosing σ_x/ω is clear, as the decay is now independent of frequency. If we had just used σ the rate at which waves decayed would depend So, making this PML transformation has changed the form of the PDE, but doesn't make it any more difficult to solve numerically.

2.1.2 Two Space Dimensions

In the two dimensional case, however, we see some of the problems of PML developing. We start with the system presentation again.

$$\frac{\partial u}{\partial t} = b\frac{\partial v_x}{\partial x} + b\frac{\partial v_y}{\partial y} = -i\omega u \qquad \frac{\partial v_x}{\partial t} = a\frac{\partial u}{\partial x} = -i\omega v_x \qquad \frac{\partial v_y}{\partial t} = a\frac{\partial u}{\partial y} = -i\omega v_y$$

The third equation will not be affected by the PML transformation in the x-direction, and we do the same process as the 1-dimensional case on the first two equations. Making the derivative transformation and clearing the denominators gives

$$b\frac{\partial v_x}{\partial x} + b\frac{\partial v_y}{\partial y}\left(1 + i\frac{\sigma_x}{\omega}\right) = -i\omega u + \sigma_x u \qquad a\frac{\partial u}{\partial x} - i\omega v_x + \sigma_x v_x$$

The second equation here is fine, and so is most of the first. There is one term that will have a problem, namely

$$bi\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}$$

since, when transformed back, the $\frac{i}{\omega}$ becomes an integral, which we have no way to represent in these equations. Therefore, in order to be able to solve these equations, we define an auxiliary function ψ, which satisfies

$$-i\omega\psi = b\sigma_x\frac{\partial v_y}{\partial y}$$

so then we can write this troublesome equation as

$$b\frac{\partial v_x}{\partial x} + b\frac{\partial v_y}{\partial y} + \psi = -i\omega u + \sigma_x u$$

Now, everything can be transformed back to the time-domain to give a system of **4** equations

$$\begin{aligned}
\frac{\partial u}{\partial t} &= b\nabla \cdot v - \sigma_x u + \psi \\
\frac{\partial v_x}{\partial t} &= a\frac{\partial u}{\partial x} - \sigma_x v_x \\
\frac{\partial v_y}{\partial t} &= a\frac{\partial u}{\partial y} \\
\frac{\partial \psi}{\partial t} &= b\sigma_x\frac{\partial v_y}{\partial y}
\end{aligned}$$

This last equation was more or less created by this PML transformation and is called an *auxiliary differential equation*, which becomes necessary in the two-dimensional case. This adds an additional differential equation to solve when trying to carry out these numerical calculations. For the three-dimensional case, doing PML in each coordinate direction requires, in the best case so far, four auxiliary functions and corresponding differential equations.

So, this PML transformation creates a different system of PDE's to solve. However, the solution will solve the standard wave equation where $\sigma_x = 0$, and will decay away rapidly outside of this region so that we can truncate the domain.

3 Helmholtz Formulation and Proofs

Now that we have an idea of how PML works, we will look at a more mathematical formulation and a proof of the fact that the PML solution of the wave equation converges to the infinite domain solution as the thickness of the PML layer goes to infinity. Therefore, if we are careful in the way we construct the PML boundary, we can have our modified solution be as close as we want to the actual infinite domain solution. This analysis will follow the work of Lassas and Somersalo.

3.1 Formulation/Notation

For this problem, we will be considering a modified electromagnetic potential, which gives rise to the Helmholtz equation. Namely, if we consider a region in $\mathbb{R}^2$ as the cross section of a cylinder, with the magnetic field parallel to the axis of the cylinder, the amplitude of this field outside of the domain satisfies

$$\Delta u + k^2 u = 0$$

and the Sommerfeld radiation condition at infinity,

$$\lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u}{\partial r} - iku\right) = 0.$$

We also assume that the obstacle is perfectly conducting, resulting in a Neumann condition on the boundary,

$$\frac{\partial u}{\partial n} \mid_{\partial\Omega} = g.$$

This work will also use double layer potentials to get some of the results. Denote by Ψ the fundamental solution of the Helmholtz equation,

$$\Psi(x, y, k) = \frac{i}{4} H_0^{(1)}(k|x - y|).$$

For Γ a curve in $\mathbb{R}^2$ and X a set disjoint from Γ, and ψ a function defined on Γ, we denote the double layer potential by

$$D_{\Gamma,X}(k)\psi(x) = \int_\Gamma \frac{\partial\Psi}{\partial n_y}(x, y, k)\psi(y)\, dS(y)$$

If X and Γ are the same set, we will only use a subscript Γ.

3.2 PML

In this instance, we will analyze the PML formulation in polar coordinates. Choose R_1 so that $\overline{\Omega} \subseteq B_{R_1}$. We then define σ (the same σ as before) to be our fictitious absorption coefficient

$$\sigma(r) = 0 \text{ for } r < R_1 \quad \sigma(r) > 0 \text{ for } r > R_1 \quad \lim_{r\to\infty} \int_{R_1}^r \sigma(t)dt = \infty$$

We then define the stretched coordinates $\tilde{r}$ by

$$\tilde{r} = \tilde{r}(r) = \begin{cases} r & r \le R_1 \\ r\left(1 + \frac{i}{\omega r}\int_{R_1}^r \sigma(t)\, dt\right) =: r\beta(r) & r > R_1 \end{cases}$$

The new solution, called the Berenger solution after the first person to develop this method, is defined as the solution to the stretched system of equations, namely, it solves

$$\begin{aligned} \frac{1}{\tilde{r}}\frac{\partial}{\partial \tilde{r}}\left(\tilde{r}\frac{\partial u_B}{\partial \tilde{r}}\right) + \frac{1}{\tilde{r}^2}\frac{\partial^2 u_B}{\partial \theta^2} + k^2 u_B &= 0 \\ \frac{\partial u_B}{\partial n} \mid_{\partial\Omega} &= g \\ |u_B| \text{ is bounded in } \mathbb{R}^2 \setminus \Omega & \end{aligned}$$

By denoting

$$\frac{\partial \tilde{r}}{\partial r} = 1 + \frac{i}{\omega}\sigma(r) =: \alpha(r)$$

we can transform variables back to see that u_B solves

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\beta}{\alpha} r \frac{\partial u_B}{\partial r}\right) + \frac{\alpha}{\beta}\frac{1}{r^2}\frac{\partial^2 u_B}{\partial \theta^2} + k^2\alpha\beta u_B = 0$$

We can also write this equation in a coordinate-less form $(\nabla \cdot A\nabla + \alpha\beta k^2)u = 0$, where the matrix A, representing a conductivity, is now non-physical. The main work of Berenger shows that this system has a unique solution that is reflectionless at the boundary. It also shows that this solution, $u_B = u_{sc}$ inside of B_1. That is, adding this PML layer did not change the value of the solution inside of the ball of radius R_1, which is exactly what we want.

Now, at this point, we have constructed an infinite PML layer that gives us the ideal result. However, this has not addressed the main problem with solving this problem numerically, that is, the unboundedness of the domain. In order to move forward with truncating the domain, we pick $R_2 > R_1$ and impose another constaint on σ, namely that for $r > R_2$

$$\sigma(r) = \sigma_0 = \frac{1}{R_2}\int_{R_1}^{R_2} \sigma(t)\ dt$$

This gives us that for all $r > R_2$,

$$\alpha(r) = 1 + \frac{i}{\omega}\sigma_0 =: \alpha_0$$

and

$$\beta(r) = 1 + \frac{i}{r\omega}\int_{R_1}^{r} \sigma(t)\ dt = 1 + \frac{i}{r\omega}\left(\int_{R_1}^{R_2} \sigma(t)\ dt + (r - R_2)\sigma_0\right) = \alpha_0$$

Therefore, by this choice of constant, we have that outside of R_2, the PDE solved by u_B reduces to

$$\Delta u_B + (\alpha_0 k)^2 u_B = 0$$

which is a uniform Helmholtz equation with complex wave number. Therefore, we can use these double layer potentials with this wave number to replace the infinite condition with a near field condition.

3.3 Double Layer Potentials

In order to use these double layer potentials, we consider the external Dirichlet problem on $\mathbb{R}^2 \setminus B_2$. Using this theory, if we want to solve this problem with

$$w \mid_{\partial B_2} = f$$

then, since the interior Neumann problem has only the trivial solution, the solution to this problem can be written as

$$w = D_{\partial B_2, \mathbb{R}^2 \setminus B_2}(\alpha_0 k)\left(\frac{1}{2} + D_{\partial B_2}\right)^{-1} f$$

In particular, we have that that the Berenger solution satisfies

$$u_B \mid_{\mathbb{R}^2\setminus B_2} = D_{\partial B_2, \mathbb{R}^2\setminus B_2}(\alpha_0 k)\left(\frac{1}{2} + D_{\partial B_2}\right)^{-1}(u_B \mid_{\partial B_2}.$$

Now, we pick some $R_3 > R_2$, and by restricting to the trace on B_3, we have that

$$u_B \mid_{\partial B_3} = P(u_B \mid_{\partial B_2}) \qquad P = D_{\partial B_2, \partial B_3}(\frac{1}{2} + D_{\partial B_2})^{-1}$$

Lassas and Somersalo then go on to prove the following

Lemma 3.1. *The restriction of u_B to the set $B_3 \setminus \Omega$ is the unique solution in H^1 that satifies*

$$\begin{aligned} (\nabla \cdot A\nabla + \alpha\beta k^2)u &= 0 \\ \frac{\partial u}{\partial n} \mid_{\partial\Omega} &= g \\ u_{\partial B_3} = P(u_B \mid_{\partial B_2}) \end{aligned}$$

This last condition is a non-local boundary condition, which specifies that it must solve the correct equation outside of B_3.

3.4 Truncating the Domain

The rest of this proof centers around this operator P and consists of two main steps. First, they show that if we take another operator P_ϵ that is close enough to P, then the solutions u_B and u_ϵ will be close. Finally, they show that truncating the domain results in an operator that is close to the original P, completing the proof.

Lemma 3.2. *Assume $P_\epsilon : H^{1/2}(\partial B_2) \to H^{1/2}(\partial B_3)$ is an operator with the property $||P_\epsilon - P|| < \epsilon$ where the norm here is the uniform operator norm on $\mathcal{B}(H^{1/2}(\partial B_2), H^{1/2}(\partial B_3))$ of bounded linear operators. If ϵ is small enough, then the previous system with P replaced by P_ϵ has a unique solution denoted u_ϵ, and we have that*

$$||u_B - u_\epsilon||_{H^1(B_3\setminus\Omega)} < C\epsilon.$$

Now, we pick some $\rho > R_3$. If we want to truncate the computation/PML domain, that is equivalent to solving the problem

$$\begin{aligned} (\nabla \cdot A\nabla + \alpha\beta k^2)u &= 0 \\ \frac{\partial u}{\partial n} \mid_{\partial\Omega} &= g \\ u_{\partial B_\rho} = 0 \end{aligned}$$

In order to relate this to the operator P, we want to define an operator $\tilde{P}$ so that it maps data on ∂B_2 to a corresponding set of data on ∂B_3 so that the solution goes to zero on B_ρ.

Lemma 3.3. *Assume $\tilde{u_B}$ satisfies the system above. Then*

$$\tilde{u_B} \mid_{\partial B_3} \tilde{P}(\tilde{u_B} \mid_{\partial B_2})$$

for some specific operator $\tilde{P}$. Conversely, if $\tilde{u_B}$ satisfies

$$\begin{aligned} (\nabla \cdot A\nabla + \alpha\beta k^2)\tilde{u_B} &= 0 \\ \frac{\partial \tilde{u_B}}{\partial n} \mid_{\partial\Omega} &= g \\ \tilde{u_B} \mid_{\partial B_3} = \tilde{P}(\tilde{u_B} \mid_{\partial B_2}) \end{aligned}$$

then $\tilde{u_B}$ satisfies the above desired system.

From this Lemma, we see that truncating the PML layer gives us a new operator $\tilde{P}$ that depends on ρ. The point of this approach is that

Lemma 3.4. *The operator $\tilde{P}(\rho)$ has the property that*

$$\lim_{\rho \to \infty} ||\tilde{P}(\rho) - P|| = 0$$

where the convergence is exponential and the norm is the uniform operator norm.

Finally, putting all of these lemmas together, we have the main theorem.

Theorem 3.1. *Assume that the fictitious absorption coefficient σ satisfies the properties from before. Then for any wave number k, there exists a $\rho_0(k)$ such that for all $\rho > \rho_0(k)$, the truncated Berenger system has a unique solution $\tilde{u_B}$. Furthermore, the solution has the approximation property*

$$\lim_{\rho \to \infty} ||u_{sc} - \tilde{u_B}||_{H^1(B_1 \setminus \Omega)} = 0$$

where the convergence is exponential.