An Improved Procedure for Selecting the Profiles of Perfectly Matched Layers

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Abstract: The perfectly matched layers (PMLs), as a boundary termination over an unbounded spatial domain, are widely used in numerical simulations of wave propagation problems. Given a set of discretization parameters, a procedure to select the PML profiles based on minimizing the discrete reflectivity is established for frequency domain simulations. We, by extending the function class and adopting a direct search method, improve the former procedure for traveling waves.

Keywords: Optimization, perfectly matched layers (PMLs), reflection coefficients.

1. Introduction

Perfectly matched layers (PMLs) are widely used as boundary terminations in problems to be solved over an unbounded spatial domain. Physically, this is an approach to surround a numerical problem domain with a layer of a material which creates as little numerical reflection as possible, while also attenuating waves that enter from the problem interior. Mathematically, when a PML is used to truncate the $x$ axis, $x$ is actually replaced by $\hat{x} = \int_{x} (1 + i\sigma(\tau))d\tau$, where $\sigma$ is a real function satisfying certain conditions.

Nevertheless, in actual numerical simulations, due to the finite thickness of the PML, reflections occur when plane waves incidence upon the PML. Note that PML is generally problem-dependent, for example, the reflection is dependent on the discretization scheme. For frequency domain simulations, based on minimizing the average discrete reflectivity, Ya Yan Lu [2] gave a practical procedure for selecting the optimal PML profile $\sigma$ where the function class is restricted to simple powers. In this paper, to further reduce the average reflectivity for traveling waves, we consider a rational function class for $\sigma$; to avoid time-consuming computations, we use the Nelder-Mead simplex method to determine the coefficients of $\sigma$. Besides, we also give a simpler $\sigma$ which is easy to optimize. Numerical simulations demonstrate that our improved procedure is much better and practical.

2. Motivations to Improve the Former Procedure

For traveling waves, we consider a two-dimensional waveguiding structure in [2]. The $y$-component of the electric field of a transverse wave satisfies a Helmholtz equation. Consider that the structure is unbounded in the negative $x$ direction and the medium is homogeneous (refractive index $n \equiv n_0$)
for \( x < G \), we then truncate the negative \( x \) axis by a PML. For \( D < H < G \), we define \( \sigma(x) \) such that \( \sigma(x) = 0 \) for \( x \geq H \) and \( \sigma(x) > 0 \) for \( x < H \) while \( \sigma(H) = 0 \) and \( \sigma'(H) = 0 \). Replacing \( x \) by \( \hat{x} = \int^x (1 + i\sigma(t))dt \) gives rise to

\[
-\frac{1}{s} \partial_x (s^{-1} \partial_x u) + \partial^2_z u + k_0^2 n_0^2 u = 0
\]

where \( k_0 \) is the free space wavenumber, and the time dependence is \( e^{-i\omega t} \). At \( x = D \), we use a simple zero boundary condition: \( u = 0 \). The actual PML is the layer \( D < x < H \). For \( H < x < G \), (1) has a plane wave solution

\[
u = e^{i(-\alpha x + \beta z)} + Re^{i(\alpha x + \beta z)} \]

where the second term is the reflected wave due to the incidence of plane waves upon the PML with reflection coefficient \( R \). When \( x \) is discretized, \( R \) depends on \( \sigma \). By a second-order finite difference approximation in the transverse direction \( x \), we can easily find \( R \) exactly by solving a linear equation system.

Thus, to select the optimal PML profile \( \sigma \) is to find a \( \sigma \) such that the following \( \overline{|R|} \) is minimized:

\[
\overline{|R|} = \frac{2}{\pi} \int_0^{\pi/2} |R(\theta)|d\theta.
\]

For convenience, let

\[
\tau(x) = \frac{x - H}{D - H}.
\]

In Lu’s procedure \([2]\), since \( \sigma \) is limited to be a simple power, i.e.

\[
\sigma = S \tau^p,
\]

we only need to determine \( p \) and the dimensionless scaling parameter \( S \) such that \( \overline{|R|} \) is minimized. The optimal values of \( S \) were computed for \( p = 2, \ldots, 5 \) respectively, among which the one giving the least \( \overline{|R|} \) was chosen to be the overall optimal PML profile.

In fact, the numerical result can be more satisfying if we give up the restriction of \( \sigma \) to be simple powers. In practice, people usually use \( \sigma = \frac{S \tau^3}{1 + \tau} \) for the PML profile \([4]\). This gives us a start to find a better profile.

After numerical computation and a little adjustment, \( \sigma = \frac{S \tau^3}{1 + \tau} \) turns out to be better in this situation. So in this paper, we first investigate into this rational function class:

\[
\sigma = \frac{a_2 \tau^2 + a_3 \tau^3 + \ldots + a_p \tau^p}{1 + \tau}, a_p > 0, p \geq 2
\]

where its coefficients are to be optimized to give a minimal value of the average discrete reflectivity \( \overline{|R|} \). Due to the condition \( \sigma > 0 \), we let \( a_p > 0 \) for simplicity while losing certain generality. However, if the PML profile is defined by such rational function, the work to determine the optimal values of its coefficients becomes much more time-consuming. To save time, we adopt the Nelder-Mead (NM) simplex method due to the fact that the problem is nonlinear and the derivative information of \( \overline{|R|} \) is unavailable.
It is natural to ask why we choose this method. We offer two answers. First, in the NM method, the objective function is evaluated at the vertices of a simplex, and movement is away from the poorest value. This method tends to work so well in practice by producing a rapid initial decrease in function values. Second, when we consider a simpler $\sigma$ with two parameters, the NM algorithm gives answer in a much shorter time. Thus, due to its powerful local descent property, we decide to adopt this method though it may not give globally optimized solution. [5]

Note that the NM method is for unconstrained problems, but $a_k > 0$ in (6) is actually a constraint. To overcome this, we define $\sigma$ as below

$$\sigma = \frac{|a_2|\tau^2 + |a_3|\tau^3 + \ldots + |a_p|\tau^p}{1 + \tau}, a_p > 0, p \geq 2. \quad (7)$$

When similar situation occurs, we will tackle it in this way again without further remarks.

Furthermore, after optimization for (6), we try to define $\sigma$ by a simpler function class which largely conserves the good properties of the former one but is much easier to optimize and more useful in practice.

3. The Improved Procedure with Numerical Results

A. General Results

In numerical simulations, we adopt the conditions in [2] so that we could compare the average discrete reflectivity $|R|$ between the two procedures. Explicitly we have the wavelength $\lambda_0 = 1 \, \mu \text{m}$, $k_0 = 2\pi/\lambda_0$, $n_0 = 1$.

Consider an example in [2]: A PML with thickness of five grids ($m = 5$), where the grid size $h = \frac{1}{2}\lambda_0 = 0.05 \, \mu \text{m}$. Under the restriction on $\sigma$ in (5): $\sigma = S\tau^p, p \leq 5$, the author obtained an optimal profile: $p = 3$ and $S = 100.4$, which gave rise to $|R| = 0.013$.

Through our improved procedure, we obtain a simple and better result: $\sigma = (23.6\tau^2 + 35.9\tau^5)/(1 - \tau)$ which gives rise to $|R| = 0.0047$, only 36% of the former one. Moreover, if we give up the simplicity and allow a higher order of the rational function, we could further get an result of 0.0031, only 24% of the former one.

B. A Rational Function Class for the PML Profile

First of all, we investigate into (6). Take note that the conditions $\sigma(0) = 0$ and $\sigma'(0) = 0$ are satisfied. Let

$$S_p = (a_2, a_3, \ldots, a_p). \quad (8)$$

In order to obtain the local optimal values of its coefficients, we carry out the NM simplex method by using a simple initial value $S_p = (0, \ldots, 0, 50)$ for all $p = 2, 3, \ldots 12$, respectively. The result is summarized in Table 1.

In general, from Table 1, it can be deduced that when $p$ gets bigger, the number of iteration gets bigger. And $|R|$ improves when $p$ increases from 2 to 10, but stopped improving when $p > 10$. The best result comes at $p = 10$ and 11 by giving $|R| = 0.0031$, only 24% of the optimal value 0.013 obtained in [2]. The number of iteration are 1279 and 715, respectively.

We also observe that: (a) in Table 1, some of the coefficients $a_3, a_4, \ldots, a_{p-1}$ are not significant when compared to $a_2$ and $a_p$; (b) when $\sigma$ gets smaller more rapidly as $\tau \to 0$ and bigger more rapidly as $\tau \to 1$, the result gets much better.
Table 1: Local optimal values of the coefficients of $\sigma$ defined by (6). Results are derived by the Nelder-Mead simplex method. At $p = 6, 9, 12$, the algorithm stops because the number of function evaluation has exceeded the preset limit of 2000. The actual number of iteration will be bigger if we increase the limit.

| $p$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $a_6$ | $a_7$ | $a_8$ | $a_9$ | $a_{10}$ | $a_{11}$ | $a_{12}$ | Iterations | $|R|$ |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----------|-----|
| 2   | 74.2  |       |       |       |       |       |       |       |       |       |       | 21        | 0.019 |
| 3   | 38.2  | 108.7 |       |       |       |       |       |       |       |       |       | 103       | 0.0131    |
| 4   | 57.1  | 0     | 222.9 |       |       |       |       |       |       |       |       | 419       | 0.009     |
| 5   | 61.8  | 0     | 2.4   | 509.7 |       |       |       |       |       |       |       | 637       | 0.0058    |
| 6   | 59.3  | 0     | 29    | 48.8  | 947.8 |       |       |       |       |       |       | 1209      | 0.0044    |
| 7   | 49.9  | 16.2  | 51.0  | 24.2  | 11.1  | 1358  |       |       |       |       |       | 741       | 0.0039    |
| 8   | 39.2  | 33    | 40.1  | 62.7  | 64.1  | 13.1  | 14.9  | 2326  |       |       |       | 959       | 0.0035    |
| 9   | 40.9  | 21.5  | 35.6  | 16.4  | 23.6  | 1.1   | 17.5  | 2685.3|       |       |       | 1279      | 0.0031    |
| 10  | 44    | 17.5  | 38.3  | 22.7  | 20.4  | 28.7  | 1.1   | 32.3  | 44.8  | 3487.2 |       | 715       | 0.0031    |
| 11  | 45.5  | 5.1   | 61.2  | 26.9  | 2.6   | 47.2  | 52.5  | 81    | 75.6  | 84.2   | 2519.2 | 1370      | 0.0031    |
| 12  |       |       |       |       |       |       |       |       |       |       |       |           |       |

C. A Simpler Function Class for the PML Profile

Based on the above observations, we try to define a simpler - in fact, better - function class for $\sigma$: due to (a), let $a_k = 0$ for $k = 3, ..., p - 1$ to reduce complexity; due to (b), let the denominator of $\sigma$ in (6) be $(1 - \tau)$, such that $\sigma \to 0$ as $\tau \to 0$ and $\sigma \to \infty$ as $\tau \to 1$. After these changes, the shape of $\sigma$ satisfies the characteristic in (b) better. Then (6) becomes

$$\sigma = \frac{a_2\tau^2 + a_8\tau^8}{1 - \tau}, p \geq 2$$

(9)

where $\sigma(0) = 0$ and $\sigma'(0) = 0$ still hold.

We carry out the NM simplex method for $\sigma$ defined in (9) again with the initial value $S_p = (0, ..., 0, 50)$ for all $p = 2, 3, ..., 12$, respectively. The local optimal values of its coefficients is listed in Table 2.

From Table 2, we can see that after simplification, the maximal number of iteration is reduced to 157. (In Contrast to Table 1, the maximal number of iteration is more than 1370.) $|R|$ gets smaller when $p$ increases from 2 to 8, but bigger when $p > 9$. The best result $|R| = 0.0037$ occurs at $p = 8$ and 9. It is bigger than $|R| = 0.0031$ obtained by (6), however, compared with its fast convergence, (9) is superior in efficiency and more practical than (6). In practice, we could choose a profile which has a lower order: for example, $p = 5$, the corresponding $|R| = 0.0047$.

D. Comparison

For more details, we plot $|R|$ as functions of $\theta$ for four different $\sigma$ in Fig. 1 and Fig. 2. In Fig. 1, we can see that $\sigma = (a_2\tau^2 + a_8\tau^8)/(1 - \tau)$ gives the lowest average of $|R|$ for $\theta > 0.3\pi/2$. In Fig. 2, for very small angles ($\theta < 0.005\pi/2$), it again distinguishes itself from the other three by giving the lowest reflectivity.

To illustrate that the NM method gives local minimizers, we plot $|R|$ as multivariable functions of $a_2$ and $a_8$ using $\sigma = (a_2\tau^2 + a_8\tau^8)/(1 - \tau)$ in Fig. 3. It can be observed that at $a_2 = 23.3$ and $a_8 = 121.3$, $|R|$ almost reaches its lowest value.
4. Conclusion

For frequency domain simulations, a procedure for selecting the optimal PML profile is established based on minimizing the average discrete reflectivity. By extending the profile to a rational function class and adopting the Nelder-Mead simplex method to calculate the profile’s coefficients, we reach a better numerical result. We also provide a simpler profile, which largely conserves the good properties of the former rational function.

For further improvements, we may use a better function class for the PML profile, or improve the convergence property of the optimization method. In addition, we may study the impact of such proposed profile in a more practical example, for instance, optical wave propagating along an optical waveguide and hitting the PMLs in different angles, or how the guided and evanescent waves behave at a waveguide discontinuity, etc.
Table 2: Local optimal values of the coefficients of $\sigma$ defined by (9). Results are derived by the Nelder-Mead simplex method.

| $p$ | $a_2$ | $a_p$ | Iterations | $|R|$  |
|-----|-------|-------|------------|-------|
| 2   | 24.9  |       | 21         | 0.0057|
| 3   | 0.0019| 28.4  | 44         | 0.0084|
| 4   | 22.5  | 14.5  | 109        | 0.0053|
| 5   | 23.6  | 35.9  | 91         | 0.0047|
| 6   | 24.4  | 76.2  | 136        | 0.0042|
| 7   | 24.3  | 113   | 157        | 0.0038|
| 8   | 23.3  | 121.3 | 150        | 0.0037|
| 9   | 23.5  | 195   | 116        | 0.0037|
| 10  | 23.2  | 180.1 | 101        | 0.0038|
| 11  | 23.5  | 221.6 | 124        | 0.0039|
| 12  | 23.5  | 223.4 | 133        | 0.0041|

Fig. 3. The average of reflectivity as functions of $a_2$ and $a_8$. The white arrow points at $a_2 = 23.3$ and $a_8 = 121.3$.

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