Long time stability of regularized PML wave equations

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***Abstract*—In this paper, we consider two dimensional acoustic wave equations in an unbounded domain and introduce a modified model of the classical perfectly matched layer (PML). In the classical PML model, an unexpected and exponential increase in energy is observed in the long-time simulation after the solution reaches a quiescent state. To address such an instability, we provide a regularization technique to a lower order regularity term employed in the auxiliary variable in the classical PML model. The well-posedness of the regularized system is analyzed with the standard Galerkin method based on the energy analysis, and the numerical stability of staggered finite difference method for its discretization is provided by using *von Neumann* stability analysis. To support the theoretical results, under various thickness and damping values, we demonstrate a long-time stability of acoustic waves in the computational domain.**

I. Introduction

It is quite important to effectively truncate an unbounded domain in wave propagation simulations in free space, where the perfectly matched layer (PML) methods that surround the domain of interest with thin artificial absorbing layers are popularly used in easy and effective ways. After the method was introduced by J. P. Bérenger [16], which involves splitting a field into two nonphysical electromagnetic fields, several studies were conducted regarding the PML method and its modified reformulations in many different wave-type equations. These include Maxwell's equations [9], [26], elastodynamics [7], [10], linearized Euler equations [12], [14], [22], [23], Helmholtz equations [28], and other types of wave equations [1], [6], [28]. Most PML models by the splitting technique, named a split PML method, yield a hyperbolic system of first order partial differential equations [8], [12], [13], [16], [29]. It is known that the split PML models demonstrate excellent overall performances from the viewpoint of applications. However, it was pointed out in [3], [5], [14] that Bérenger's split, as well as other split models, transform Maxwell's equations from being strongly hyperbolic into weakly hyperbolic. These transforms imply a transition from strong to weak well-posedness in the Cauchy problem and may lead to ill-posedness under low-order damping functions or thin layers [15]. The authors of [4], [12] mention that the use of artificial dissipation is necessary to stabilize the numerical scheme of such formulations for long-time simulations.

The resulting concerns about the well-posedness and stability of the split PML models have prompted the development of other PMLs. Some examples of such developments, without splitting the fields, include un-split PML models using convolution integrals [24], [25] and auxiliary variables [2], [3], [20]. In contrast to the split PML models, it is known that the un-split PML wave equations are more effective at time discretization [20] and does not make the use of additional memory for the nonphysical field variables. However, it has been found that the un-split PML models are susceptible to developing gradual instabilities in long-time simulations [4], [28]. These issues are the motivation for the mathematical study of the well-posedness and stability for the un-split PML models. Contrary to the many existing claims, the PML model may generate instability when the solution is quiescent or nearly quiescent in the PML layers, which is demonstrated numerically in Section II. This instability causes the wave energy to exponentially increase in the computational domain, which depends on the damping and layer thickness in the experiments.

The main contribution of this study is not only to introduce a regularized system of the second order PML acoustic wave equation that exhibits well-posedness without losing the non-reflection property of PMLs, but also to demonstrate its numerical stability. To construct the system, we adopt a regularization technique in the term $\nabla\cdot\vec{q}$ that has a lower regularity, to regularize the PML model for the Maxwell equation, where $\vec{q}$ is the auxiliary variable (see (II.3)). The standard Galerkin approximation and energy estimation of the solution are used to show the well-posedness of the regularized system. For its numerical scheme, we use a family of finite difference schemes using half-step staggered grids in space and time with central finite differences that maintain the second order approximation in both space and time, respectively. A concrete *von Neumann* stability analysis for the numerical scheme indicates that the scheme is stable under the Courant-Friedrichs-Lewy (CFL) condition. The novel features of this study include the good performance of the solution that presents a long-time stability compared to the classical PML model, which is numerically illustrated by presenting the energy behavior for the solutions in Section IV.

II. Motivation of Study

The target problem we consider is a general second order acoustic wave equation with a variable sound speed $c(\mathbf{x}) > 0$ described by

$$u_{tt}(\mathbf{x},t) - c^2(\mathbf{x})\Delta u(\mathbf{x},t) = 0, \quad \forall(\mathbf{x},t) \in \mathbb{R}^2 \times (0,T] \quad \text{(II.1)}$$

with initial conditions $u(\cdot,0) = u_0$ and $u_t(\cdot,0) = 0$, where $supp(u_0)$ is a subset of a domain Ω_0 included in the computational domain $\Omega_{comp} := [-a,a] \times [-b,b]$ in $\mathbb{R}^2$ for some $a,b > 0$. Here, $T > 0$ and the sound speed $c(\mathbf{x})$ is assumed to be bounded by

$$0 < c_* \leq c(\mathbf{x}) \leq c^* < \infty. \quad \text{(II.2)}$$

Suppose that a domain $\Omega = [-a-L_x, a+L_x] \times [-b-L_y, b+L_y]$ consists of Ω_{comp} surrounded by PMLs, where $L_x, L_y > 0$. Using a complex coordinate stretch, Grote and Sim [11] introduced the following two dimensional acoustic PML wave model: find $(u, \vec{q})$ satisfying, for $(\mathbf{x},t) \in \Omega \times (0,T]$,

$$\begin{cases} \frac{1}{c^2}u_{tt} + \alpha u_t + \beta u - \nabla \cdot \vec{q} - \Delta u = 0, \\ \vec{q}_t + A\vec{q} + B\nabla u = 0 \end{cases} \quad \text{(II.3)}$$

with initial and boundary conditions $u(\cdot,0) := u_0$, $u_t(\cdot,0) := u_1 = 0$, $\vec{q}(\cdot,0) := \vec{q}_0 = \vec{0}$, $u(\mathbf{x},\cdot)|_{\partial\Omega} = 0$, where $\vec{q}$ denotes the auxiliary variable and the coefficients are given by $\alpha := \frac{\sigma_x+\sigma_y}{c^2}$, $\beta := \frac{\sigma_x\sigma_y}{c^2}$, $A = \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_y \end{pmatrix}$, and $B = \begin{pmatrix} \sigma_x - \sigma_y & 0 \\ 0 & \sigma_y - \sigma_x \end{pmatrix}$. Here, the damping terms $\sigma_x := \sigma_x(x)$ and $\sigma_y := \sigma_y(y)$ are assumed to be nonnegative functions that vanish in the computational domain Ω_{comp} in the sense of the analytical continuation of the PML [17]. It is noted that the Cauchy problem for the model problem (II.3) is strongly stable in [11]. We also note that the model problem turns into an initial boundary problem by the artificial carving of the computational domain, which generates the boundary. From this artificial building of the boundary, therefore, the wave propagation should be affected by its condition. To demonstrate these effects, we use the energy method, introduced in [18], and numerically examine the well-posedness and stability of the model (II.3) by observing the behavior of the acoustic wave energy defined by

$$\mathcal{E}(t) = \frac{1}{2}\int_{\Omega_{comp}} \left(\frac{1}{c^2}u_t(t)^2 + \nabla u(t) \cdot \nabla u(t) \right) d\mathbf{x}. \quad \text{(II.4)}$$

For this purpose, we use the computational domain $\Omega_{comp} = [-1,1] \times [-1,1]$ surrounded by a PML layer with thickness $L_x = L_y = L$. In the absorbing layer, we consider the constant case ($\beta = 0$) in the following damping function of the form;

$$\sigma_{x_k}(x_k) = \begin{cases} 0, & |x_k| < 1, \\ \sigma_0 \left(\dfrac{|x_k - 1|}{L} \right)^\beta, & 1 \leq |x_k| \leq 1 + L, \end{cases} \quad \text{(II.5)}$$

where $x_k = x, y$ $(k = 1,2)$, $\beta = 0,1,2$, σ_0 is a given constant, and L denotes the thickness of the layers. The smooth initial value u_0 for our numerical tests is adopted as

$$u_0(x,y) = \begin{cases} e^{-0.6\left((x-x_0)^2+(y-y_0)^2\right)} & \text{if } (x,y) \in \Omega_{comp}, \\ 0 & \text{otherwise,} \end{cases} \quad \text{(II.6)}$$

and a constant sound speed $c(x,y) = 1$ is assumed. With

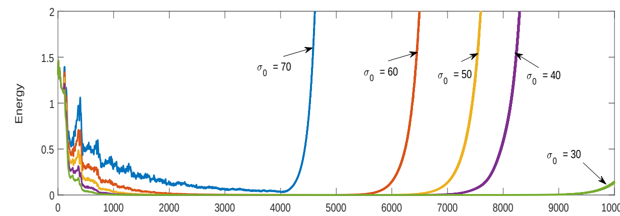

Fig. 1: $\mathcal{E}(t)$ when a fixed $L = 0.125$ and various dampings

these conditions, we first discretize equations (II.3) with the staggered finite difference scheme in time and space under a uniform spatial grid size $h = \triangle x = \triangle y = 0.025$. In addition, we choose a time step size $\triangle t$ of $h/3$, which satisfies the CFL condition (III.5) to guarantee the stability of the staggered finite difference scheme for equation (II.3). The first order backward and second order central finite differences in time and space, respectively, are used to discretize the energy $\mathcal{E}(t_n)$ of (II.4) at each time step t_n.

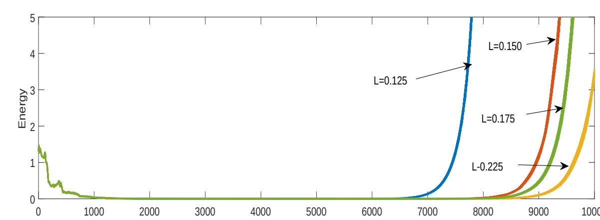

Fig. 2: $\mathcal{E}(t)$ when $\sigma_0 = 50, \beta = 0$ and various thicknesses L

We investigate the behavior of the energy for a long-time simulation at time $t_n = 10000$ according to the thickness of the layers and magnitude of the damping. The numerical results are displayed in Fig. 1 and 2: the energy for a fixed thickness $L = 0.125$ with various dampings $\sigma_0 = 30, 40, 50, 50, 60, 70$ (Fig. 1) and the energy for a fixed damping $\sigma_0 = 50$ with various thicknesses $L = 0.125, 0.15, 0.175, 0.225$ (Fig. 2). The results indicate that the numerical stability of the PML model is quite susceptible to both the thickness of the layers and magnitude of the damping, as noted in [27]. Furthermore, in the long-time simulation, one can observe that the wave energy unexpectedly and exponentially increase in the computational domain. These phenomena indirectly show that the stability argument of the energy developed by [18] is not clearly answered. Furthermore, the experiments indicate that the stability analysis [11] for the Cauchy problem for the model (II.3) is not sufficient.

The unexpected phenomena detailed above is likely to occur due to the non-physical auxiliary variable $\vec{q}$, or a lower regularity term $\nabla \cdot \vec{q}$ in the layers of the un-split PML model (II.3). This experiment makes it necessity to further develop the PML model, which is a motivation to the study.

III. Regularized System

Based on the motivation discussed in Section II, the aim of this section is to introduce a regularized system overcoming the instability that occurs in the classical PML model (II.3) for the acoustic wave equation (II.1).

Let $H^1(\Omega) = \{\varphi : \varphi, \partial_x\varphi, \partial_y\varphi \in L^2(\Omega)\}$ and $H^{-1}(\Omega)$ denote the Sobolev space and dual space of $H_0^1(\Omega)$, respectively. First, note that $\nabla \cdot \vec{q} \in H^{-1}(\Omega)$, which does not have a sufficient regularity so that the weak solution $(u, \vec{q})$ of (II.3) is included in $H_0^1(\Omega) \times \mathbb{L}^2(\Omega)$, where $\mathbb{L}^2(\Omega) := [L^2(\Omega)]^2$. To handle this problem of lower regularity, we define a linear bounded regularization operator δ_ε satisfying $\delta_\varepsilon \to \mathbf{1}$ as $\varepsilon \to \infty$ and $\|\delta_\varepsilon(\varphi)\|_{L^2(\Omega)} \le C_{\delta_\varepsilon}\|\varphi\|_{H^{-1}(\Omega)}$ for some $C_{\delta_\varepsilon} > 0$. Following [19], [22], we introduce a regularized system of the classical PML model (II.3) by using δ_ε in the term $\nabla \cdot \vec{q}$, which is given by, for $(\mathbf{x}, t) \in \Omega \times (0, T]$

$$\begin{cases} \dfrac{1}{c^2}u_{tt} + \alpha u_t + \beta u - \delta_\varepsilon \nabla \cdot \vec{q} - \Delta u = 0, \\ \vec{q}_t + A\vec{q} + B\nabla u = 0 \end{cases} \tag{III.1}$$

with initial and boundary conditions $u(\cdot, 0) := u_0$, $u_t(\cdot, 0) := u_1 = 0$, $\vec{q}(\cdot, 0) := \vec{q}_0 = \vec{0}$, $u(\mathbf{x}, \cdot)|_{\partial\Omega} = 0$. The remainder details the analysis of the well-posedness of the solution to the regularized system (III.1) based on the energy estimation under the assumption of the dampings σ_x, $\sigma_y \in L^\infty(\Omega)$.

A. Well-posedness of weak solution

We assume that the damping functions satisfy $\sigma_x, \sigma_y \in L^\infty(\Omega)$ and $c(\mathbf{x}) = 1$ in the layers of the PML model (II.3). Under these assumptions, we define the weak solution of (III.1) in the sense that $u \in L^2(0, T; H_0^1(\Omega))$, $\vec{q} \in L^2(0, T; \mathbb{L}^2(\Omega))$ with $u_t \in L^2(0, T; L^2(\Omega))$, $u_{tt} \in L^2(0, T; H^{-1}(\Omega))$, $\vec{q}_t \in L^2(0, T; \mathbb{L}^2(\Omega))$, which satisfies

$$\begin{cases} \left\langle \frac{1}{c^2}u_{tt}, w\right\rangle + (\alpha u_t + \beta u - \delta_\varepsilon \nabla \cdot \vec{q}, w) + (\nabla u, \nabla w) = 0, \\ (\vec{q}_t, \vec{v}) + (A\vec{q}, \vec{v}) + (B\nabla u, \vec{v}) = 0 \end{cases} \tag{III.2}$$

for each $w \in H_0^1(\Omega)$, $\vec{v} \in \mathbb{L}^2(\Omega)$, and almost everywhere $0 \le t \le T$ and the initial data satisfy $(u(0), w) = (u_0, w)$, $\langle u_t(0), w\rangle = (u_1, w)$, $(\vec{q}(0), \vec{v}) = (\vec{q}_0, \vec{v})$ for each $w \in H_0^1(\Omega)$, $\vec{v} \in \mathbb{L}^2(\Omega)$. Here, $\langle\cdot, \cdot\rangle$ denotes the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$, and $(\cdot, \cdot)$ is the inner product in $L^2(\Omega)$. In addition, the time derivatives are understood in a distributional sense. To investigate the weak solution of (III.1) that satisfies (III.2) with the initial condition, we can show the well-posedness of the regularized system (III.1) using the standard Galerkin approximation and estimate the energy of the solution. Let $\mathcal{U}_k$ be the subspace generated by the c^{-2}-weighted orthogonal basis of $H_0^1(\Omega)$ in the sense that

$$\left(c^{-2}w_j, w_k\right) + (\nabla w_j, \nabla w_k) = 0 \quad \text{if } j \ne k.$$

Let us also denote $\mathcal{Q}_k$, which is the space generated by the smooth functions $\{\vec{v}_1, \vec{v}_2, \cdots, \vec{v}_k\}$ such that $\{\vec{v}_k : k \in \mathbb{N}\}$ is an orthonormal basis of $\mathbb{L}^2(\Omega)$. We construct approximate solutions $\left(u^k, \vec{q}^k\right), k = 1, 2, 3, \cdots$, in the form

$$u^k(t) = \sum_{j=1}^{k} g_j^k(t)w_j, \qquad \vec{q}^k(t) = \sum_{j=1}^{k} h_j^k(t)\vec{v}_j, \tag{III.3}$$

whose coefficients $g_j^k(t),\ h_j^k(t),\ j = 1, 2, \cdots, k$, are chosen so that $g_j^k(0) = (u_0, w_j)$, $(g_j^k)_t(0) = (u_1, w_j)$, $h_j^k(0) = (\vec{q}_0, \vec{v}_j)$ and

$$\begin{cases} \left(\frac{1}{c^2}u_{tt}^k + \alpha u_t^k + \beta u^k - \delta_\varepsilon \nabla \cdot \vec{q}^k, w_j\right) + \left(\nabla u^k, \nabla w_j\right) = 0, \\ \left(\vec{q}_t^k, \vec{v}_j\right) + \left(A\vec{q}^k, \vec{v}_j\right) + \left(B\nabla u^k, \vec{v}_j\right) = 0 \end{cases} \tag{III.4}$$

are satisfied for all $w_j \in \mathcal{U}_k$, $\vec{v}_j \in \mathcal{Q}_k$, $j = 1, \cdots, k$. For each integer $k = 1, 2, \cdots$, the standard theory of ordinary differential equations guarantees the existence of the approximation $\left(u^k(t),\ \vec{q}^k(t)\right)$ satisfying (III.3) and (III.4). The following theorem gives a uniform bound of energy of the approximate solutions (III.3), which allows us to send $k \to \infty$.

Theorem 3.1: There exists a constant $C_T > 0$ that depends only on σ_x, σ_y, Ω, and T such that for $k \ge 1$

$$\max_{0\le t\le T} E_k(t) + \left\|u_{tt}^k\right\|_{L^2(0,T;H^{-1}(\Omega))} + \left\|\vec{q}_t^k\right\|_{L^2(0,T;\mathbb{L}^2(\Omega))} \le C_T\left(\|u_0\|_{H_0^1(\Omega)}^2 + \|u_1\|_{L^2(\Omega)}^2 + \|\vec{q}_0\|_{\mathbb{L}^2(\Omega)}^2\right),$$

where the energy $E_k(t)$ is defined by

$$E_k(t) = \|\frac{1}{c}u_t^k(t)\|_{L^2(\Omega)}^2 + \|\nabla u^k(t)\|_{\mathbb{L}^2(\Omega)}^2 + \|\vec{q}^k(t)\|_{\mathbb{L}^2(\Omega)}^2.$$

Passing to the limit from the bounds, we obtain the following theorem.

Theorem 3.2: (Existence and Uniqueness) Assume that the initial conditions $(u_0, u_1, \vec{q}_0) \in H_0^1(\Omega) \times L^2(\Omega) \times \mathbb{L}^2(\Omega)$. Then, the system (III.4) has a unique weak solution provided by $\sigma_x, \sigma_y \in L^\infty(\Omega)$. (see [19] for detail proof of uniqueness).

B. Numerical Scheme

For the staggered finite difference method, we use a family of finite difference schemes [21] with half-step staggered grids in space and time. All spatial derivatives are discretized with the centered finite differences over two or three cells, which guarantees a second order approximation in space. For the time discretization, we also use the centered finite differences for the first and second order time derivatives on a uniform mesh, which is also of the second order approximation in time. Based on the standard *von Neumann* stability analysis technique, we analyze the stability of the numerical scheme and obtain its CFL condition. To obtain the stability condition of the staggered finite difference scheme defined above, we restrict our concern to the constant damping case with $\sigma_x = \sigma_y = \sigma_0 \ge 0$ for simplicity in our analysis. The stability condition for the scheme in the computational domain is as follows.

Remark 3.3: The CFL condition of the staggered scheme in the computational area $(i.e., \sigma_x = \sigma_y = 0)$ is

$$c\frac{\triangle t}{h} \le \frac{1}{\sqrt{2}}$$

for $\triangle x = \triangle y = h$ from the standard *von Neumann* stability analysis technique.

Generally the stability condition for the staggered finite difference scheme can be obtained as follows.

Theorem 3.4: Assume that $\sigma_x = \sigma_y = \sigma_0 > 0$ and the sound speed c are constants. Then, the discrete scheme is stable if the CFL condition

$$c\triangle t \leq \frac{h}{\sqrt{2}} \frac{1}{(1+\frac{{\sigma_0}^2 h^2}{8c^2})^{1/2}} \tag{III.5}$$

is satisfied for $\triangle x = \triangle y = h$. (see [19] for detail proof)

IV. Numerical Result

The aim of this section is to provide numerical evidence of the well posedness of the regularized system and discuss the numerical stability in the long-time simulation for the staggered finite difference method. To do this, we demonstrate the behavior of the acoustic wave energy $\mathcal{E}(t)$ defined in (II.4) in the computational domain. For the numerical simulation, we use the same initial condition defined by (II.6) and, in the absorbing layer, the damping function of the form in (II.5). For the sound speed $c(x, y)$, we consider the constant form as well as variable sound speeds. For a comparison with the numerical results for the classical PML system (II.2), we first simulate the regularized system under the same conditions for the damping σ_0 with $\beta = 0$ and thickness L of the layers shown in Section II. The numerical results of formulae (II.2) and (III.1) are displayed in Fig. 3 and 4. As shown in the figures, it can be observed that the wave energy $\mathcal{E}(t)$ for the regularized system exhibits an outstanding stability performance in the long-time simulation independent of both the magnitude of the damping σ_0 and thickness L. For further investigation, using variable sound speeds, the nonconstant damping values of (II.4) with $\beta = 1, 2$, and the different magnitudes $\sigma_0 = 30, 50, 80$, we examine the long time behaviors of $\mathcal{E}(t)$ for formulae (II.2) and (III.1), and display the numerical results in Fig. 5. It can be observed that an unexpected and exponential growth of $\mathcal{E}(t)$ of the classical PML model occurs in the long time simulation, similar to the case of $\beta = 0$ shown in Section II. In contrast to the classical one, however, the wave energy $\mathcal{E}(t)$ of the regularized system are consistently stable in the long-time simulation regardless of the damping, thickness, and sound speed.

In summary, the regularized system demonstrates a good numerical stability performance in terms of the measure $\mathcal{E}(t)$ for a long-time simulation under the various damping, layer thickness, and sound speed values. This provides proof of the well-posedness of the developed system and numerical stability for the finite difference method. These numerical results show the extent to which the solution of the classical PML model is affected by the regularization $\delta_\epsilon \nabla \cdot \vec{q}$ for the divergence of the auxiliary variable $\vec{q}$, which has a lower regularity in $H^{-1}(\Omega)$. Contrary to the theoretical claim of [18], however, the classical PML model presents an instability of $\mathcal{E}(t)$, for certain damping and thickness values, which may come from the lower regularity of $\nabla \cdot \vec{q}$.

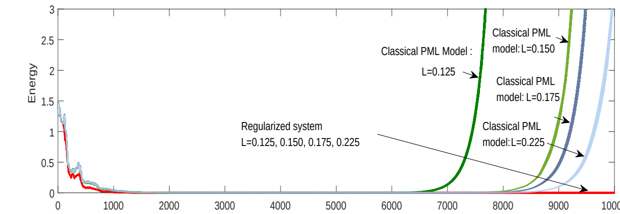

Fig. 3: $\mathcal{E}(t)$ when $\sigma_0 = 50, \beta = 0$ and various thickness L

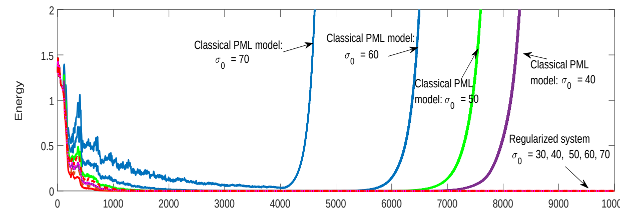

Fig. 4: $\mathcal{E}(t)$ when $L = 0.125, \beta = 0$ and various damping σ_0

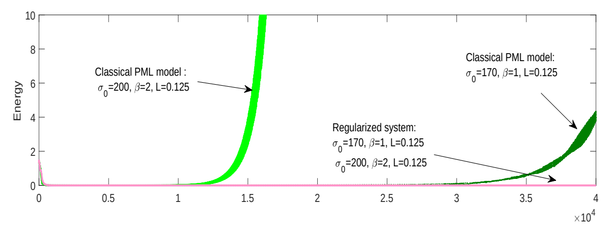

Fig. 5: $\mathcal{E}(t)$ when various damping values and variable sound speed

Conclusions

We have introduced a new and efficient formulation related to the acoustic wave equation based on the regularization of the un-split PML wave equation. By regularizing the lower order regularity term in the original equation and the standard *von Neumann* stability analysis, we have achieved well-posedness as well as numerical stability, even in the long-time simulation, of the solution in the new formulation. We have demonstrated the extent to which the regularization is important in the long time stability by several numerical tests. We summarize the main novelty and results of this study as follows: (1) We have proved the analytical well-posedness of our formulation without any restriction of damping terms; (2) several numerical tests suggest that the formulation exhibhits a long-time stability regardless of damping terms, layer thickness, and sound speeds; (3) we have demonstrated that the lower order regularity term in the up-split PML formulation highly affects the long-time stability; this is a strong motivation for the regularization.

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