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Lacunae based stabilization of PMLs

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Abstract

Perfectly matched layers (PMLs) are used for the numerical solution of wave propagation problems on unbounded regions. They surround the finite computational domain (obtained by truncation) and are designed to attenuate and completely absorb all the outgoing waves while producing no reflections from the interface between the domain and the layer. PMLs have demonstrated excellent performance for many applications. However, they have also been found prone to instabilities that manifest themselves when the simulation time is long. Hereafter, we propose a modification that stabilizes any PML applied to a hyperbolic partial differential equation/system that satisfies the Huygens' principle (such as the 3D d'Alembert equation or Maxwell's equations in vacuum). The modification makes use of the presence of lacunae in the corresponding solutions and allows us to establish a temporally uniform error bound for arbitrarily long-time intervals. At the same time, it does not change the original PML equations. Hence, the matching properties of the layer, as well as any other properties deemed important, are fully preserved. We also emphasize that besides the aforementioned PML instabilities per se, the methodology can be used to cure any other undesirable long-term computational phenomenon, such as the accuracy loss of low order absorbing boundary conditions.

Keywords: Perfectly matched layer (PML); Long-time stability; Weak well-posedness; Wave propagation; Hyperbolicity; The Huygens' principle; Lacunae; Maxwell's equations; Artificial boundary conditions (ABCs); Numerical solution

1. Introduction

Numerical solution of infinite-domain problems requires truncation of the unbounded domain for the purpose of constructing a finite-dimensional discretization. In doing so, one clearly needs to set some artificial boundary conditions (ABCs) at the outer boundary of the finite computational domain [1,2]. The ABCs shall provide a closure for the truncated formulation and guarantee that its solution will not differ much from the corresponding fragment of the original infinite-domain solution (ideally, will coincide with it).

For the problems of propagation of electromagnetic waves, a very efficient closure mechanism was introduced by Bérenger [3,4]. He proposed to surround the computational domain by a layer of artificial material

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capable of rapidly damping all the outgoing waves while generating no reflections from the interface between the domain and the layer, regardless of the wave's frequency or angle of incidence. It was called a perfectly matched layer (PML). The PML capabilities were attained in work [3,4] by splitting the field components, i.e., introducing additional unknowns and equations in the layer, and then using the resulting extra degrees of freedom for the development of an efficient waves' attenuation strategy. Subsequently, similar techniques were proposed for other wave propagation problems, such as acoustics [5] and elasticity. Note that the PML never alters the propagation speed as it would immediately create a scattering mechanism for the waves, it only reduces their amplitude.

It has also been noticed [6], however, that the Bérenger's split transforms the strongly hyperbolic (symmetric) Maxwell's equations into a weakly hyperbolic system, which, in turn, implies transition from strong well-posedness to weak well-posedness of the Cauchy problem [7].[1] A weakly well-posed system can become ill-posed under a low order perturbation, and an example of such a perturbation for the Bérenger's equations was given in [6]. Even though it has later been shown [9] that the actual form of the Bérenger's system does not lead to ill-posedness, the system still remains only weakly well-posed, *and a linear growth of the split field components inside the PML is possible*. This behavior may also lead to a purely numerical instability of the discretization. In particular, it has been proved in [6] that the very popular Yee scheme [10] becomes unconditionally unstable in the PML [3,4], with the powers of the amplification matrices growing linearly as the number of time steps increases.

From the standpoint of applications, the split field PML of [3,4] has demonstrated an overall excellent performance. However, concerns about its well-posedness and stability have prompted the development of other types of PMLs for computational electromagnetism [11–13] and other areas (e.g., acoustics [14]). These alternative strategies do not require splitting the field components in the PML, although they still introduce additional unknowns inside the layer. Later, however, *the unsplit PMLs have also been found susceptible to gradually developing instabilities [15]*. They have first been predicted theoretically and then *corroborated by the actual computations*, e.g., for the two-dimensional TE polarized Maxwell's equations [15]. A systematic experimental study of the long-time performance of unsplit PMLs with several commonly used explicit second order schemes has been conducted in our recent paper [16].

Note that if some components of the solution begin to grow inside the PML, the resulting numerical artifacts from the layer may or may not contaminate the computational domain, depending on the particular application and the design of the scheme. As mentioned, e.g., in [17], the Yee scheme can keep the instability inside the layer, whereas a higher order scheme of [15] propagates it back to the domain. As, however, has been noticed in [18], for the reason of improving the numerical performance on parallel platforms, a code that includes a split field PML is often designed in such a way that the equations solved inside the domain (not in the layer) are also split, although with no damping factors. In this case, even the Yee scheme appears capable of allowing the contamination from the layer into the domain.

An approach has been proposed in [15] to cure the long-time instability of unsplit PMLs. This approach is based on changing the governing equations in the layer. It has been experimentally shown to work well, but theoretically it is unclear whether the modified layer remains perfectly matched and absorbing.

Other remedies can also be found in the literature. For example, the non-linear PML of [19] guarantees boundedness of the energy integrals and strong well-posedness of the governing equations in the layer. However, its practical implementation requires a certain regularization to keep the denominators away from zero. Again, computationally it has been shown to perform well, but the analysis does not extend to this case. The complex frequency-shifted PML introduced in [20,21] and analyzed in detail in [17] also guarantees boundedness of the energy integrals and strong well-posedness.[2] However, the frequency shift in the PML leads to the loss of frequency independent absorption [17].

Altogether, the aforementioned stabilizing changes inside the PML often show no detrimental effect of any kind in the experiments, even when the supporting analysis is lacking. Moreover, according to a number of authors (see, e.g., [8]), the long-time instability of the PMLs may only have a limited negative effect in practical

[1] In fact, weak well-posedness characterizes all split field PMLs, see, e.g., [8].
[2] For the analysis of well-posedness see also [22].