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Absorbing boundary conditions for time harmonic wave propagation in discretized domains

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ABSTRACT

While many successful absorbing boundary conditions (ABCs) are developed to simulate wave propagation into unbounded domains, most of them ignore the effect of interior discretization and result in spurious reflections at the artificial boundary. We tackle this problem by developing ABCs directly for the discretized wave equation. Specifically, we show that the discrete system (mesh) can be stretched in a non-trivial way to preserve the discrete impedance at the interface. Similar to the perfectly matched layers (PML) for continuous wave equation, the stretch is designed to introduce dissipation in the exterior, resulting in a PML-type ABC for discrete media. The paper includes detailed formulation of the new discrete ABC, along with the illustration of its effectiveness over continuous ABCs with the help of error analysis and numerical experiments. For time-harmonic problems, the improvement over continuous ABCs is achieved without any computational overhead, leading to the conclusion that the discrete ABCs should be used in lieu of continuous ABCs.

1. Introduction

Many problems of wave propagation involve computing the solution in a finite region of an unbounded domain in an efficient way. The finite region of interest is usually called the *interior* and the rest of the unbounded domain is called the *exterior*. The problem is then finding an efficient way to model the effect of the exterior on the interior. In the absence of any sources in the exterior, the exterior absorbs energy entering the medium and does not emit any energy into the interior. Artificial boundary conditions developed to mimic this behavior are called absorbing boundary conditions (ABCs). Several successful boundary conditions have been proposed for this purpose. However, most of the ABCs are designed for the underlying continuous wave equation and do not consider the discretization of the interior, resulting in some spurious reflections. This paper presents a systematic derivation of ABCs that accurately considers the discretization of the interior, thus mitigating these reflections (we refer to these boundary conditions as *discrete ABCs*, while the boundary conditions derived for continuous equations are called *continuous ABCs*).

While discrete ABCs are more commonly considered for the Schrödinger equation (see, e.g. [1]), most of the work on ABCs for wave propagation has been in developing continuous ABCs (see, e.g. [2,3]). In what follows, we give a brief and non-exhaustive summary of existing methods, focusing on polygonal interiors (straight computational boundaries with corners).

1.1. The exact boundary condition

For the problem without any sources in the exterior, the exact boundary condition at the truncation boundary is written as a relation between the Dirichlet data and the Neumann data. The operator relating the Dirichlet data to the Neumann data is referred to as the *DtN map* or the *half-space stiffness* in the context of straight boundaries. Another commonly used term is the *characteristic impedance* which relates the velocity to the traction at the boundary. While the stiffness and impedance are different, there is a one-to-one mapping between the two and thus both terms are often used interchangeably. The DtN map in the continuous case can be derived using Fourier transform, while the discrete case requires the Z-transform. In both cases, however, the exact DtN map is non-local in space and time, and is prohibitively expensive. ABCs are essentially various tractable approximations of the exact boundary condition and can be classified based on the nature of the approximation. The major classifications are as follows.

1.2. Global or nonlocal ABCs

These methods rely on reducing the computational cost by truncating the extent of non-local coupling in space and convolution in time. However, accurate simulation requires rather long-range coupling in space and/or time and the computation is expensive even after such truncation. A review of the various methods

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can be found in [2] for continuous case, and [1] for the discrete case in the context of the Schrödinger equation. Furthermore, global ABCs usually require the knowledge of the analytic form of the DtN map. Although in some cases the DtN map can be numerically approximated (see, e.g. [4] for continuous waves and [5–7] for discrete waves) it is in general expensive and cannot easily handle geometric complexities such as corners.

1.3. Rational ABCs

Originally introduced independently by Lindman [8] and Engquist and Majda [9], this class of continuous ABCs approximate the exact DtN map, which is a pseudo-differential operator, using rational functions to derive local ABCs in a differential form. Also worth noting are the ABCs developed by Higdon [10]; albeit coming from a different viewpoint of multi-directional absorption of waves, Higdon showed that his ABCs are generalizations of the ABCs of Lindman and Engquist–Majda. While the theoretical development has been done decades back, the implementation of high-order versions of these boundary conditions were only developed relatively recently (see, e.g. [11]). With respect to discrete systems, rational absorbing boundary conditions and related ideas have been explored in [12,13], and more recently in [14]. The development of these discrete ABCs are relatively less mature compared to continuous ABCs and treatment of corner regions is an important open question.

1.4. Perfectly matched layers (PML)

The PML, also a continuous ABC, involves replacing the exterior with an attenuating medium (PML region) that perfectly matches in impedance with the interior [15], and truncated at some distance. Due to the perfect matching of impedance, there are no reflections at the interface, and due to attenuation in the PML region, the reflection due to truncation is minimal. PML is a widely used continuous ABC due to its flexibility and generality. However, it has been recently shown that PML may not be as efficient as rational ABCs [16,17]. While extension of PML to discrete systems exist [18], these do not preserve the perfect matching property of PML. In Remark 4 (Section 3), we explain briefly the loss of perfect matching when coordinate stretching is applied in a direct manner.

1.5. Perfectly matched discrete layers (PMDL)

Our research on ABCs has resulted in a class of continuous ABCs called perfectly matched discrete layers (PMDL) that link PML to rational ABCs. Essentially, PMDL is a specially discretized PML that is equivalent to rational ABCs. Specifically, PMDL is a PML discretized using linear finite elements with midpoint integration [19]. It has been shown that, *with respect to approximating the DtN map*, the error due to midpoint integration exactly cancels the discretization error, thus resulting in perfect matching even after the discretization of the exterior (hence the name, perfectly matched discrete layers – PMDL). The only error in the DtN map is due to the truncation of PMDL, which converges to zero exponentially as the number of layers increases. PMDL is shown to be algebraically equivalent to rational ABCs and can be considered an efficient way to implement rational ABCs (in fact, initial development of PMDL started as an efficient implementation of rational ABCs [20]). Given its close links to PML and rational ABCs, PMDL can be considered as a unification of PML and rational ABCs, thus inheriting their respective advantages of flexibility and efficiency. Notwithstanding these attractive features, most of the PMDL development has been largely limited to continuous wave equations.

Motivated by molecular dynamics applications, we recently proposed an extension of PMDL [21] for the semi-discrete (discrete in space) wave equation in time domain. In this paper, we apply the discrete PMDL for the discretized Helmholtz equation and claim that discrete PMDL is a better choice than continuous ABCs. Note that discrete PMDL contains two *discrete*'s in its name (when expanded). The first *discrete* refers to the fact that the PMDL is designed for discrete interiors and thus considers the discretization error in the interior. The second *discrete* refers to the exterior discretization that preserves the perfect matching (thus called perfectly matched discrete layers – PMDL).

The proposed discrete PMDL is based on the observation that, just like in the case of continuous PML, there exist a class of exteriors, both continuous and discrete, which have the same DtN map as uniformly discretized half-space but different propagation characteristics. These equivalent exteriors include semi-infinite meshes of non-uniform and arbitrary lengths. Similar to the original development of PMDL, the flexibility in choosing arbitrary lengths allows the use of complex coordinate stretching ideas of PML to damp out propagating waves and large real elements to damp out evanescent waves [22,19]. Since the waves are damped out in the exterior, the exterior can be truncated depending on the required accuracy in the interior. Given that the proposed discrete PMDL is perfectly matched with discretized interiors, as expected, it is shown to be more accurate than the continuous PMDL. Furthermore, the computational costs of continuous and discrete PMDL are comparable, leading us to advocate the use of discrete PMDL as the ABC for numerical simulations in frequency domain.

The rest of the paper contains more precise formulation of the proposed discrete PMDL. Section 2 lays down the details of continuous and discrete wave equations, both with respect to solution behavior and ABCs. Section 3 outlines the basic intuition that triggered the current development and an argument that continuous ABCs can be modified to work for discrete systems. Given that the this paper extends PMDL to discrete wave equations, the continuous PMDL is briefly reviewed in Section 4. A detailed procedure to extend PMDL to discrete systems in 1-D is presentation in Section 5. Section 6 contains the extension of the 1-D formulation for 2-D rectangular mesh, along with some comments related to extension to non-rectangular and higher order meshes. The paper is concluded with closing remarks in Section 7.

2. Preliminaries

2.1. Model problem

Consider the propagation of a wave in full-space, $x \in (-\infty, \infty)$ (Fig. 1a), and assume that we are interested in the solution in the left half-space, $x \in (-\infty, 0)$, when there are no sources in the right half-space. The usual procedure to solve such a problem is to break the full-space into left and right half-spaces and replace the right half-space by applying an absorbing boundary condition (ABC) at the interface $x = 0$ (Fig. 1b). The problem can now be solved using a numerical method like the finite element method (FEM), which involves discretizing the left half-space. However, once the left half-space is discretized, we now have two different systems at the interface (Fig. 1c): a discrete half-space on the left and a continuous half-space on the right (mimicked by the ABC). Since a change in medium leads to reflections at the interface, this treatment of the right half-space is not ideal. The ideal way to handle the problem is to consider the propagation in a discrete full-space (Fig. 1d) and then replace the right half-space with a Discrete ABC that captures the discreteness of the medium (Fig. 1e). Thus, we seek a way to develop ABCs for a discrete half-space.

Before discussing the proposed method, we first present the governing equations and some basic definitions that will be used in the rest of the paper. For simplicity, we consider the 1-D case first and extend the ideas to higher dimensions in Section 6.