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APPROXIMATION, STABILITY AND FAST EVALUATION OF EXACT ARTIFICIAL BOUNDARY CONDITION FOR THE ONE-DIMENSIONAL HEAT EQUATION*

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Abstract

In this paper we consider the numerical solution of the one-dimensional heat equation on unbounded domains. First an exact semi-discrete artificial boundary condition is derived by discretizing the time variable with the Crank-Nicolson method. The semi-discretized heat equation equipped with this boundary condition is then proved to be unconditionally stable, and its solution is shown to have second-order accuracy. In order to reduce the computational cost, we develop a new fast evaluation method for the convolution operation involved in the exact semi-discrete artificial boundary condition. A great advantage of this method is that the unconditional stability held by the semi-discretized heat equation is preserved. An error estimate is also given to show the dependence of numerical errors on the time step and the approximation accuracy of the convolution kernel. Finally, a simple numerical example is presented to validate the theoretical results.

Mathematics subject classification: 65N12, 65M12, 26A33.
Key words: Heat equation, Artificial boundary conditions, Fast evaluation, Unbounded domains.

1. Introduction

There are a large number of problems modeled by partial differential equations defined on unbounded domains. When numerically solving this kind of problems, a common practice is to limit the computation to a finite domain by introducing artificial boundaries. To make complete the "truncated" problem on the finite domain, artificial boundary conditions (ABCs) should be designed and applied. They are called exact if the solution of the truncated problem is exactly the same as that of the original problem on the unbounded domain. ABCs were first derived by Engquist and Majda [8] for hyperbolic systems. Since then, their idea has been extended and refined for numerous applications. Givoli [10] and Tsynkov [20] made thorough reviews on this topic.

This paper is concerned with the numerical issues related to the heat equation on one-dimensional unbounded domains. Much attention has been paid on the numerical solution to the Schrödinger equation, both linear [1, 2, 4, 6, 13, 15, 21] and nonlinear [3, 23]. Comparatively, the attention paid on the heat equation is much less [12, 14, 19, 22]. Actually, these two equations share many similarities. One lies in the fact that for one-dimensional problems on unbounded domains, both their exact ABCs (in a form of Dirichlet-to-Neumann mapping) involve the nonlocal half-order derivative operator. To well understand these two equations with exact ABCs, a key point is to explore the properties of this operator. Correspondingly, to

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well resolve their solutions numerically, a key point is to approximate the half-order derivative operator by an efficient and stable method.

So far, there are two different numerical methods for evaluating this half-order derivative operator. The first one was proposed by Baskakov and Popov [6]. They approximated the integrands with piecewise linear interpolating functions at the discrete time points. This idea presents a 1.5th-order approximation to the half-order derivative operator, but its generalization has to be very careful. Mayfield [18] showed that even cooperated with the classical unconditionally stable Crank-Nicolson scheme for the interior discretization of the Schrödinger equation, this idea adapted for the exact ABCs in the Neumann-to-Dirichlet form can only guarantee the stability on some disjoined intervals of $\Delta t/\Delta x^2$ (Δt is the time step, and Δx the spatial step). Comparatively, when cooperated with a delicately designed finite difference scheme for the heat equation, Wu and Sun [22] proved the unconditional stability. Another idea to approximate the half-order derivative operator was proposed by Yevick et. al [21], Antoine and Besse [2]. The starting point is the semi-discretization of time variable with the Crank-Nicolson method for the Schrödinger equation on the whole space. By using the $\mathcal{Z}$-transform, an exact semi-discrete ABC is then derived. There are two highlights about this method. First, it presents an approximation of second-order accuracy for the half-order derivative operator, which is more accurate than the direct integration method. Second, the reduced problem with this semi-discrete ABC is unconditionally stable. Moreover, if a conforming Galerkin method is employed for the spatial discretization, this stability is automatically maintained.

No matter which method is employed, the approximate discrete half-order derivative operator involves convolution operations. If the number of time steps is large, these operations become very costly, which justifies the use of fast evaluation methods. Two candidates have been appeared in the literature. The first one was proposed by Jiang and Greengard [15]. They divided the convolution into a local part and a history part. The local part is approximated with the Baskakov-Popov method, while the history part is approximated by a sum of convolutions with decaying exponential kernels, thus fast evaluation is straightforward. The second method was given by Arnold et. al [5]. Based on their discrete transparent boundary conditions, they approximated convolution coefficients with a sum of exponentials directly. These exponentials were determined by equating a number of elements with their corresponding convolution coefficients. Both of these two methods work well for some problems, as their numerical tests demonstrated, but up to now, neither of them can ensure stability in a rigorous mathematical way.

In this paper, following the idea of [2, 21], we will derive the exact semi-discrete ABC for the one-dimensional heat equation. Stability of the reduced problem will be proved, and we will show that this semi-discrete approximation is of second-order accuracy, which is superior to the scheme proposed by Wu and Sun [22]. A new fast evaluation method will be proposed for the half-order derivative operator. We will rigorously prove its stability and present an error estimate which shows the dependence of numerical error on the time step and the approximating accuracy of the convolution kernel.

2. Preliminary

The $\mathcal{Z}$-transform of a complex sequence $\mathbf{f} = \{f_0, f_1, \cdots\}$ is defined as the power series

$$\mathcal{Z}\{\mathbf{f}\}(z) = \sum_{n=0}^{+\infty} f_n z^{-n}. \tag{2.1}$$