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A GPU-Accelerated Cartesian Grid Method for the Heat, Wave and Schrödinger Equations on Irregular Domains

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Abstract. Based on Ying's kernel-free boundary integral (KFBI) method [1], a second-order method for general elliptic partial differential equations (PDEs), this paper develops a GPU-accelerated KFBI method for the heat, wave and Schrödinger equations on the irregular domain. Since the limitation of time steps imposed by CFL conditions in the explicit scheme and the inadequate accuracy generated by the fully implicit scheme for the Laplacian operator, the paper selects a series of second-order time discrete schemes, and the Laplacian operator is split into explicit and implicit mixed ones. The Crank-Nicolson method is used to discretize the heat equation in temporal dimension while the implicit θ-scheme is for the wave equation. The Strang splitting method is applied to the Schrödinger equation. After discretizing the temporal dimension implicitly, the heat, wave and Schrödinger equations are transformed into a sequence of elliptic equations. The Laplacian operator on the right-hand side of the elliptic equation is obtained from the numerical scheme instead of being discretized and corrected by the five-point difference method. A Cartesian grid-based KFBI method is used to solve the resulting elliptic equations. The KFBI method is accelerated by the graphics processing unit (GPU) with a parallel Cartesian grid solver, achieving a high degree of parallelism. Numerical results show that the proposed method has a second-order accuracy for the heat, wave, and Schrödinger equations. Additionally, the GPU-accelerated solvers for the three types of time-dependent equations are 30 times faster than CPU-based solvers.

AMS subject classifications: 65M80

Key words: GPU-accelerated kernel-free boundary integral method, time discretization scheme, irregular domains.

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1 Introduction

The heat, wave, and Schrödinger equations encountered many scientific and engineering applications. Examples include biological systems and option pricing associated with the heat equation [2–5], electromagnetic wave propagation and underwater acoustics related to the wave equations [6–8], and quantum mechanics issues associated with the Schrödinger equation [3, 4, 9, 10]. Over the past few decades, there have been extensive studies in numerical methods for those three types of time-dependent PDEs, including the finite element method [11, 12], the finite difference method [13, 14], the pseudo-spectral method [15] and the boundary integral method (BIM) [16, 17]. The primary purpose of this work is to present an efficient GPU-accelerated and second-order accurate kernel-free boundary integral (KFBI) method combined with an implicit time discretization scheme as an alternative for the approaches above in solving the heat, wave and Schrödinger equations.

One can distinguish three approaches of BIM to the application of the heat, wave and Schrödinger problems, space-time boundary integral equation methods [17–20], Laplace-transform methods [17–21], and time-stepping methods [16, 17, 20, 22, 23]. For the space-time boundary integral method, the original equation is reformed as a space-time boundary integral equation by Green's third identity, then the boundary element method (BEM) [24], Galerkin method [25] and collocation method [26] can be applied to solve the space-time boundary integral equation. Remarkably, because the numerical methods constructed from these space-time boundary integral equations are global in time, the solution can be obtained in one step for the entire time interval [20]. However, the difficulty of obtaining Green's functions for general domains and the high cost of solving the large discrete system matrix and higher-dimensional integrals prevent it from becoming a universal method [20]. For the Laplace transform method, the primal problem is transformed to an elliptic boundary value problems in the frequency domain with an eigenvalue parameter λ depending on the frequency ω by taking the Laplace transform of the variable. Then the elliptic boundary value problems in the finite frequency domain are solved by the BIM. Finally, the solution in the frequency domain space is converted back to the time domain space through the inverse Laplace transform. Due to the good characteristics of the Laplacian operator, this method's solution process is relatively simple [27]. However, there will be some ω_l with large absolute value, which means large negative real parts for $\lambda(\omega_l)$ [20]. An alternative to solving the three types of time-dependent equations is first to discretize the temporal dimension by an implicit scheme, then solve the resulting elliptic equations for each time step by boundary integral method. Significantly, a careful treatment of time discretization and spatial discretization at each time step is of utmost importance to ensure the long-term numerical stability of the discrete scheme.

Since the hyperbolicity of wave and Schrödinger equations, it is expected that the discrete schemes employed in time-stepping methods respect the dissipative properties enjoyed by the original systems. Structure-preserving algorithms are achieved by con-