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A GPU-Accelerated Cartesian Grid Method for PDEs on Irregular Domain

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Abstract. The kernel-free boundary integral (KFBI) method has successfully solved partial differential equations (PDEs) on irregular domains. Diverging from traditional boundary integral methods, the computation of boundary integrals in KFBI is executed through the resolution of equivalent simple interface problems on Cartesian grids, utilizing fast algorithms. While existing implementations of KFBI methods predominantly utilize CPU platforms, GPU architecture's superior computational capabilities and extensive memory bandwidth offer an efficient resolution to computational bottlenecks. This paper delineates the algorithms adapted for both single-GPU and multiple-GPU applications. On a single GPU, assigning individual threads can control correction, interpolation, and jump calculations. The algorithm is expanded to multiple GPUs to enhance the processing of larger-scale problems. The arrowhead decomposition method is employed in multiple-GPU settings, ensuring optimal computational efficiency and load balancing. Numerical examples show that the proposed algorithm is second-order accurate and efficient. Single-GPU solver runs 50-200 times faster than traditional CPU, and the parallel efficiency of a multiple-GPU distributed solver within the same NUMA node reaches up to 80%.

AMS subject classifications: 65M80

Key words: GPU-accelerated kernel-free boundary integral method, GPU parallel computing, arrowhead decomposition method, irregular domains.

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1 Introduction

Graphics Processing Units (GPU) are co-processors originally devoted to accelerate graphics processing. In the last years, they are extensively used as massively parallel platforms to run general-purpose programs. This practice is mostly known as General-Purpose computing on Graphics Processing Units (GPGPU). This growing trend is confirmed by the number of computers in the top500 ranking that are provided of GPUs, which on November 2023 was 186 [1].

One of the areas taking advantage of the capabilities of this kind of accelerators is scientific computing. There are many recent publications describing works that successfully port code from CPU to GPU, achieving significant speedups [2, 3]. Elliptic type problems are widely applied in the fields of electrochemistry [4,5], electromagnetism [6], computational fluid dynamics [7, 8], shape optimisation problems [9, 10] and other areas in science [11–14], Solving these problems often requires a substantial computational cost [15].

An effective and accurate approach for solving elliptical PDEs is the kernel-free boundary integral (KFBI) method [16–18], which originates from boundary integral methods. Unlike traditional boundary integral approaches, the KFBI method embeds complex domains into larger, regular computational areas (such as square regions), which are subsequently partitioned using Cartesian grids. The KFBI method not only benefits from the well-conditioning property of the boundary integral equation(BIE) but also avoids explicitly calculating Green's function directly, which is challenging in complex domains [17,19]. In recent years, the KFBI method has been extensively applied [19–23].

The substantial memory bandwidth and abundant cores in GPU architecture enable the concurrent execution of thousands of computational tasks, leading to significant acceleration. This renders it an efficient solution for addressing computing bottlenecks. More importantly, the GPU architecture suits the Cartesian grid method since each thread easily controls one grid node. Several related works have addressed the GPU acceleration of Cartesian grid methods in the last ten years [24–27]: the GPU-accelerated VOF by Rajesh Reddy and R. Banerjee [24], the CUDA-Based IB method by S. K. Layton, A. Krishnan and L. A. Barba [25], the TVD Runge–Kutta method on multiple GPUs by S. Liang, W. Liu and L. Yuan [26], the multiple-GPU based lattice Boltzmann algorithm by C. Huang, B. Shi, N. He and Z. Chai [27].

As a Cartesian grid method, the critical procedure of the KFBI method involves correction at irregular points and control points on the interface individually, making it inherently well-suited for GPU-accelerated parallel processing. Furthermore, the KFBI method utilizes an FFT-based solver, well-documented in literature for its suitability with GPU or GPU clusters [28–32], to enhance the efficiency of interface problem computations in iterative procedures. In fact, due to the simple grid topology on Cartesian grids, building a highly parallel GPU-accelerated Cartesian grid solver based on the KFBI method is straightforward. The implementation details of the KFBI solver for a single-GPU version are concisely delineated in Section 3, with the corresponding numerical results presented