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A Highly Scalable Boundary Integral Equation and Walk-On-Spheres (BIE-WOS) Method for the Laplace Equation with Dirichlet Data

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Abstract. In this paper, we study a highly scalable communication-free parallel domain boundary decomposition algorithm for the Laplace equation based on a hybrid method combining boundary integral equations and walk-on-spheres (BIE-WOS) method, which provides a numerical approximation of the Dirichlet-to-Neumann (DtN) mapping for the Laplace equation. The BIE-WOS is a local method on the boundary of the domain and does not require a structured mesh, and only needs a covering of the domain boundary by patches and a local mesh for each patch for a local BIE. A new version of the BIE-WOS method with second kind integral equations is introduced for better error controls. The effect of errors from the Feynman-Kac formula based path integral WOS method on the overall accuracy of the BIE-WOS method is analyzed for the BIEs, especially in the calculation of the right hand sides of the BIEs. For the special case of flat patches, it is shown that the second kind integral equation of BIE-WOS method can be simplified where the local BIE solutions can be given in closed forms. A key advantage of the parallel BIE-WOS method is the absence of communications during the computation of the DtN mapping on individual patches of the boundary, resulting in a complete independent computation using a large number of cluster nodes. In addition, the BIE-WOS has an intrinsic capability of fault tolerance for exascale computations. The nearly linear scalability of the parallel BIE-WOS method on a large-scale cluster with 6400 CPU cores is verified for computing the DtN mapping of exterior Laplace problems with Dirichlet data for several domains.

AMS subject classifications: 65C05, 65N99, 78M25, 92C45

Key words: Dirichlet-to-Neumann (DtN) mapping, meshless methods, parallel BIE-WOS method, Monte Carlo method, walk-on-spheres (WOS), boundary integral equations, Laplace equation, Dirichlet problem.

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1 Introduction

The prevalence of many-core teraflops computing platforms makes scalability the principal concerns for developing new numerical algorithms for solving Laplace and Helmholtz equations, encountered in many engineering and scientific problems. Capacitance extractions of very large scale integral (VLSI) circuits in a full-chip, for example, solve the Laplace equation with Dirichlet boundary conditions in an extremely large scale. Boundary element methods (BEMs) or finite element methods (FEMs), widely used in capacitance extractions of VLSI circuits [2–7], are highly accurate and versatile, however, belonging to the deterministic and global methods, which need expensive surface or volume mesh generations of whole domains. Moreover, high scalability of BEMs and FEMs on millions of CPU cores is challenging in storing and solving large linear systems, prompting many research works [8, 9].

Random methods, based on Feynman-Kac probabilistic formula for the solutions, however, can offer local solutions of the Laplace equation [1,10–12] as well as natural parallelism. Potentials or charge densities are expressed as a weighted average of boundary Dirichlet data visited by multiple Brownian motion paths, sampled efficiently with the walk-on-spheres (WOS) method [23]. In fact, the industrial golden capacitance extraction tool QuickCap NX [13] is a practical example of such random methods [14, 15].

However, a naive application of the Feynman-Kac formula for the Dirichlet data is not applicable for an efficient calculation of the Neumann data on the boundary, as the Dirichlet boundary will absorb quickly the random particles starting near the boundary. To overcome such a drawback, we combined a deterministic boundary integral equation (BIE) and the probabilistic Feynman-Kac formula based walk-on-spheres (WOS) method, termed BIE-WOS [1], which allows us to compute the Neumann data over local patches of the domain boundary efficiently, while still maintaining the merit of natural parallelism of random methods. The BIE-WOS superimposes a hemisphere intersected with the boundary of interest and sets a local BIE over the subdomain enclosed by a part of the hemisphere and the intersected boundary. Using a homogeneous Green's function of a sphere results in the BIE involving only Dirichlet data over the hemisphere, which can be calculated by WOS algorithms. With the given Dirichlet data and unknown Neumann data on the patch surface, collocation methods can be employed to solve the integral equations on the aforementioned patch surface to yield the required Neumann data.

In this paper, we will present a new version of BIE-WOS with a well-conditioned integral equation of second kind (IESK), which has a much better error control related to the computation of the right hand side by the Feynman-Kac based WOS method. With the new IESK BIE-WOS, a highly scalable communication-free boundary domain decomposition BIE-WOS scheme is developed for the Laplace equation with Dirichlet data. The main highlights of this paper are summarized as follows. (1) First, we exam the original BIE-WOS method [1], which uses the integral equation of first kind (IEFK), even with its well-known ill-conditioned issue in the resulting linear systems, still much used in practice due to its simplicity. In fact, the first kind integral equation is still widely used in