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A p-Adaptive Treecode Solution of the Poisson Equation in the General Domain

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Abstract. Raising the order of the multipole expansion is a feasible approach for improving the accuracy of the treecode algorithm. However, a uniform order for the expansion would result in the inefficiency of the implementation, especially when the kernel function is singular. In this paper, a p-adaptive treecode algorithm is designed to resolve the efficiency issue for problems defined on a general domain. Such a p-adaptive method is realized through i). conducting a systematical error analysis for the treecode algorithm, ii). designing a strategy for a non-uniform distribution of the order of multipole expansion towards a given error tolerance, and iii). employing a hierarchy geometry tree structure for coding the algorithm. The proposed p-adaptive treecode algorithm is validated by a number of numerical experiments, from which the desired performance is observed successfully, i.e., the computational complexity is reduced dramatically compared with the uniform order case, making our algorithm a competitive one for bottleneck problems such as the demagnetizing field calculation in computational micromagnetics.

AMS subject classifications: 65D30, 35A08

Key words: Treecode, p-adaptive method, hierarchy geometry tree, Poisson equation.

1 Introduction

The solution of Poisson equation is a critical task in many fields of science and engineering from quantum physics and chemistry to materials science and biology [15, 21, 27]. In these fields, problems such as the computation of the demagnetizing field in micromagnetism and the computation of Hartree potential in quantum physics often require a fast and accurate solution of Poisson equation. However, the use of direct numerical

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integration methods to compute the fundamental solution of the Poisson equation with long-range interactions leads to a computational complexity of $\mathcal{O}(N^2)$, where N is the number of mesh elements in computational domain Ω. When N is large, this complexity is unacceptable.

To address this issue, a series of fast algorithms have been proposed as potential solutions to the Poisson equation, including Multigrid method [25], Finite Element Method (FEM) [17], Fast Fourier Transform (FFT) [29], nonuniform fast Fourier transform (NUFFT) [11], treecode algorithm [7,8], and the Fast Multipole Method (FMM) [10], etc. These algorithms reduce the complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(N\log N)$ even $\mathcal{O}(N)$, respectively. While both the multigrid method and FEM are very efficient in solving the Poisson equation, approximation of boundary values with an integral form by direct summation is an $\mathcal{O}(N^{4/3})$ operation in three dimensions, such as the calculation of the demagnetizing field in the Landau-Lifshitz-Gilbert (LLG) equation [30,31]. In addition, FFT is an efficient solver for Poisson equation based on the potential theory with complexity of $\mathcal{O}(N\log N)$ but is limited to regular computational domains, such as rectangular grids and periodic boundary conditions. In practical applications, computational domains are often complex and irregular, such as when simulating dynamic magnetization in ferromagnetic materials with defects [6]. NUFFT is easy to deal with irregular domain, but the accuracy of this approach is hampered due to the singularity in the interaction kernel, such as 3D Coulomb interaction. Therefore, a high-order discretization by generalized Gaussian quadrature [20] or coordinate transform [2,13] has to be used for canceling the singularity, which unavoidably adds some computational costs. Treecode is a competitive one for problems defined in complex domain with $\mathcal{O}(N\log N)$, and FMM is even better due to its optimal computational complexity $\mathcal{O}(N)$. However, in parallel environment, due to the translation method used in FMM, the two method, treecode and FMM, are comparable [32]. In addition to these fast algorithms, there are a number of h-adaptive techniques that have also been used for the acceleration of the long-range interaction problem, for details please refer to [28,34].

There is a challenge for solving Poisson equation based on the potential theory, where singularity is encountered in modeling a variety of problems. One of the typical cases is the Coulomb interaction arising in Schrödinger equation and Kohn–Sham equation [3,14,23]. Dipole-dipole interactions with same or different dipole orientation arises in quantum chemistry, dipolar Bose-Einstein condensation, etc. [1,12,16]. As a result, an accurate quadrature has to be used in order to handle the singularity of kernel function. However, a direct use of the standard FFT or NUFFT, a phenomenon know as "numerical locking" occurs, limiting the achievable precision [26]. The treecode originally approximate the interaction with low expansion for efficiency. In addition to the accuracy issue, the approximation of the treecode algorithm lacks global continuity, which leads to energy drift when the order in multipole expansion is low, such as in molecular dynamics simulations [4,22,24].

Uniformly increasing the expansion order improves the accuracy and stability of the treecode algorithm but incurs a computational cost of $\mathcal{O}(p^3)$, where p is the expansion