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A Linear Scaling in Accuracy Numerical Method for Computing the Electrostatic Forces in the N-Body Dielectric Spheres Problem

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Abstract. This article deals with the efficient and accurate computation of the electrostatic forces between charged, spherical dielectric particles undergoing mutual polarisation. We use the spectral Galerkin boundary integral equation framework developed by Lindgren et al. (J. Comput. Phys. 371 (2018): 712-731) and subsequently analysed in two earlier contributions of the authors to propose a linear scaling in cost algorithm for the computation of the approximate forces. We establish exponential convergence of the method and derive error estimates for the approximate forces that do not explicitly depend on the number of dielectric particles N. Consequently, the proposed method requires only $\mathcal{O}(N)$ operations to compute the electrostatic forces acting on N dielectric particles up to any given and fixed relative error.

AMS subject classifications: 65N12, 65N15, 65N35, 65R20

Key words: Boundary integral equations, error analysis, N-body problem, linear scaling, polarisation, forces.

1 Introduction

Predicting the motion of a large number of objects interacting under the influence of a potential field, commonly known as the N-body problem, is one of the most well-known problems of classical physics. The N-body problem first arose due to the desire of astronomers to explain the motion of celestial objects interacting due to gravity [54, 57] but the problem is also ubiquitous in physical phenomena involving large-scale electrostatic interactions. Thus, understanding the behaviour of charged colloidal particles (see, e.g., [5, 17, 35, 41, 52, 53]) or the fabrication of binary nanoparticle superlattices and

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so-called Coulombic crystals (see, e.g., [7, 10, 29, 37, 50, 60, 65]), or the assembly of proteins and other cellular structures (see, e.g., [18,20,56,63,68,71]) all require knowledge of Coulomb interactions between a large number of physical objects.

Many such electrostatic phenomena involve interactions between charged, spherical dielectric particles embedded in a dielectric medium, undergoing mutual polarisation. One is then typically interested in either the total electrostatic energy of the system or the electrostatic force acting on each particle, both of which can be derived from knowledge of the electric potential generated by these particles. Knowledge of the forces in particular is required if one wishes to perform molecular dynamics simulations or study assembly processes of charged particles (see, e.g., [15,40,58,72] as well as the references on superlattices given above). In contrast to the much simpler case of point-charges however, a full description of the electric potential generated by such polarisable particles cannot be obtained as simply the sum of pairwise interactions. Instead, the potential is realised as the solution to a PDE, posed on the full three-dimensional space with interface conditions on the boundaries of the spherical particles (see, e.g., [10,31,43]). Since this PDE cannot generally be solved analytically, it becomes necessary to use some numerical method to first compute the *approximate* electric potential and then use this to obtain *approximations* to either the total energy or the force acting on each particle. It is therefore of great interest to develop efficient numerical algorithms that can yield approximations to the energy and the forces with theoretically quantifiable error estimates.

A number of different approaches to this so-called *N-body dielectric spheres electrostatic interaction* problem have been proposed in the literature (see, e.g., [6, 14, 23, 46, 48, 53, 59, 70]). Unfortunately, many of these methods suffer from the handicap that they may become computationally prohibitive if the number of particles is very large. Additionally, these method have typically been formulated in a manner that makes them unsuitable for a systematic numerical analysis. As a consequence, it is usually not possible to theoretically evaluate the accuracy of these methods and, in particular, to explore the dependence of the accuracy on the number of dielectric particles N. These drawbacks are particularly regrettable since the quality of an N-body numerical method is assessed precisely by considering how the accuracy and computational cost of the algorithm scale with N. Indeed, given a family of geometrical configurations with varying number of dielectric spheres N, using the terminology stated in [11]:

- We say that an N-body numerical method is *N-error stable* if, for a fixed number of degrees of freedom per object, the relative or average error in the approximate solution for different geometrical configurations does not increase with N.
- We say that an N-body numerical method is *linear scaling in cost* if, given a geometrical configuration with N spheres and for a fixed number of degrees of freedom per object, the numerical method requires $\mathcal{O}(N)$ operations to compute an approximate solution with a given and fixed tolerance.
- Finally, we say that an N-body numerical method is *linear scaling in accuracy* if it is both N-error stable and linear scaling in cost.