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On the Numerical Analysis of a Linear Scaling Numerical Method for the N-body Dielectric Spheres Problem

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Many phenomena in chemical physics involve calculating the electrostatic interaction between charged dielectric particles embedded in a polarisable continuum undergoing mutual polarisation. In order to tackle this problem, E. Lindgren et al. (J. Comput. Phys. 371 (2018): 712-731) have proposed a numerical method based on a Galerkin discretisation of a boundary integral equation (BIE) of the second kind. The proposed method is general enough to treat any homogeneous dielectric medium containing an arbitrary number of spherical particles of any size, charge, dielectric constant and position in three-dimensional space. Furthermore, numerical experiments indicate that the algorithmic complexity of the method scales linearly with respect to the number of particles thanks to the use of a modified Fast Multipole Method (FMM).

The current talk will present results on the numerical analysis of this algorithm with a focus on proving that the method is linear scaling in accuracy with respect to the number of spheres N, i.e., in order to compute physical quantities of interest up to fixed relative error, the computational cost of the algorithm scales as $\mathcal{O}(N)$. As a first step, we obtain N-independent continuity and (discrete) inf-sup constants for the BIE. This allows us to derive relative error estimates that do not explicitly depend on N and to demonstrate, in addition, exponential convergence under suitable regularity assumptions. Next, we analyse the conditioning of the solution matrix associated with the Galerkin discretisation, and show that the maximum number of Krylov solver iterations required to obtain a solution (up to a given tolerance) is also independent of N. Combining this analysis with an FMM implementation that allows computing matrix vector products in $\mathcal{O}(N)$ yields the required linear scaling in accuracy.

Time permitting, we will also mention some extensions including linear scaling computation of the forces, and extending the model to include external electric fields and point-charges on the surfaces of the dielectric particles.

References:

1. M. Hassan and B. Stamm. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part I: Numerical Analysis**, *ESAIM:M2AN (2020) (https://doi.org/10.1051/m2an/2020030).*
2. B. Bramas, M. Hassan, and B. Stamm. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part II: Complexity Analysis**, *ESAIM:M2AN (2020)(https://doi.org/10.1051/m2an/2020055)*
3. M. Hassan, and B. Stamm. **A Linear Scaling in Accuracy Numerical Method for Computing the Electrostatic Forces in the N-Body Dielectric Spheres Problem**, *to appear in Communications in Computational Physics (2020), arXiv preprint arXiv:2002.01579.*

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