Incorporating surface polarization effects into large-scale coarse-grained Molecular Dynamics simulation

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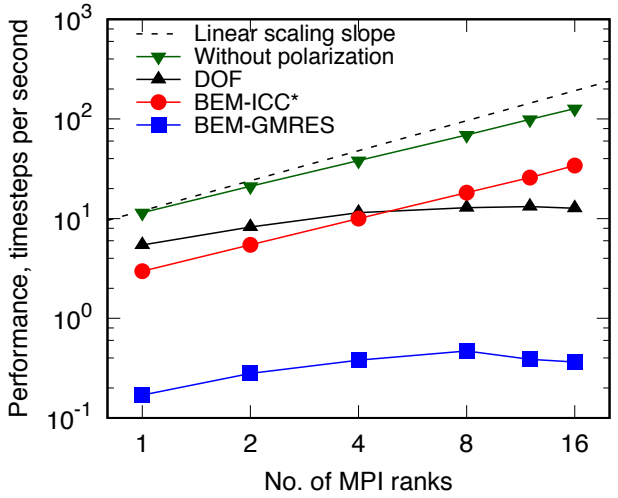
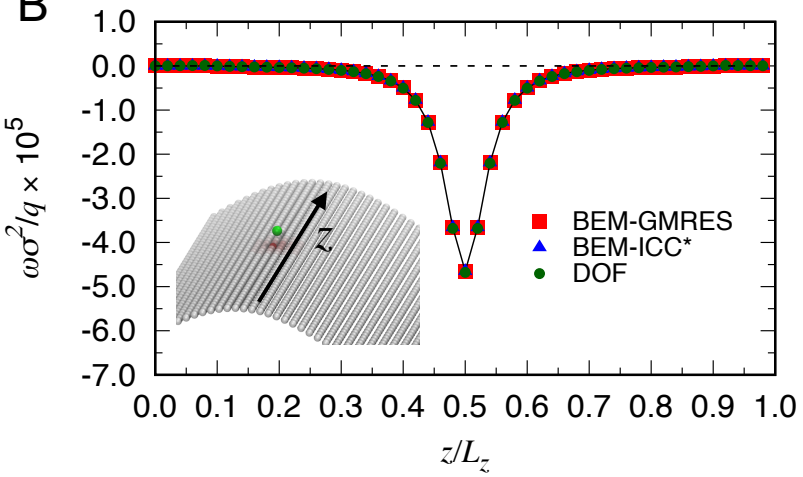
Nanoscopic and mesoscopic systems that are partitioned into domains with different dielectric constants are ubiquitous in nature and present in a wide variety of nanotechnology applications. Notable examples include, but are not limited to, ionic liquids in contact with graphene or silica substrates, polyelectrolytes confined between capacitors, and biomolecules captured inside protein capsids. Nevertheless, accurately and efficiently evaluating electrostatic interactions in such dielectrically heterogeneous systems remains challenging for most modeling and computational studies. One of the main reasons comes from the polarization effects at the interface due to dielectric mismatch between the media.

We implement and extend three methods for incorporating surface polarization effects into coarse-grained Molecular Dynamics simulations for LAMMPS: the boundary element method using the generalized minimum residual (GMRES) solver for solving the Poisson equation, the induced charge computation method using the successive over relaxations scheme (ICC*), and the direct optimization of an energy functional of induced charge density (DOF). Our implementations exhibit excellent strong scaling and are employed successfully in several case studies. The codes can be found at https://bitbucket. org/ndtrung/lammps.

A



B



A) Strong scaling behavior of three implemented methods
B) Case study: A point charge near a curved interface

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