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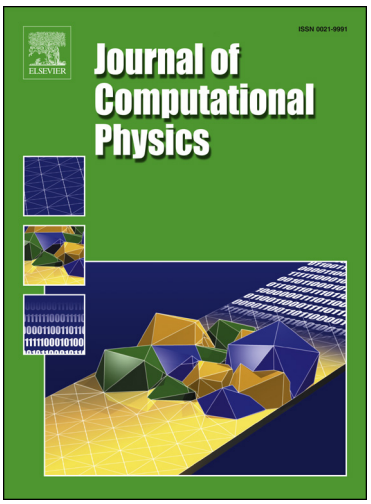

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James Cheung, Amalie L. Frischknecht, Mauro Perego, Pavel Bochev

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A Hybrid, Coupled Approach for Modeling Charged Fluids from the Nano to the Mesoscale

James Cheung[a,c], Amalie L. Frischknecht[b,c,*], Mauro Perego[a,c], Pavel Bochev[a,c,*]

[a] *Center for Computing Research*
[b] *Center for Integrated Nanotechnologies*
[c] *Sandia National Laboratories, Albuquerque, NM 87185, USA*

Abstract

We develop and demonstrate a new, hybrid simulation approach for charged fluids, which combines the accuracy of the nonlocal, classical density functional theory (cDFT) with the efficiency of the Poisson-Nernst-Planck (PNP) equations. The approach is motivated by the fact that the more accurate description of the physics in the cDFT model is required only near the charged surfaces, while away from these regions the PNP equations provide an acceptable representation of the ionic system. We formulate the hybrid approach in two stages. The first stage defines a coupled hybrid model in which the PNP and cDFT equations act independently on two overlapping domains, subject to suitable interface coupling conditions. At the second stage we apply the principles of the alternating Schwarz method to the hybrid model by using the interface conditions to define the appropriate boundary conditions and volume constraints exchanged between the PNP and the cDFT subdomains. Numerical examples with two representative examples of ionic systems demonstrate the numerical properties of the method and its potential to reduce the computational cost of a full cDFT calculation, while retaining the accuracy of the latter near the charged surfaces.

Keywords: Charged fluids, hard sphere model, PNP, classical density functional theory, Alternating Schwarz method.

1. Introduction

Predictive simulations of steady-state flows of ionic solutions are important for a variety of technological applications, including flow through microfluidic and nanofluidic devices [1, 2], and flow through ion-separation membranes [3]. These systems possess an electric double layer near surfaces, whose thickness depends on ion concentration and surface charge, but is typically in the range of 1–10 nm. Devices of interest, by contrast, can have dimensions ranging from tens of nm up to microns or larger. These devices often operate in a regime where the details of the electric double layer near surfaces are important to the physics

*Corresponding authors
Email addresses: jcheung@sandia.gov (James Cheung), alfrisc@sandia.gov (Amalie L. Frischknecht), mperego@sandia.gov (Mauro Perego), pbboche@sandia.gov (Pavel Bochev)