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A Long-Range Electric Field Solver for Molecular Dynamics of Fluid-Solid Interfaces Based on Atomistic-to-Continuum Modeling[1]
JEREMY TEMPLETON, REESE JONES, JONATHAN ZIMMERMAN, BRYAN WONG, Sandia National Laboratories, Livermore CA, JONATHAN LEE, Rice University — Understanding charge transport processes at a molecular level using computational techniques is currently hindered by a lack of appropriate models for incorporating anistropic electric fields, as occur at charged fluid/solid interfaces, in molecular dynamics (MD) simulations. In this work, we develop a model for including electric fields in MD using an atomistic-to-continuum framework. Our model represents the electric potential on a finite element mesh satisfying a Poisson equation with source terms determined by the distribution of the atomic charges. The method is verified using simulations where analytical solutions are known or comparisons can be made to existing techniques. A Calculation of a salt water solution in a silicon nanochannel is performed to demonstrate the method in a target scientific application.

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Jeremy Templeton
Sandia National Laboratories, Livermore CA

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