Abstract Submitted
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Molecular simulation of electrokinetic flows JIN LIU, Department of Mechanical Engineering, The Johns Hopkins University, Baltimore, MD 21218, MORAN WANG, EES-6 and T-13, Los Alamos National Laboratory, Los Alamos, NM 87545, SHIYI CHEN, Department of Mechanical Engineering, The Johns Hopkins University, Baltimore, MD 21218, MARK O. ROBBINS, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 — We develop a highly accurate and efficient molecular approach to simulate micro and nano electrokinetic flows. We calculate the long range Coulombic interactions using Particle-Particle Particle-Mesh (P^3M) approach. The Poisson equation for charge potential is solved in physical space using an iterative multi-grid technique. We demonstrate our approach through simulation of electro-osmotic channel flows with nano roughness on the walls. By comparing the flow rate with traditional pressure driven flows, our results indicate that in electro-osmotic flow the roughness affects the flow through altering the charge density distribution in the electrical double layer (EDL).

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