

Abstract Submitted
for the DFD07 Meeting of
The American Physical Society

Hybrid modeling of electromagnetic forces in microfluidic devices

JUSTYNA CZERWINSKA, IPPT, Polish Academy of Sciences, Warsaw, Poland, MOHAMED GAD-EL-HAK, Virginia Commonwealth University, Richmond, Virginia, USA — Many flows in microdevices operate under condition in which electromagnetic fields are essential driving force. The majority of research in that field is experimental due to the extreme complexity of the theoretical approach. To enhance understanding as well as to help direct design in such flows, there is a need to develop fast and efficient simulation techniques. For many practical operational conditions of MEMS and NEMS, the continuum approximation breaks down. Pure atomistic modeling is too computationally intensive to be possible in the near future but for the smallest of devices. Hence, there are two approaches that can be proposed: mesoscale modeling such as DSMC, LBM, DPD and RD; and hybrid molecular dynamics–continuum approach, which we focus on herein. Non-equilibrium molecular dynamics simulations are applied to all fluid molecules in the immediate vicinity of the charged particles' molecules. The Navier–Stokes equations are applied in the rest of the flow field, linked to the Maxwell equations. Adding to the complexity is the fact that electromagnetic forces are long range while molecular interactions are short range, presenting an additional multiscale challenge. Our results are validated using simple flows with immersed charged particles.

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Date submitted: 31 Jul 2007

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