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Coupled multiphysics simulations of charged particle electrophoresis for massively parallel supercomputers

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Abstract

We introduce a novel coupled algorithm for massively parallel direct numerical simulations of electrophoresis in microfluidic flows. This multiphysics algorithm employs an Eulerian description of fluid and ions, combined with a Lagrangian representation of moving charged particles. The fixed grid facilitates efficient solvers and the employed lattice Boltzmann method can efficiently handle complex geometries. Validation experiments with more than 70 000 time steps are presented, together with scaling experiments with over $4 \cdot 10^6$ particles and $1.96 \cdot 10^{11}$ grid cells for both hydrodynamics and electric potential. We achieve excellent performance and scaling on up to 65 536 cores of a current supercomputer.

Keywords: Parallel simulation, electrokinetic flow, electrophoresis, fluid-particle interaction, MPI

1. Introduction

1.1. Motivation

The motion of charged particles in fluids under the influence of electric fields occurs in a wide range of industrial, medical, and biological processes. When the charged particles are immersed in liquids, their migration caused by electric fields is termed electrophoresis. Due to the complex interplay of the physical effects involved in such particle-laden electrokinetic flows, numerical simulations are required to analyze, predict, and optimize the behavior of these processes. To this end, we present a parallel multiphysics algorithm for direct numerical simulations of electrophoretic particle motion.

Industrial applications that involve electrophoretic effects are electrofiltration [1, 2, 3] and electro-dewatering [4]. Moreover, electrophoresis is utilized

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