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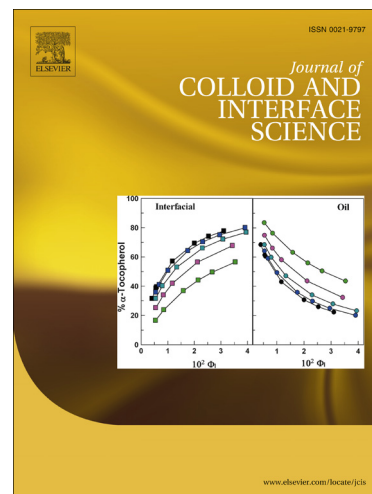
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Simulation of Chaotic Electrokinetic Transport: Performance of Commercial Software versus Custom-built Direct Numerical Simulation Codes

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Abstract

Many microfluidic and electrochemical applications involve chaotic transport phenomena that arise due to instabilities stemming from coupling of hydrodynamics with ion transport and electrostatic forces. Recent investigations have revealed the contribution of a wide range of spatio-temporal scales in such electro-chaotic systems similar to those observed in turbulent flows. Given that these scales can span several orders of magnitude, significant numerical resolution is needed for accurate prediction of these phenomena. The objective of this work is to assess accuracy and efficiency of commercial software for prediction of such phenomena. We have considered the electroconvective flow induced by concentration polarization near an ion selective surface as a model problem representing chaotic electrokinetic phenomena. We present detailed comparison of the performance of a general-purpose commercial computational fluid dynamics (CFD) and transport solver against a custom-built direct numerical simulation code that has been tailored to the specific physics of unsteady electrokinetic flows. We present detailed statistics including velocity and ion concentration spectra over a wide range of frequencies as well as time-averaged statistics and computational time required for each simulation. Our results indicate that while accuracy can be guaranteed with proper mesh resolution and avoiding numerical dissipation, commercial solvers are generally at least an order of magnitude slower than custom-built direct numerical simulation codes.

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