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Abstract Submitted
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Continuum Navier-Stokes modelling of water flow past fullerene molecules J. H. WALTHER, Technical University of Denmark, Denmark, A. POPADIC, National Institute of Chemistry, Slovenia, P. KOUMOUTSAKOS, ETH Zurich, Switzerland, M. PRAPROTNIK, National Institute of Chemistry, Slovenia — We present continuum simulations of water flow past fullerene molecules. The governing Navier-Stokes equations are complemented with the Navier slip boundary condition with a slip length that is extracted from related molecular dynamics simulations. We find that several quantities of interest as computed by the present model are in good agreement with results from atomistic and atomistic-continuum simulations at a fraction of the computational cost. We simulate the flow past a single fullerene and an array of fullerenes and demonstrate that such nanoscale flows can be computed efficiently by continuum flow solvers, allowing for investigations into spatiotemporal scales inaccessible to atomistic simulations.

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