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Simulation of flow through nanochannels: a novel multi-scale approach[1] FREDERIKE JAEGER, ALEX WRAY, ERICH MULLER, Imperial College London, PIETRO POESIO, University of Brescia, OMAR MATAR, Imperial College London — A novel method for the simulation of flow through nanochannels is proposed. We use molecular dynamics (MD) simulations to determine relations between the pressure, shear and bulk viscosities and the density, as well as the slip length for different fluid-wall combinations. These relations are then plugged into a steady, two-dimensional continuum-scale model that allows the simulation of a compressible (Lennard-Jones) fluid through channels. No restrictive assumptions are made on the nature of the fluid and its flow behaviour (e.g. fully-developed, parabolic velocity profiles for incompressible fluids). Direct comparisons between the MD and the continuum-scale predictions for the channel flow show good agreement. A major advantage of the proposed method is its computational efficiency, which allows for complex flow geometries to be studied whilst still retaining the accuracy of MD-based simulations. Furthermore, through the use of the statistical fluid associating theory (SAFT), more complex fluids can be modelled, providing a computational framework capable of representing realistic experimental set-ups.

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