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Fluid flows in nano/micro network configurations: a multiscale molecular-continuum approach[1] MATTHEW BORG, University of Strathclyde, DUNCAN LOCKERBY, University of Warwick, JASON REESE, University of Strathclyde — We present a new hybrid molecular-continuum methodology for resolving multiscale flows emergent in nano-/micro-scale networks, in particular for NEMS/MEMS applications. The method models junction and channel components of the network using independent MD micro elements. Long channels with uniform or gradually varying nano-scale sections along the direction of flow, contribute the most towards the highest computational savings, by replacing them with much smaller MD simulations. Junction components, however, do not exhibit any length-scale separation and are modelled in their entirety. All micro elements are coupled together in one hybrid simulation using standard continuum fluid-dynamics equations, that dictate the overall macroscopic flow in the network. In the case of isothermal, incompressible, low-speed flows we use the conservative continuity and momentum equations. An iterative algorithm is presented that computes at each iteration the new constraints on the pressure differences applied to individual micro elements, in addition to enforcing overall continuity in the network. We show that the hybrid simulation of various small network cases converge quickly to the result of a full MD simulation over just a few iterations, with significant computational savings.

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