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A multiscale method for modeling high-aspect-ratio micro/nano flows[1] DUNCAN LOCKERBY, University of Warwick, MATTHEW BORG, JASON REESE, University of Strathclyde — In this paper we present a new multiscale scheme for simulating micro/nano flows of high aspect ratio in the flow direction, e.g. within long ducts, tubes, or channels, of varying section. The scheme consists of applying a simple hydrodynamic description over the entire domain, and allocating micro sub-domains in very small "slices" of the channel. Every micro element is a molecular dynamics simulation (or other appropriate model, e.g., a direct simulation Monte Carlo method for micro-channel gas flows) over the local height of the channel/tube. The number of micro elements as well as their streamwise position is chosen to resolve the geometrical features of the macro channel. While there is no direct communication between individual micro elements, coupling occurs via an iterative imposition of mass and momentum-flux conservation on the macro scale. The greater the streamwise scale of the geometry, the more significant is the computational speed-up when compared to a full MD simulation. We test our new multiscale method on the case of a converging/diverging nanochannel conveying a simple Lennard-Jones liquid. We validate the results from our simulations by comparing them to a full MD simulation of the same test case.

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