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A particle-based multiscale model for submicron fluid flows SAUMYADIP MUKHOPADHYAY, JOHN ABRAHAM, Purdue University — A particle-based multiscale model for submicron fluid flows is proposed in this work. The model is based on a combination of a dissipative-particle dynamics (DPD) model for the mesoscales and molecular dynamics (MD) for the atomistic scales. The coarse-graining procedure involved in deriving DPD from MD is systematically exploited in this work, to transition from the atomistic region to the mesoscale region. Increasing levels of coarse-graining represent increasing length and time scales. The continuity of thermodynamic and transport properties across the interface is facilitated by appropriate selection of model parameters, and the modeling of particle flux across layers. The model is applied to solve Poiseuille and Couette flows, flow over a rough wall, and microscale flows with slip at the wall. Results are compared with analytical/full-scale MD simulations. In the case of the Poiseuille and Couette flows, the results are found to differ from the analytical solutions by less than 10%. The differences with full-scale MD simulation results are within 5% for flow over an obstacle. The reduction in computational cost with increasing coarse-graining is also evaluated.

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