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A seamless multiscale model coupling dissipative particle dynamics and molecular dynamics ANUPAM TIWARI, JOHN ABRAHAM, School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907 — Dissipative particle dynamics (DPD) is a mesoscopic method in which coarse-graining is done at the molecular level to capture physics at the mesolevel. DPD includes thermal fluctuations which are important at the lower scales of the mesolevel. This feature makes DPD an attractive choice for seamless multiscale simulations at the sub-micron level. In this work we propose a multiscale model coupling DPD and molecular dynamics (MD). We demonstrate the applicability of this model by a Poiseuille flow simulation in which MD is used in the region close to walls, while DPD is used to model the bulk fluid. Comparison of the simulation results with the analytical solution will be provided.

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