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Coupling Strategy for Multi-Scale Simulations in Micro-Channels

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Abstract : With the development of micro-electro-mechanical systems (MEMS), understanding fluid flow and heat transfer at the micrometer scale is crucial. In the case where the flow characteristic length scale is narrowed to around ten times the mean free path of gas molecules, the classical fluid mechanics and energy equations are still valid in the bulk flow, but particular attention must be paid to the gas/solid interface boundary conditions. Indeed, in the vicinity of the wall, on a thickness of about the mean free path of the molecules, called the Knudsen layer, the gas molecules are no longer in local thermodynamic equilibrium. Therefore, macroscopic models based on the continuity of velocity, temperature and heat flux jump conditions must be applied at the fluid/solid interface to take this non-equilibrium into account. Although these macroscopic models are widely used, the assumptions on which they depend are not necessarily verified in realistic cases. In order to get rid of these assumptions, simulations at the molecular scale are carried out to study how molecule interaction with walls can change the fluid flow and heat transfers at the vicinity of the walls. The developed approach is based on a kind of heterogeneous multi-scale method: micro-domains overlap the continuous domain, and coupling is carried out through exchanges of information between both the molecular and the continuum approaches. In practice, molecular dynamics describes the fluid flow and heat transfers in micro-domains while the Navier-Stokes and energy equations are used at larger scales. In this framework, two kinds of micro-simulation are performed: i) in bulk, to obtain the thermo-physical properties (viscosity, conductivity, ...) as well as the equation of state of the fluid, ii) close to the walls to identify the relationships between the slip velocity and the shear stress or between the temperature jump and the normal temperature gradient. The coupling strategy relies on an implicit formulation of the quantities extracted from micro-domains. Indeed, using the results of the molecular simulations, a Bayesian regression is performed in order to build continuous laws giving both the behavior of the physical properties, the equation of state and the slip relationships, as well as their uncertainties. These latter allow to set up a learning strategy to optimize the number of micro simulations. In the present contribution, the first results regarding this coupling associated with the learning strategy are illustrated through parametric studies of convergence criteria, choice of basis functions and noise of input data. Anisothermic flows of a Lennard Jones fluid in micro-channels are finally presented.

Keywords : multi-scale, microfluidics, micro-channel, hybrid approach, coupling
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