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MOLECULAR DYNAMICS PRE-SIMULATION METHODOLOGY FOR NANO-SCALE COMPUTATIONAL FLUID DYNAMICS

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Nanofluidic technology is advancing rapidly and with it a range of new technical opportunities are emerging. For example, desalination of water using carbon nanotubes [1, 2], heat removal and control in some high heat-flux systems such as micro/nanoelectronics mechanical systems (MEMS/NEMS), and micro chemical reactions [3, 4]. However, the prediction of mass flow rate and heat transfer in nano-scale systems presents a major barrier to their design. The existence of non-continuum effects, such as molecular layering and velocity slip near to liquid-solid interfaces, seemingly precludes efficient continuum Computational Fluid Dynamics (CFD). On the other hand, more-accurate Molecular Dynamics (MD) simulations are extremely costly in terms of the computational resources they require. To simulate the liquid over large scales is beyond the reach of current computational capabilities, and certainly prevents using the simulations within an iterative design process.

A procedure will be presented that uses a single MD simulation framework to provide essential fluid and interface properties for subsequent use in CFD calculations of nano-scale fluid flows. The MD pre-simulation enables an equation of state, constitutive relations, and boundary conditions for any given fluid/solid combination, in a form that can be conveniently implemented within a Navier-Stokes solver.

Results will be presented demonstrating that these enhanced CFD simulations are then capable of obtaining good flow field results in a range of complex geometries at the nano-scale.Comparison is with full-scale MD simulations but the computational cost of the CFD is negligible in comparison with the MD.

Two different sets of cases will be presented. The first set of results consist of two reser-

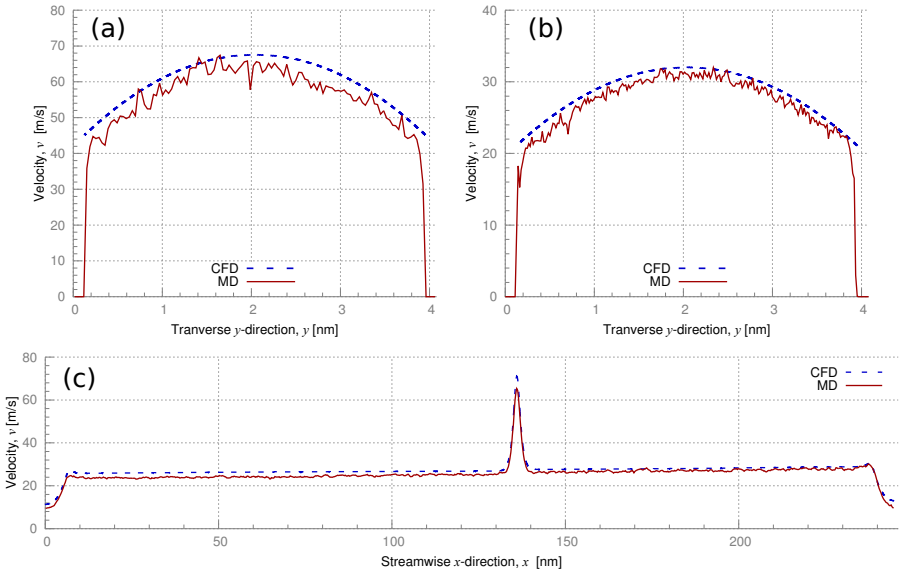

Figure 1: Streamwise velocity profiles for (a) a short channel at the centre; (b) a long channel at the centre; and (c) a channel with an irregularity.

voirs connected by either a short, a long or a defected channel. Accurate predictions for velocity (see figure 1) and mass flow rate (about 2% above the MD simulations) are achieved for these cases despite the large amount of fluid layering at the walls in the MD simulations. More importantly, accurate predictions can be obtained in geometries that are more complex than the planar MD pre-simulation geometry that provides the nano-scale fluid properties. The robustness of the nano-scale CFD is tested by application to water flow through a (15,15) carbon nanotube (CNT) and it is found that useful flow information is obtained.

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