Advances in Hybrid Molecular/Continuum Methods forMicro and Nano Flows

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We discuss our new methods for improving the efficiency of hybrid molecular/continuum models of multiscale flows, in particular at the micro and nano scales. We focus on producing general solutions to the problems associated with simulating flow regions that are typically either a) scale-separated in space and time, or b) non-scale-separated. Identifying the Heterogeneous Multiscale Method (HMM) [1] as more appropriate for most practical flow situations than conventional domain decomposition, we first present a method to make the HMM more effective for multiscale flows of arbitrary time-scale separation. Our method has an adaptability that enables the most desirable aspects of existing schemes to be applied only in the appropriate conditions, as well as a leapfrog coupling between the 'macro' and 'micro' components of the hybrid model to improve numerical accuracy over a standard simultaneous approach [2]. The test case demonstrator for this method is a micro-jet actuator for aerodynamic drag reduction applications. In this case we combine a kinetic treatment in a small flow region where rarefaction is important, with a simple continuum-conservation model in the much larger actuating domain. Our new time-stepping method consistently demonstrates as good as, or better, performance than existing schemes.

We then discuss a spatial coupling method in which the individual molecular solvers are not coupled with the continuum grid at nodes (i.e. point-wise coupling), but instead coupling occurs over distributed heterogeneous fields (i.e. field-wise coupling) [3]. This generalizes HMM to flows with arbitrarily-varying degrees of spatial scale separation (e.g. the flow from a large reservoir into a nano-channel). As the position of molecular elements does not need to be collocated with nodes of the continuum grid, the resolution of the microscopic correction can be adjusted independently of the resolution of the continuum model. This in turn means the computational cost and accuracy of the molecular correction can be independently controlled and optimised. The test case we demonstrate this method on is the Poiseuille (nano)flow of both Newtonian (Lennard-Jones) and non-Newtonian (FENE) fluids, which finds application in nanoscale filtration of contaminated liquids, such as seawater. Our multiscale method converges very quickly (within 3–4 iterations) and is an order of magnitude more computationally efficient than a full-scale Molecular Dynamics simulation.

References

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