Keynote Lecture: Hybrid atomistic-continuum formulations for small scale hydrodynamics

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Summary

By limiting the molecular treatment to the regions where it is needed, a hybrid method allows the simulation of complex thermo-fluid phenomena at the microscale without the prohibitive cost of a fully molecular calculation. In this talk we will discuss and review hybrid atomistic-continuum methods for multiscale hydrodynamic applications. Both dense fluid and dilute gas formulations will be considered and coupling to representative simulation methods, namely molecular dynamics (MD) and direct simulation Monte Carlo (DSMC) respectively, will be discussed.

We will show that to a large extent, the two major issues in developing a hybrid method is the choice of a coupling method and the imposition of boundary conditions on the molecular simulation. Generally speaking, these two can be viewed as decoupled: the coupling technique can be developed on the basis of matching two compatible and equivalent (over some region of space) hydrodynamic descriptions, while boundary condition imposition can be posed as the general problem of imposing "macroscopic" boundary conditions on a molecular simulation. In our opinion, the latter is a very challenging problem that has not been, in general, resolved to date completely satisfactorily. This is discussed further in [1].

Particular emphasis will be given to the "selection" of the coupling approach between the two descriptions. As will be illustrated by examples, powerful and robust hybrid methods can be developed by using already developed continuum-continuum coupling techniques (recall that the molecular and continuum description can only be coupled in regions where both are valid, namely in regions where the continuum assumption holds). Existing continuum coupling techniques have the additional advantages of being mathematically rigorous and performing optimally for the application they have been developed for.

One of the most important messages of this talk is that there is no general hybrid method that can be applied to all hydrodynamic problems. On the contrary, similarly to continuum numerical solution methods, hybrid methods need to be tailored to the *flow physics* of the problem at hand. Perhaps the most important consideration in this respect is that of timescale decoupling originally discussed by Hadjiconstantinou in [2]: explicit integration of the molecular subdomain at the molecular timestep to the global solution time (or steady state) is very computationally expensive if not infeasible if the continuum subdomain is appropriately large. This is because the molecular timestep is significantly smaller (MD–dense fluids) or at best smaller (DSMC–dilute gases) than the Courant-Friedrich-Lewy (CFL) stability timestep at typical discretization levels.

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We show [1] that the above considerations are intimately linked to the flow physics: compressible flow physics have characteristic timescales that scale with the compressible CFL timestep [3] which is not very different from a DSMC timestep in a dilute gas simulation. In this manner, explicit time integration with a finite-volume-type technique is possible as a natural extension of the continuum solution methods (see [4] and references therein) as long as the problem of interest is not too large. The use of a compressible formulation for liquids is obviously not a wise choice for *typical* applications. On the other hand, incompressible flow physics have characteristic timescales that are much longer than the CFL timestep and thus explicit integration at the molecular timestep is more prohibitive. Implicit methods are thus required that provide solutions without the need for explicit integration in time. One such implicit method for steady state problems has been proposed for liquids [5] [2] and gases [6]; it is based on a domain decomposition approach known as the Schwarz alernating method [7]. A hybrid method based on this coupling approach was recently used to simulate flow through microfluidic filters [8] yielding significant computational savings.

We will present examples of recently developed hybrid methods appropriate for both compressible [4] and incompressible flow physics. These methods will be compared and contrasted. Finally, recent work towards the development of second-generation adaptive hybrid methods will be presented. These methods introduce the molecular description adaptively in the regions where it is needed in complete analogy with adaptive refinement approaches found in continuum methods. An important prerequisite for such capabilities is robust criteria for continuum breakdown and a complete understanding of the effect of molecular fluctuations.

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