HYBRID ATOMISTIC–CONTINUUM FORMULATIONS FOR MULTISCALE HYDRODYNAMICS

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Hybrid atomistic-continuum formulations allow the simulation of complex hydrodynamic phenomena at the nano and micro scales without the prohibitive cost of a fully atomistic approach. Hybrid formulations typically employ a domain decomposition strategy whereby the atomistic model is limited to regions of the flow field where required and the continuum model is implemented side-by-side in the remainder of the domain within a single computational framework. This strategy assumes that non-continuum phenomena are localized and that coupling of the two descriptions can be achieved in a spatial region where both formulations are valid. In this article we review hybrid atomistic-continuum methods for multiscale hydrodynamic applications. Both liquid and gas formulations are considered. The choice of coupling method and its relation to the fluid physics as well as the differences between incompressible and compressible hybrid methods are discussed using illustrative examples.

1. Background

While the fabrication of MEMS devices has received much attention, transport mechanisms at the nano and micro scale environment are currently poorly understood. Furthermore, efficient and accurate design capabilities for nano and micro engineering components are also somewhat limited since design tools based on continuum formulations are increasingly reaching their limit of applicability.

For gases, deviation from the classical Navier–Stokes behavior is typically quantified by the Knudsen number, $Kn = \frac{\lambda}{L}$ where $\lambda$ is the atomistic mean free path (≈ 4.9 × 10^{-8} m for air) and $L$ is a characteristic dimension. The Navier–Stokes formulation is found to be invalid for $Kn \gtrsim 0.1$. Ducts of width 100 nm or less which are common in N/MEMS correspond to Knudsen numbers of order 1 or above [1]. The Knudsen number for Helium leak detection devices and mass spectrometers can reach values of up to 200 [2]. Also material processing applications such as chemical vapor deposition and molecular beam epitaxy involve high Knudsen number flow regimes [3]. The Navier–Stokes description also deteriorates in the presence of sharp gradients. One example comes from Navier–Stokes formulations for high Mach number shock waves which are known to generate spurious post-shock oscillations [4, 5]. In such cases, a Knudsen number can be defined using the characteristic length scale of the gradient. A significant challenge therefore exists to develop accurate and efficient design tools for flow modeling at the nano and micro scales.

Liquids in nanoscale geometries or under high stress and liquids at material interfaces may also exhibit deviation from Navier–Stokes behavior [6]. Examples of problems which require modeling at the atomistic scale include the moving contact-line problem between two immiscible liquids [6], corner singularities, the breakup and merging of droplets [7], dynamic melting processes [8], crystal growth from a liquid phase and polymer/colloid wetting near surfaces. Accurate modeling of wetting phenomena is of particular concern in predicting microchannel flows.

While great accuracy can be obtained by an atomistic formulation over a broader range of length scales, a substantial computational overhead is associated with this approach. To mitigate this cost, “hybrid” atomistic-continuum simulations have been proposed as a novel approach to model hydrodynamic flows across multiple length and time scales. These hybrid approaches limit atomistic models to regions of the flow field where needed, and allow continuum models to be implemented in the remainder of the domain within a single computational framework. A hybrid method therefore allows the simulation of complex hydrodynamic phenomena which require modeling at the microscale without the prohibitive cost of a fully atomistic calculation.

In what follows we provide an overview of this rapidly expanding field and discuss recent developments. We begin by discussing the challenges associated with hybrid formulations, namely the choice of the coupling method and the imposition of boundary conditions on atomistic simulations. We then illustrate hybrid methods for incompressible and compressible flows by describing recent archetypal approaches. Finally we discuss the effect of statistical fluctuations in the context of developing robust criteria for adaptive placement of the atomistic description.