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Multiscale simulation of heat transfer in a rarefied gas

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ABSTRACT

We present a new hybrid method for dilute gas flows that couples a continuum-fluid description to the direct simulation Monte Carlo (DSMC) technique. Instead of using a domain-decomposition framework, we adopt a heterogeneous approach with micro resolution that can capture non-equilibrium or non-continuum fluid behaviour both close to bounding walls and in the bulk. A continuum-fluid model is applied across the entire domain, while DSMC is applied in spatially-distributed micro regions. Using a field-wise coupling approach, each micro element provides a local correction to a continuum sub-region, the dimensions of which are identical to the micro element itself. Interpolating this local correction between the micro elements then produces a correction that can be applied over the entire continuum domain. Key advantages of this method include its suitability for flow problems with varying degrees of scale separation, and that the location of the micro elements is not restricted to the nodes of the computational mesh. Also, the size of the micro elements adapts dynamically with the local molecular mean free path. We demonstrate the method on heat transfer problems in dilute gas flows, where the coupling is performed through the computed heat fluxes. Our test case is micro Fourier flow over a range of rarefaction and temperature conditions: this case is simple enough to enable validation against a pure DSMC simulation, and our results show that the hybrid method can deal with both missing boundary and constitutive information.

1. Introduction

While the conventional hydrodynamic equations are generally excellent for modelling the majority of fluid flow problems, the presence of localised regions of non-continuum or non-equilibrium flow can result in some degree of inaccuracy. Such regions appear when the flow is far from local thermodynamic equilibrium, for example, when there are large gradients in fluid properties, or when surface effects become dominant. Although molecular simulation tools can provide an accurate modelling alternative in these cases, they are usually much too computationally expensive for resolving engineering spatial and temporal scales. Multiscale methodologies that exploit 'scale separation' have therefore been developed over the past decade. Scale separation occurs when the variation of hydrodynamic properties across small regions of space or periods of time is only very loosely coupled with the flow behaviour on a much larger spatial or temporal scale.

Often referred to as 'hybrids', these multiscale methods combine continuum and molecular descriptions of the flow. A traditional continuum description is employed in macro flow regions, and a molecular treatment is applied in small-scale micro or nano regions. Essentially, the aim is to combine the best of both solvers: the computational efficiency associated with continuum methods, and the detail and accuracy of molecular techniques.

In the literature, two different hybrid frameworks have emerged for fluid flows: (a) the domain-decomposition technique, and (b) the Heterogeneous Multiscale Method (HMM). For liquids, molecular dynamics (MD) is the appropriate molecular simulation tool. This deterministic method is, however, inefficient for dilute gas flows, and the direct simulation Monte Carlo (DSMC) method (Bird, 1998) can instead provide a coarse-grained molecular description. Founded on the kinetic theory of dilute gases, DSMC reduces computational expense by adopting a stochastic approximation for the molecular collision process.

Typically, thermodynamic non-equilibrium effects occur in the vicinity of bounding surfaces or other interfaces. Recognising this behaviour, domain-decomposition has become the most popular hybrid framework for both liquids (O'Connell and Thompson, 1995; Hadjiconstantinou and Patera, 1997; Flekkøy et al., 2000; Delgado-Buscalioni and Coveney, 2003; Werder et al., 2005) and dilute gases (Wadsworth and Erwin, 1990; Hash and Hassan,

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1996; Garcia et al., 1999; Aktas and Aluru, 2002; Roveda et al., 1998; Sun et al., 2004; Sun and Boyd, 2002; Wijesinghe et al., 2004; Wu et al., 2006; Schwartzentruber et al., 2007; Lian et al., 2008). In this method, the simulation domain is partitioned — a molecular solver is applied in the regions closest to the surfaces, while a conventional continuum fluid solver is implemented in the remainder. These micro and macro sub-domains are independent but communicate through an overlap region that enables mutual coupling. This coupling is typically established by matching fluxes of fluid mass, momentum, and energy, or by matching state properties. However, despite its popularity, a fundamental disadvantage of this micro–macro decomposition approach is that computational efficiency can only be increased above that of a full molecular simulation when non-continuum flow is confined to 'near-wall' regions. In highly non-equilibrium flows, or when the temperature dependence of fluid properties such as dynamic viscosity or thermal conductivity is not known *a priori* (for example, in unusual chemically-reacting gas mixtures), the traditional fluid constitutive relations may be inaccurate in the bulk of the domain.

Domain-decomposition techniques are also inappropriate for simulating flow through micro or nanoscale geometries that have a high aspect ratio, e.g. one dimension of the geometry is orders of magnitude larger than another. This class of flow presents a challenge as it requires simultaneous solution of the microscopic processes occurring over the smallest dimension and the macroscopic processes occurring over the largest dimension, and is often too computationally intensive for a full molecular approach. Such flows are generally beyond the reach of domain-decomposition as the majority (or perhaps all) of the flowfield can be considered 'near-wall'.

The less-common HMM framework overcomes the limitations of domain-decomposition by adopting a micro-resolution approach that can be employed anywhere in the domain — near bounding surfaces, or in the bulk flow. In this case, a continuum model is applied across the entire flow field, and the molecular solver is applied in spatially-distributed micro regions. These micro regions provide the missing data that is required for closure of the local continuum model, either in the form of unknown boundary conditions, or unknown constitutive information. Existing HMM studies in the literature are mainly for liquid flows, using MD as the molecular solver (Ren and E, 2005; Yasuda and Yamamoto, 2008; Asproulis et al., 2012; Borg et al., 2013). Generally, these studies consider flow problems where momentum transport is dominant and the transfer of heat is negligible. Coupling is therefore based on momentum: velocity fields or strain-rates are prescribed in each micro region, and the resultant stress is used to apply a correction back into the hydrodynamic momentum equation (Ren and E, 2005; Yasuda and Yamamoto, 2008). Each HMM micro region supplies information to a computational node on the continuum mesh. This *point-wise coupling* approach (Asproulis et al., 2012) is ideal when there is a large degree of spatial scale separation in the system, providing significant computational savings over a pure molecular simulation. However, in flow problems with smaller, or mixed, degrees of spatial scale separation, the molecular resolution required can result in the micro elements overlapping, making HMM more expensive and less accurate than a pure molecular treatment.

Despite its advantages over domain-decomposition techniques, there has been little development of HMM-type hybrids that use DSMC as the molecular treatment. In 2010, Kessler et al. (2010) proposed the Coupled Multiscale Multiphysics Method (CM^3) that couples both momentum and heat transfer, with DSMC providing corrections to both the hydrodynamic momentum and energy equations. This method was, however, developed to simulate transient flows where a time-accurate solution is sought, and so any computational advantage over a full DSMC simulation is achieved only through decoupling of the time scales; the length scales remain fully coupled, with both the continuum description and DSMC employed over the same region of space. More recently, Patronis et al. (2013) adapted the Internal-flow Multiscale Method (IMM) to simulate dilute gas flows with DSMC. Originally developed by Borg et al. (2013) for liquid flows, IMM adopts a framework similar to HMM but is tailored to model flows in high-aspect-ratio channels. Although large computational savings are presented, this method is tailored specifically to deal with cases where the length scale in the direction of flow is significantly larger than the length scales transverse to the flow direction.

In this paper we propose a new form of the HMM technique, with DSMC providing the molecular description. We adopt the field wise coupling (HMM–FWC) approach developed by Borg et al. (2013) for liquid flows: rather than supplying a correction to a node on the continuum mesh, each micro element instead corrects a continuum sub-region, the spatial dimensions of which are identical to those of the micro element itself. This means that, unlike point wise coupling, HMM–FWC is suitable for dealing with flow problems with varying degrees of spatial scale separation. Also, the location of each micro element is not restricted to the nodes of the computational mesh: both the position and size of the micro elements can be optimised for each problem, independently of the continuum mesh.

Our method is designed to cope with inaccuracy in the traditional flow boundary conditions and/or constitutive relations, and is therefore able to deal with problems that are beyond the reach of domain-decomposition. This includes problems where the fluid behaviour is unknown in the bulk, i.e. the traditional constitutive relations fail due to non-equilibrium effects (for example, in the wake of a re-entry vehicle), or the transport properties are unknown (for example, in unusual gas mixtures). The method is also suitable for simulating high aspect ratio geometries. While the IMM is designed to simulate problems where the largest length scale is in the flow direction, our new method has no such restriction and so provides a more general approach. It could therefore be useful when the largest length scale is transverse to the flow direction; for example, the flow through microscale cracks that can appear in valves.

The form of the method we present in this paper is tailored to model heat transfer problems in dilute gas flows. As a starting point we consider problems in which the gas is essentially motionless, with large applied temperature gradients placing the focus on heat transfer. With negligible transport of momentum, our coupling is performed through the heat flux: we impose the local temperature fields on the micro elements and measure the consequent heat flux from the relaxed DSMC particle ensembles. A suitable correction is then applied to the hydrodynamic conservation of energy equation. (Full coupling of mass, momentum, and heat transfer is a subject for future work.)

The level of translational non-equilibrium in a rarefied gas is generally characterized by the Knudsen number *Kn*, defined as the ratio of the gas molecular mean free path λ to a characteristic system dimension *L*. Typically, the traditional 'no-temperature-jump' boundary condition at a bounding surface (wall) is only valid when $Kn < 0.001$; the flow is then in thermodynamic equilibrium as the frequency of both intermolecular and molecule-wall collisions is very high. As *Kn* increases above 0.001, this collision frequency decreases, resulting in a temperature discontinuity between the wall and its adjacent gas. For low *Kn*, the conventional conservation equations can be extended to account for this by employing von Smoluchowski temperature-jump boundary conditions (von Smoluchowski, 1898). However, as *Kn* increases, molecule-wall collisions become more frequent than intermolecular collisions and the thermal Knudsen layer becomes significant. This is essentially a region of non-equilibrium that extends from the