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Coupling heterogeneous continuum-particle fields to simulate non-isothermal microscale gas flows

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ABSTRACT

This paper extends the hybrid computational method proposed by Docherty et al. (2014) for simulating non-isothermal rarefied gas flows at the microscale. Coupling a continuum fluid description to a direct simulation Monte Carlo (DSMC) solver, the original methodology considered the transfer of heat only, with validation performed on 1D micro Fourier flow. Here, the coupling strategy is extended to consider the transport of mass, momentum, and heat, and validation in 1D is performed on the high-speed micro Couette flow problem. Sufficient micro resolution in the hybrid method enables good agreement with an equivalent pure DSMC simulation, but the method offers no computational speed-up for this 1D problem. However, considerable speed-up is achieved for a 2D problem: gas flowing through a microscale crack is modelled as a microchannel with a high-aspect-ratio cross-section. With a temperature difference imposed between the walls of the cross-section, the hybrid method predicts the velocity and temperature variation over the cross-section very accurately; an accurate mass flow rate prediction is also obtained.

1. Introduction

The behaviour of fluid flows through and around micro- and nano-scale devices is still not well understood; traditional continuum fluid mechanics is often inaccurate due to the importance of the fluid's molecular nature at these scales. Deterministic molecular dynamics (MD) may be employed to model liquid flows at the nano-scale, while the stochastic direct simulation Monte Carlo (DSMC) method is the most popular computational tool for dilute gases at the micro- or nano-scale. Both of these techniques are, however, too computationally intense to resolve the spatial and temporal scales in real engineering flow problems. The DSMC method is significantly cheaper than MD, but the expense of tracking and computing collisions between thousands/millions of DSMC particles can require months (or even years) of computing time. Therefore, continuum-molecular 'hybrid' methods are being developed to reduce this expense. Hybrid methods combine the efficiency of a continuum-fluid description with the resolution and accuracy of a molecular treatment: the molecular tool is applied over micro/nano scales to resolve the molecular flow behaviour, while the continuum-fluid description is employed over macro scales to resolve macroscopic flow variations.

The majority of current continuum-molecular hybrid methods are based on a domain decomposition (DD) framework [2–6], where the molecular solver is applied in a 'micro' sub-domain (which is typically close to a bounding wall) and the continuum-fluid solver is applied in the remaining 'macro' sub-domain; an overlap region then enables coupling of the two solvers, as illustrated in Fig. 1(a). These DD methods are, however, limited to flow problems where microscopic resolution is required only in localised regions. The less common 'equation-free' [7] and 'heterogeneous' [8] multiscale approaches are able to simulate problems that require the molecular solver to provide information to the continuum solver everywhere in the flow, i.e. when the conventional linear fluid-constitutive relations fail in the bulk of a flowfield — this could be the case if non-equilibrium flow appears in the bulk, or if the transport properties are unknown in an unusual gas mixture. In this case, a continuum-fluid description is applied across the entire flowfield, and spatially-distributed micro elements (in which the molecular solver is implemented) are then deployed to 'correct' this continuum description.

The Heterogeneous Multiscale Method (HMM) [8] uses a 'point-wise coupling' approach, illustrated in Fig. 1(b). The micro elements supply information (consisting of updated boundary conditions and fluid-constitutive information) directly to the nodes of the macro grid, both at the bounding walls and in the bulk. At the same time, each micro element is constrained by the local

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Nomenclature

a	acceleration
d	molecular diameter
e	specific energy
$\mathbf{f}$	external body force per unit volume
G	number of DSMC time-steps
H	separation between bounding walls
$H_{\text{lower/bulk/upper}}$	vertical extents of micro elements
I	number of iterations
Kn	Knudsen number
l	characteristic dimension
M_x	number of macro nodes
Ma	Mach number
$\dot{m}$	mass flow rate
p	pressure
$\mathbf{q}$	heat flux vector
S	computational speed-up
T	temperature
t_{cl}	average clock time per DSMC time step
$\mathbf{u}$	gas velocity
u, v, w	gas velocity spatial components
W	separation between bounding walls, or the channel width
$W_{\text{left/bulk/right}}$	horizontal extents of micro elements

Greek symbols

Δx	horizontal macro node spacing
Δy	vertical macro node spacing
δt	DSMC time step
δx	bin width
δy	bin height
$\bar{\epsilon}$	mean percentage error
ζ	convergence parameter
ζ_{tol}	convergence tolerance
κ	thermal conductivity
λ	mean free path
μ	dynamic viscosity
Π	number of micro elements
ρ	density
$\boldsymbol{\tau}$	viscous stress
$\boldsymbol{\Phi}$	heat flux correction
$\boldsymbol{\Omega}$	stress correction
ω	viscosity exponent

Subscripts

av	averaged property
corr	corrected property from hybrid method
pure	property from pure DSMC simulation
gl	global flow property
hyb	property of a hybrid simulation
l	local flow property
NSF	Navier–Stokes–Fourier property
ref	reference property
tot	total
VHS	Variable Hard Sphere property
wall	bounding wall property
x, y, z	directional components of vectors

continuum solution at the collocated macro node. This point-wise coupling means that the position and size of the micro elements is restricted by the placement and density of the macro nodes. It also means that, while the HMM is effective when the spatial scales are highly separated (i.e. when the variation of the flow properties relative to the physical extent of a micro element is small), it is inefficient and potentially inaccurate for flow problems that exhibit mixed degrees of spatial scale separation.

To overcome the restrictions of point-wise coupling, the HMM with field-wise coupling (HMM-FWC) was proposed by Borg et al. [9], which builds on the equation-free [7] and heterogeneous [8] multiscale frameworks. A continuum description is again applied over the entire flowfield, but each micro element now represents a field that correlates directly with an identically-sized continuum sub-region. The coupling is then performed via fields rather than nodal points: the local continuum property fields are imposed over the micro elements, and local constitutive *correction fields* (i.e. corrections to properties derived from linear constitutive-fluid relations) are extracted[1]; these local corrections are then interpolated to provide global corrections across the entire flowfield. Essentially, the HMM-FWC takes advantage of the fact that properties like stress and heat flux (and hence their corrections) often vary slowly in space, and so computational savings can be made by interpolating these fields between micro elements that are more sparsely located than the macro nodes. As in the HMM, near-wall micro elements also provide the continuum-fluid description with updated boundary information. The HMM-FWC can be considered a more general heterogeneous approach than the HMM — the position and size of the micro elements is not restricted by the macro nodes, as indicated in Fig. 1(c), and flows with mixed degrees of spatial scale separation can be simulated efficiently.

A specific class of the HMM-FWC has recently been developed to simulate efficiently the flow through long micro/nanochannels, which are a fairly common feature of emerging micro and nano devices. Presented by Borg et al. [10], the framework and coupling strategy of the Internal-flow Multiscale Method (IMM) is tailored to exploit the large length scale separation that exists in the streamwise direction of these flows. A continuum-fluid description is applied over the entire channel, and very short micro elements occupying the entire cross-section (i.e. the full channel height in 2D problems) are distributed along the channel length, as shown in Fig. 1(d). Compared with the other heterogeneous methods, the coupling is simplified — pressure gradients are imposed over the periodic micro elements via body-forcing, and the resulting mass flux is used to correct the continuum description.

Both the HMM-FWC and the IMM were originally implemented using MD as the micro solver for the simulation of liquids, and with assumptions of incompressible and isothermal flow. The IMM has seen significant development since: it has been implemented for a continuum–DSMC coupling [11,12], and extended to compressible [11], non-isothermal [12], and unsteady flows [13]. Note, however, that the non-isothermal coupling strategy in [12] is not general, and is applicable only to the long micro/nanochannel flows tackled by the IMM.

In 2014, Docherty et al. [1] adapted the HMM-FWC for a continuum–DSMC coupling, tailoring the constraint of the micro elements to suit the use of a DSMC solver. The focus was on heat transfer problems, and non-isothermal coupling was achieved via the conservation of energy. However, this coupling strategy limited the method to 'stationary' heat transfer problems, i.e. where the

[1] Note that a benefit of coupling via correction fields, rather than the stress and heat flux fields directly, is that the correction fields are able to provide an indication of the system's departure from thermodynamic equilibrium.