Journal of Computational Physics 255 (2013) 558–571

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Hybrid continuum–molecular modelling of multiscale internal gas flows ☆

Alexander Patronis [a], Duncan A. Lockerby [a,*], Matthew K. Borg [b], Jason M. Reese [b]

[a] School of Engineering, University of Warwick, Coventry CV4 7AL, UK
[b] Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow G1 1XJ, UK

ARTICLE INFO

Article history:
Received 27 February 2013
Received in revised form 16 June 2013
Accepted 19 August 2013
Available online 28 August 2013

Keywords:
Multiscale modelling
Continuum–molecular simulation
Continuum–particle simulation
Hybrid methods
Rarefied gas dynamics
Micro gas flows
Compressibility

ABSTRACT

We develop and apply an efficient multiscale method for simulating a large class of low-speed internal rarefied gas flows. The method is an extension of the hybrid atomistic–continuum approach proposed by Borg et al. (2013) [28] for the simulation of micro/nano flows of high-aspect ratio. The major new extensions are: (1) incorporation of fluid compressibility; (2) implementation using the direct simulation Monte Carlo (DSMC) method for dilute rarefied gas flows, and (3) application to a broader range of geometries, including periodic, non-periodic, pressure-driven, gravity-driven and shear-driven internal flows. The multiscale method is applied to micro-scale gas flows through a periodic converging–diverging channel (driven by an external acceleration) and a non-periodic channel with a bend (driven by a pressure difference), as well as the flow between two eccentric cylinders (with the inner rotating relative to the outer). In all these cases there exists a wide variation of Knudsen number within the geometries, as well as substantial compressibility despite the Mach number being very low. For validation purposes, our multiscale simulation results are compared to those obtained from full-scale DSMC simulations: very close agreement is obtained in all cases for all flow variables considered. Our multiscale simulation is an order of magnitude more computationally efficient than the full-scale DSMC for the first and second test cases, and two orders of magnitude more efficient for the third case.

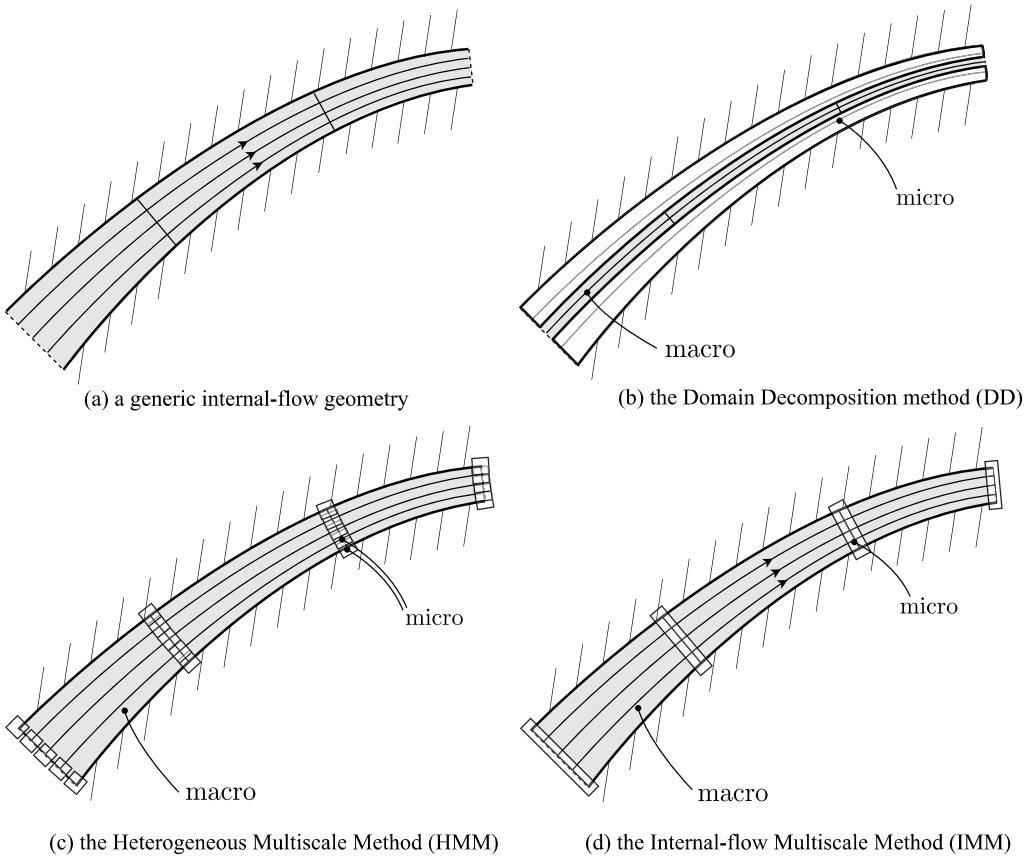
1. Introduction

The flow of gases through micro-scale internal geometries (e.g. micro channels) is critical to a range of future technologies, including: micro heat exchangers for cooling integrated circuits, micro-jet actuators for flow control in aerospace, hand-held gas chromatography systems, micro-reactors to generate small quantities of chemicals, and a host of other 'lab-on-a-chip' devices.

Numerical simulation of the gas flow through such non-trivial internal geometries is, however, extremely challenging. This is because conventional continuum fluid dynamics, which assumes that locally a gas is close to a state of thermodynamic equilibrium, becomes invalid or inaccurate as the smallest characteristic scale of the geometry (e.g. the channel height) approaches the mean distance between molecular collisions, λ [1]. An accurate and flexible modelling alternative for these cases is the direct simulation Monte Carlo method (DSMC) [2]. However, DSMC can be prohibitively expensive

* Corresponding author.
E-mail address: duncan.lockerby@warwick.ac.uk (D.A. Lockerby).

0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.08.033



(a) a generic internal-flow geometry

(b) the Domain Decomposition method (DD)

(c) the Heterogeneous Multiscale Method (HMM)

(d) the Internal-flow Multiscale Method (IMM)

Fig. 1. Schematic of different types of hybrid methods applied to (a) a generic internal-flow problem: (b) the domain-decomposition (DD) method, e.g. [3], (c) the heterogeneous multiscale method (HMM), e.g. [18] and (d) the internal-flow multiscale method (IMM) [28].

for internal-flow applications, which typically have a geometry of high-aspect ratio (i.e. are extremely long, relative to their cross-section). The high-aspect ratio creates a formidable multiscale problem: processes need to be resolved occurring over the smallest characteristic scale of the geometry (e.g. a channel's height), as well as over the largest characteristic scale of the geometry (e.g. the length of a long channel network), simultaneously.

To tackle such multiscale flow problems, simulation methods that combine a molecular treatment with a continuum description are often employed: these are known as hybrid methods. The main hybrid techniques developed so far can be grouped as follows: (a) domain-decomposition methods (e.g. for liquids [3–8] and for gases [9–17]) and (b) heterogeneous multiscaling (e.g. for liquids [18–21] and for gases [22]). Note, in this paper we restrict our attention to steady flows, but for transient problems temporal scale separation is also possible, see e.g. [23–25].

Domain decomposition (DD) is a methodology that applies a molecular-based model where non-equilibrium/non-continuum effects are located (statically or dynamically); for example, in the vicinity of boundaries, interfaces and moving shock waves. This localised molecular treatment is coupled to a continuum model applied over the rest of the domain (often an Euler solver for rarefied gas flows); the coupling is typically performed by matching hydrodynamic flux or state properties in an overlapping region (see Fig. 1(a), (b)). Despite their demonstrated success in a number of applications, DD methods have some disadvantages in certain classes of flow [26]. For example, a major disadvantage of using domain decomposition to solve the kind of highly-confined micro-/nano-channel problems we investigate in this paper is that the majority (if not all) of the flow can be considered 'near-wall', and thus highly non-equilibrial. As illustrated in Fig. 1(b) for a generic flow geometry, the molecular component (e.g. DSMC) would need to describe the entire length of the channel walls in order to capture the slip and other near-wall phenomena. As a consequence this severely restricts the maximum channel lengths (and the minimum channel heights) that can be usefully tackled by DD-type methods.

The heterogeneous multiscale method, known as HMM [27], is the main hybrid alternative to DD (see Fig. 1(c)). In HMM a continuum description is regarded as applicable in the whole domain and defined everywhere (although no assumptions regarding constitutive models or boundary conditions are made). Small 'micro elements' (individual molecular solvers) are dispersed on the nodes of the continuum computational grid, with the sole objective to provide the microscopic information that the macro model requires for closure (i.e. constitutive and boundary information). For a flow in a channel or pipe, for example, molecular micro elements would be placed on the bounding surfaces and in the fluid region, as illustrated in Fig. 1(c). Molecular simulations are performed using the local continuum strain-rate as a constraint, and from which only