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Application a hybrid solver to gas flow through a slit at arbitrary pressure ratio

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ABSTRACT

A hybrid solver, dynamically coupling the direct numerical solution of the kinetic equation and hydrodynamic Navier–Stokes equations is applied for numerical investigation of the gas flow through a slit at pressure ratio of 0.1, 0.5 and 0.9, including flow into vacuum and Knudsen number from slip to transitional regime. The coupling is achieved by matching half fluxes at the interface of kinetic and Navier–Stokes sub-domains, which are decomposed based on the local Knudsen number and macroparameters gradients. The solver efficiency is increased via MPI (Message Passing Interface) parallelization. The improvement in accuracy over Navier–Stokes equations and the computational efficiency of the proposed solver are assessed via comparison with pure kinetic solution in terms of mass flow and local parameters. The capability of hybrid solver to apply for vacuum science problems is demonstrated.

1. Introduction

Current developments in micro and nano technologies have dramatically increased possible applications of micro scale flow simulations, from micro-electro-mechanical-systems (MEMS) devices to genuinely multiscale problems. The coexistence of rarefied and continuum flow regime areas is a typical feature of gas flow in micro systems. Unfortunately, kinetic solvers, even for model equations, involve a considerable effort in terms of CPU time and memory requirements, due to the discretization in both physical and velocity spaces. On the other hand, hydrodynamics Euler or Navier–Stokes equations, describing the flow in terms of mere average gas velocity, density and temperature, are much more efficient, but less accurate in rarefied areas. However, in many applications rarefied areas cover only a limited portion of the whole computational domain; therefore, the development of hybrid solvers combining kinetic and continuum models has become an important area of research over the last decade, e.g. [1–13].

Potential applications of such solvers range from gas flows in complex micro systems to aerospace applications, such as high altitude flights. Major challenges in the development of hybrid code are the identification of kinetic and continuum domains and the choice of the coupling technique. The key parameter defining the choice of the appropriate physical model is usually related to some definition of a local Knudsen number, although more complex approaches have been suggested [7].

Different methods presented so far in the open literature can be classified into three categories. The first relies on domain decomposition in physical space: the computational domain is thus decomposed into kinetic and continuum sub-domains using appropriate criteria [1–11]. The second is based on domain decomposition in velocity space, where fast and slow particles are treated separately [12]. The third category includes hybrid models: both kinetic and fluid equations are solved in the entire domain, using velocity distribution function to compute transport coefficients for fluid equations [13]. Most of published works fall into the first category.

Typically, particle methods such as DSMC or Molecular Dynamics are used in regions with strong deviations from equilibrium, and a continuum fluid dynamics CFD (Euler or NS, depending on problem features) solver is used elsewhere, e.g. [1–6]. Nonetheless, in authors' opinion, the Direct Numerical Solution (DNS) of kinetic equations is a viable alternative to DSMC method and may be preferable to DSMC, for coupling purposes, since both kinetic and continuum models use similar numerical techniques. A combination of numerical solution of the Boltzmann equation and its model with kinetic schemes of continuum fluid dynamics was presented in Refs. [8,9]. In Refs. [10,11] a direct Boltzmann solver was combined with a NS solver using a priori decomposition of the domain, chosen on the basis of a previous continuum solution and not updated during the computation.

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The present work is a sequel to works presented in Refs. [10,11] and focuses on the efficient, consistent and accurate use of hybrid solver to simulate gas flow through a slit. The hybrid method was improved and dynamically decomposes the physical domain into kinetic and continuum sub-domains by computing gradient-length Knudsen number Kn_{GL} based on the local Knudsen number and macroparameters gradients [6,7]. The size of these domains is here dynamically updated during the transient depending on the current Kn_{GL}. The solution is advanced in time simultaneously in both kinetic and continuum domains: the coupling is achieved by matching half fluxes at the interface of kinetic and NS domains, thus taking care of the conservation of momentum, energy and mass through the interface. The fluxes matching technique allows the combination of existing in-house codes for numerical solution of both S-model kinetic equation based on the discrete velocity method and a finite-difference finite volume scheme for NS equations. Furthermore, solver efficiency is increased via MPI (Message Passing Interface) parallelization.

The chosen application, gas flow through a slit, is a relatively simple flow configuration representative of several real engineering applications, encountered, e.g., in vacuum equipment, micro/nano devices, spacecraft design, and metrology of gas flow. In addition, the flow through the slit is a popular numerical benchmark test for the validation of numerical methods. Despite its geometrical simplicity, in fact, the numerical study of the pressure-driven gas flow through the slit is not a trivial task due to possible local transition from continuum to rarefied regimes in the flow near the slit, requiring the use of hybrid simulation methods. Since the pressure drop ratio may vary from 1 to thousands (flow into vacuum), the molecular mean free path changes correspondingly from tens of nanometres to millimetres.

In the open literature kinetic approaches, allowing to describe all flow regimes from continuum to free-molecular, are commonly adopted to study the slit flow. In particular, numerical solutions of linearized BGK and S model kinetic equations for the slit problem have been reported in Refs. [14,15]. Nonlinear BGK and S-model kinetic equations were implemented for the simulation of the flow through the slit into vacuum in Ref. [16] and at arbitrary pressure ratios in Refs. [17,18], ranging from free-molecular to hydrodynamic regime. Rarefied gas flow through a slit was studied on the basis of the direct simulation Monte Carlo (DSMC) method at arbitrary pressure ratio including flow to the vacuum over the whole range of gas rarefaction in Ref. [19]. Moreover, in Ref. [16] it was stated that nonlinear BGK and S-model provide a solution close to DSMC results, at a lower computational cost and avoiding the statistical scattering typical of DSMC solutions in the case of small flow velocities.

The direct numerical solution of the Boltzmann equation was compared with BGK results in Ref. [17] and with S-model ones in Ref. [18] for the gas rarefaction range from the free-molecular to the hydrodynamic regime and for the reservoir pressure ratios leading to either the subsonic or supersonic outflow. It was shown that nonlinear BGK and S-model equations provide the same value of the mass flow rate as the Boltzmann equation within the relative difference of the order of 1%.

In Ref. [4] a hybrid CFD/DSMC solver was applied to predict gas flow and pressure in axisymmetric micro-thruster nozzles for throat Knudsen number varying from 0.008 to 0.125. It was shown that CFD simulations, even when thermal and velocity slip at the walls were accounted for in the boundary conditions, could not properly predict gas velocities and pressures in micro-nozzles. The high efficiency of solver was demonstrated: simulations can be performed in 5–25% of the CPU time required for a full DSMC simulation whereas predicted outflow macroparameters (pressures and velocities) differed less than 1–2%. The hybrid Euler/DSMC solver has been applied for unsteady evolution of a jet from a slit subjected to a pressure differential in Ref. [5]. The approach allowed one to resolve complicated transient flow structures. In Ref. [9] an adaptive hybrid kinetic–fluid solver was implemented for pressure-driven flow through a slit for rarefaction level ranging from transition to slip regime and pressure ratios 0.9 and 0.99.

In the present work a hybrid solver is applied for numerical investigation of the gas flow through a slit at pressure ratio of 0.1, 0.5 and 0.9, including flow into vacuum and Knudsen number from slip to transitional regime. The accuracy and computational efficiency of the proposed approach are assessed via comparison with both NS and pure kinetic solutions.

2. Statement of the problem

The planar monoatomic gas flow through a slit of height H cut in an infinitely thin partition at the plane $x = 0$ separating two containers (see Fig. 1) is considered. The gas far from the slit is in equilibrium at pressures p_0 in the inlet plenum and p_e in the outlet one, with $p_0 > p_e$, and the same temperature T_0. The slit is considered as infinite in the z direction. Since the main aim of the paper is the assessment of the coupling procedure, only monoatomic pure gas consisting of hard sphere molecules is considered. Any extension to mixtures or polyatomic gas, although in principle possible, is thus outside the scope of the paper and not yet considered or discussed here.

Two large areas of radius R before and after the slit are included in the computation, simulating the upstream and downstream reservoirs. Thus, the computational domain has the shape of a circle of radius R surrounding a slit of size H. Due to the symmetry of the problem about $y = 0$ only a half of the circle and a slit ($-H/2 \le y \le 0$), shown in Fig. 1, will be considered. The bold line I_c in Fig. 1 is the moving interface between kinetic and NS sub-domains, and its position is updated during the computation.

The difference between upstream p_0 and downstream p_e reservoirs pressures induces mass flow through the slit. The static inlet pressure p_i is the result of computation, although, due to the low inlet velocity, it almost coincides with p_0. A global characteristic of the flow, namely dimensionless mass flow rate W, is introduced as:

$$W = \frac{\dot{m}}{\dot{m}_{fm}}, \quad \dot{m}_{fm} = \frac{Hp_0}{\sqrt{\pi}v_0}, \tag{1}$$

where $\dot{m}_{fm}$ is the analytically deduced mass flow rate in the limit of free molecular regime and the mass flow rate through the slit is computed as:

$$\dot{m} = 2\int_{-H/2}^{0} \rho(0,y)u(0,y)dy. \tag{2}$$

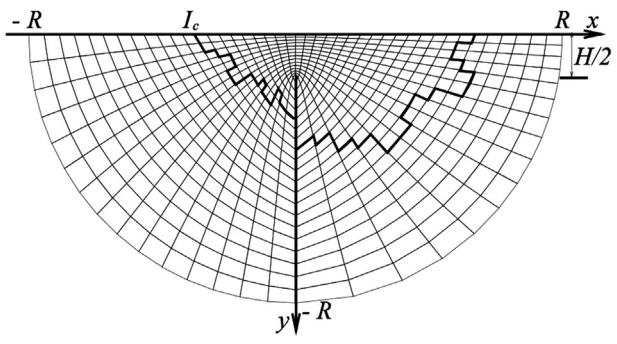

Fig. 1. Computational domain sketch.