Simulations of Low Speed Flows with Unified Flow Solver

V.V.Aristov, A.A.Frolova, S.A.Zabelok, V.I.Kolobov and R.R.Arslanbekov

Dorodnicyn Computing Center of the Russian Academy of Sciences,
Moscow, Russia
Computational Fluid Dynamics Research Corporation,
Huntsville, AL, USA

Abstract. Low speed gas flows are studied using a Unified Flow Solver (UFS) that automatically selects continuum-fluid-dynamic and kinetic solvers for near-equilibrium and kinetic domains. Direct Numerical Solution of the Boltzmann equation is used in the kinetic domains at moderate and high *local* Knudsen number, while kinetic schemes for Euler or Navier Stokes equations are used in the continuum domains. The adaptive mesh refinement and automatic domain decomposition are the key components of the UFS. This paper illustrates the UFS capabilities for external and internal subsonic flow problems including temperature and pressure driven flows of interest to micro-devices.

Keywords: Unified Flow Solver, Direct methods for the Boltzmann equation, Slow subsonic flows.
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INTRODUCTION

Interest to modeling low speed gas flows in micro-scale devices has stimulated increased attention to solving the Boltzmann equation. Micro channels of MEMS devices frequently operate at Knudsen numbers ($0.1<Kn<10$) for which the Navier-Stokes equations with slip boundary conditions are not reliable. Potential advantages of direct kinetic methods over statistical particle methods for low speed flows come from the large statistical noise of traditional DSMC methods for flow velocities comparable to thermal velocity of molecules. We have used the Unified Flow Solver (UFS) developed in [1] to study subsonic flows at low Mach number around plates, flows between non-uniformly heated plates with periodic temperatures along the plates for a wide range of conditions from near-continuum to free molecular regimes. We have also simulated pressure driven gas flows through an orifice and flows in channels and in micronozzles.

HYBRID METHODS FOR TRANSITIONAL LOW SPEED FLOWS

A number of recent papers have been devoted to the development of hybrid methods for subsonic flows, see, e.g., [2,3,4]. In [3], DSMC code is coupled to the Navier-Stokes (NS) code for analysis of transitional flow in a long channel. The NS solver is used in the inlet regions with high pressure and the DSMC is used in the outlet regions with low pressure. In [4], a hybrid method combining a BGK-type kinetic model equation with the NS equations has been proposed. In this approach, either kinetic scheme or continuum scheme is selected *a priory* for each computational cells. At interfaces between kinetic and continuum domains, the Chapman-Enskog distribution functions of the kinetic model equation are passed from the continuum side to the kinetic side, while macroscopic flow quantities are simply passed from the kinetic side to the continuum side. Using the hybrid method, the number of time steps required to obtain a steady-state solution as well as computational memory and CPU time are reduced.

Selection of appropriate continuum breakdown criteria and threshold value of the breakdown parameter for low speed flows are not simple. In [2], a breakdown criteria based on maximum values of the heat flux and stress tensor has been used. In our UFS studies, we tested different criteria for switching kinetic and continuum solvers. For example, the gradient switching criterion was used for flows in a short channel and micronozzle. Figure 1 shows kinetic (red) and continuum (white) domains in these cases.

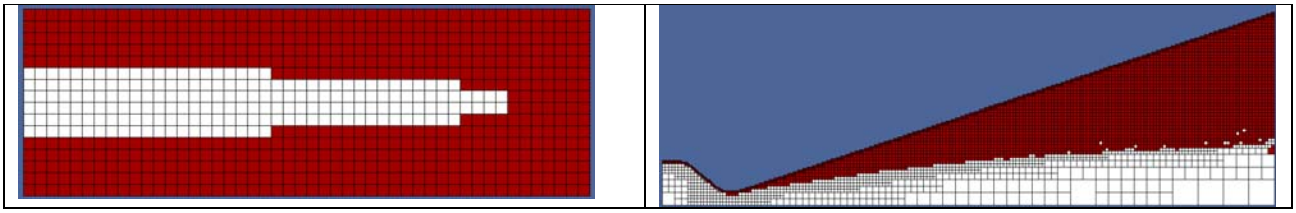

FIGURE 1. Mesh and domain decomposition of the UFS in a channel (left) and in a micronozzle (right)

BOLTZMANN SOLVERS FOR LOW SPEED FLOWS

The Boltzmann solvers have some specifics for low speed flows. Recently, an effort has been made to construct methods utilizing small deviation of the velocity distribution function from the equilibrium [5,6,7,8]. In Ref. 8, a method has been proposed for near-equilibrium flows at small Knudsen numbers, which can be applied for flows at small Mach numbers and small deviation from equilibrium.

We have compared our Boltzmann results with Tcheremissine's results [9] for flow around a cold plate (the temperature of the plate is equal to the temperature of free flow) at Mach number M=0.001 and Knudsen number Kn=0.1 (a molecular model of hard spheres, diffuse reflection at the plate surface). In Figure 2, contours of longitudinal and transverse velocities respectively are presented. The plate is located between x=0 and x=1, i.e. the dimensionless value is given through the length of the plate. The results are in a good agreement with the results of [9] confirming adequate characteristics of our Boltzmann solver for low speed flows.

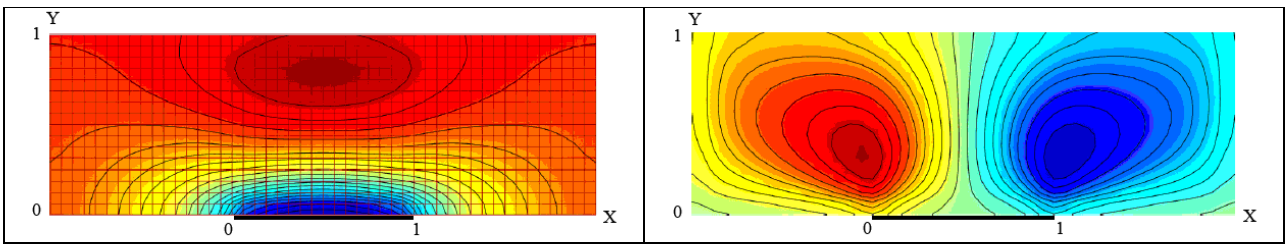

FIGURE 2. Longitudinal velocity contours and ccomputational mesh, 0.00025< u < 0.00099 (on the left) and transverse velocity contours, -0.00012 <v< 0.00012 (on the right)

FLOWS DRIVEN BY TEMPERATURE GRADIENTS

Heat transfer in micro-devices and gas flows induced by temperature gradients are important for many practical applications. We have performed analysis of heat transfer and gas flows between non-uniformly heated plates using UFS. Consider two parallel plates with nonuniform temperature along the plate surfaces (T=1 at y=0.5 and T=1-0.5sin($2\pi x$) at y=-0.5). The problem has been studied by Sone [10] using asymptotic theory. Recently, Filbert and Russo [11] performed calculations using Boltzmann equation for hard sphere molecules with 2D velocity space. As described by Sone, traditional NS equations (with traditional slip wall boundary conditions) give zero flow velocity and symmetric distribution of gas temperature in this case. As pointed out in [12], the Maxwell-Burnett boundary condition can predict the phenomenon of thermal-stress slip flow. In our simulations, the computational domain consisted of a unit box with symmetry (specular) boundary conditions at x=-0.5 and x=0.5. Diffuse reflection at the top and bottom boundaries (y=0.5 and y=-0.5) was assumed. We solved this problem for different Kn numbers using the Boltzmann solver (with BGK collision operator and the HS model), the NS kinetic solver with the kinetic boundary conditions, and the UFS. The kinetic NS scheme uses half-fluxes at cell faces and half-fluxes at the boundaries determined by integration of the velocity distribution function.

We have performed numerical solution of this problem for different Kn numbers using BGK collision model. Distributions of temperature and mean flow velocity for Kn=0.01 was obtained with (40,40,1) nodes in velocity space. The maximal value of the mean flow velocity is 0.09 in units of thermal velocity. Numerical analysis for different *Kn* numbers has shown that the velocity amplitude decreases proportionally to *Kn* number (Figure 3). For *Kn*=0.05 results of two calculations with different meshes are presented.

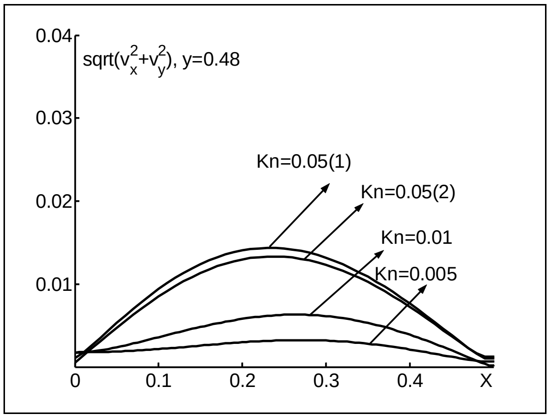

FIGURE 3. Flow velocity for different Kn numbers (and two different mesh for Kn=0.05).

The results of calculations using the Boltzmann, kinetic NS and UFS solvers for a similar problem are presented in Figure 4. In this case, the temperature of the right wall increases linearly from 1 to 1.7 from top to bottom, the temperatures of the left and top walls are set to 1, and a symmetry BC is assumed at the bottom boundary. The arrows show the mean flow velocity vectors, the color indicates the magnitude of the mean flow velocity. One can see that there is a well-formed vortex in the middle of computational domain. This vortex is temperature-driven. The simulation with the kinetic NS solver reproduced well results of the Boltzmann (BGK) solver and permitted to obtain the same vortex structure. The UFS results for Kn=0.06 are also shown in Figure 4 on the right with kinetic (broun) and continuum (white) domains illustrated in the left top corner.

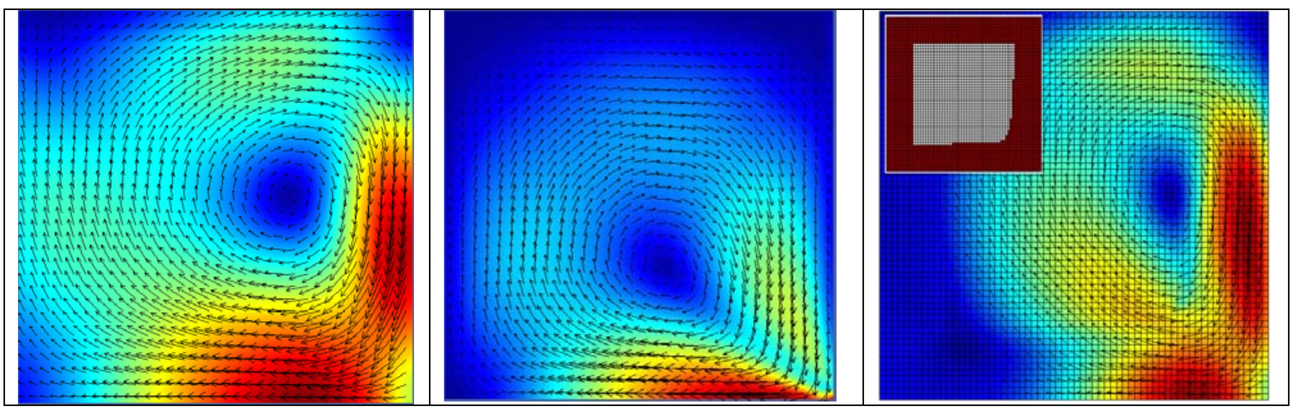

FIGURE 4. Temperature driven vortex flows: left – Boltzmann solver for *Kn*=0.3, center NS solver for *Kn*=0.01, right - UFS results for *Kn*=0.06. Shown are flow velocity vector fields and velocity amplitude. Domain decomposition into kinetic and continuum parts is shown in the left top corner.

Analytical Solution for the Collisionless Case

An analytical solution for the velocity distribution function was obtained for a collisionless gas contained between two nonuniformly heated plates with diffuse reflection of atoms at the boundaries. The temperatures along the plate surfaces are T=1 at y=1 and T=1-0.5sin($2\pi x$) at y=0. To derive an analytical solution, consider the number of particles $N(x)$ arriving at a unit surface near a point x per unit time. Due to the non-penetration condition, this number is also equal to the number of reflected particles at the point x. For the diffuse reflection, the density of reflected particles is expressed through this quantity *N(x)* as $n(x) = N(x)\sqrt{\frac{2\pi}{T(x)}}$. The velocity distribution of the reflected particles at any point *(x,y)* between the plates $(-\infty < x < +\infty, 0 < y < 1)$ is found as

$$f(x,y,\xi) = N(x_1)\sqrt{\frac{2\pi}{T(x_1)}}\frac{1}{(2\pi T(x_1))^{3/2}}\exp(-\frac{\xi^2}{2T(x_1)}), \quad (1)$$

where $\xi = (\xi_x, \xi_y, \xi_z)$ and x_1 is the coordinate of the point on the plate from which the particle with a given velocity arrives to the given point. We have

$$x_1 = x - \frac{\xi_x}{\xi_y} y \text{ at } \xi_y > 0 \quad \text{and} \quad x_1 = x - \frac{\xi_x}{\xi_y}(1-y) \text{ at } \xi_y < 0. \quad (2)$$

For the case of similar temperature profiles along both plates, the equation for the quantity *N(x)* was obtained in the form of an integral equation

$$N(x) = \frac{1}{2}\int_{-\infty}^{\infty} N(y)\frac{1}{(1+(y-x)^2)^{3/2}}dy. \quad (3)$$

It is obvious that *N(x)*=const is a solution to this equation, which we assume below (it is interesting to note that the Fredholm equation (3) can possess, in principle, non-unique solution, in particular, the linear function *N(x)*=*x* is another solution to this equation which is similar to the equation describing gas flow in an infinite tube, see [5]).

For the case of non-uniform temperature distributions along both plates, we introduce two functions, $N_t(x)$ and $N_b(x)$ for the top and bottom plates, correspondingly. We can obtain the system of two integral equations

$$N_b(x) = \frac{1}{2}\int_{-\infty}^{\infty} N_t(z)\frac{1}{(1+(z-x)^2)^{3/2}}dz$$

$$N_t(x) = \frac{1}{2}\int_{-\infty}^{\infty} N_b(z)\frac{1}{(1+(z-x)^2)^{3/2}}dz.$$

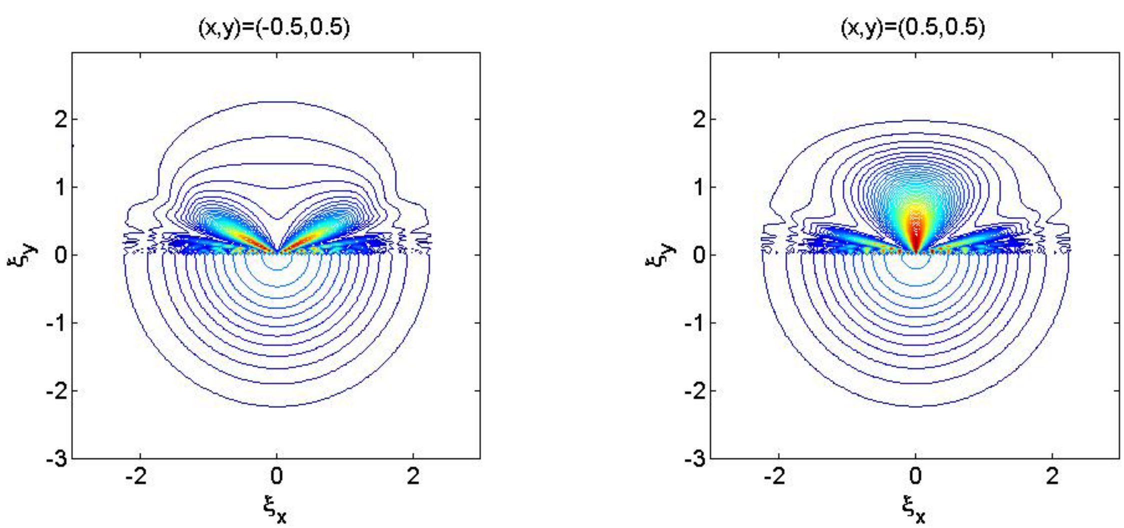

FIGURE 5. Velocity distribution functions for a free-molecular flow

The analytical solution (1)-(3), is shown in Figure 5 for two different *x* and *y*=0.5 It is seen that the velocity distribution function has a rather complex structure, with sharp peaks at certain angles. The fine structure is observed for gliding particles moving at small angles along the surfaces.

By introducing cylindrical coordinates $\xi_x = \xi\cos\theta, \xi_y = \xi\sin\theta$, we obtain for the mean velocity component

$$u_x = \int_0^{\pi}\cos\theta d\theta\int_0^{\infty} f\xi^2 d\xi$$

The second integral is calculated analytically, using $\int_0^{\infty}\xi^2 d\xi e^{-\alpha\xi^2} = \frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}}$ giving zero mean velocity.

PRESSURE DRIVEN FLOWS

Pressure driven micro-flows are one of the interesting problems in rarefied gas dynamics [13]. In the transitional regime ($0.1<Kn<10$) rarefied effects are significant, and Computational Fluid Dynamics (CFD) methods are not reliable. We have simulated flows through an orifice and a channel for various values of the pressure ratio. Many authors studied this problem but until now no results have been obtained for a wide range of pressure ratio and rarefaction parameter. Recently, reliable results have been obtained by Sharipov [14] using DSMC for regimes from a free-molecular flow to Kn=0.01 and for the pressure ratio from 0 to 0.9. However for the pressure ratio larger than 0.9, DSMC did not allow solving this problem with a sufficient accuracy [14]. We have simulated flows through an orifice for various values of the pressure ratio. Figure 6 shows selected results of 2D simulations with our Boltzmann solver for different pressure ratios in the chambers (all calculations were made for pressure ratios P_l/P_0=0.99, 0.95, 0.9, 0.5, 0.1). The isothermal case is considered (temperatures in boundary chambers are equal and the pressure drop is due to the density drop). Note that for the right plot the temperature is changed and its minimum is near the center of a slit (a blue spot in the bottom of the right plot), that is correspondent to the same problem but for an orifice from [14]. The subscript 0 denotes the values in the left chamber (inlet) and the subscript 1 – in the right chamber (outlet).

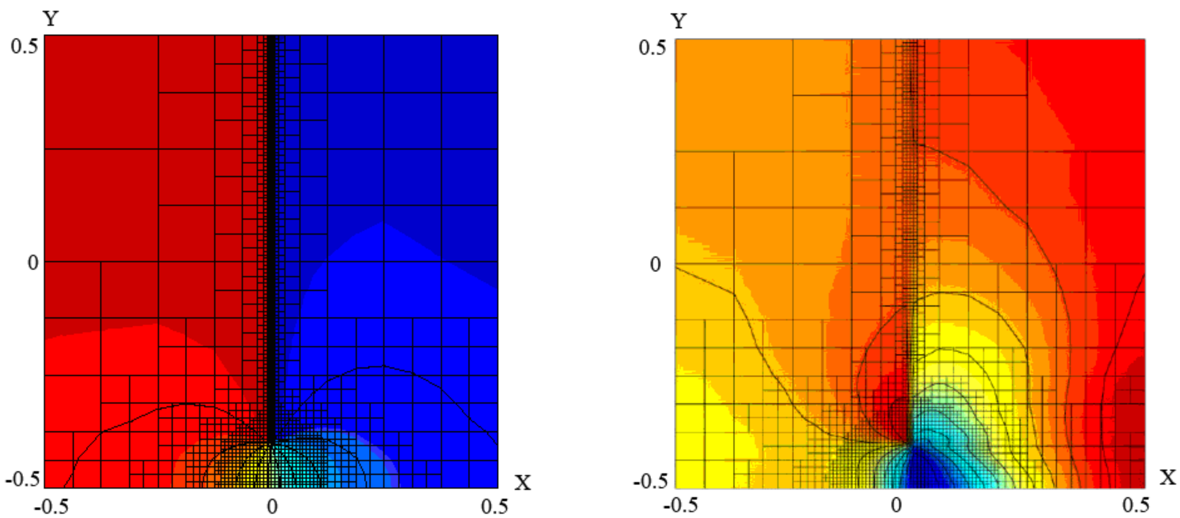

FIGURE 6. Computational mesh and density contours for the isothermal flow through a slit at P_1/P_0=0.95, T_0=T_1=1 in both chambers, n_0=1 – left chamber, n_1=0.95 – right chamber (left plot) and computational mesh and temperature contours at P_1/P_0=0.5, T_0=T_1=1 in both chambers, n_0=1 – left chamber, n_1=0.5 – right chamber (right plot).

We have also simulated pressure driven flows through channel for various pressure ratios. Figure 7 shows results for a channel with the length/width ratio L/d=21 (isothermal conditions for different Kn numbers at the outlet, the Lennard-Jones model of inter-molecular interactions). The Knudsen minimum is observed in both cases, at P0/P1=2 (left) and at P0/P1=1.5 (right).

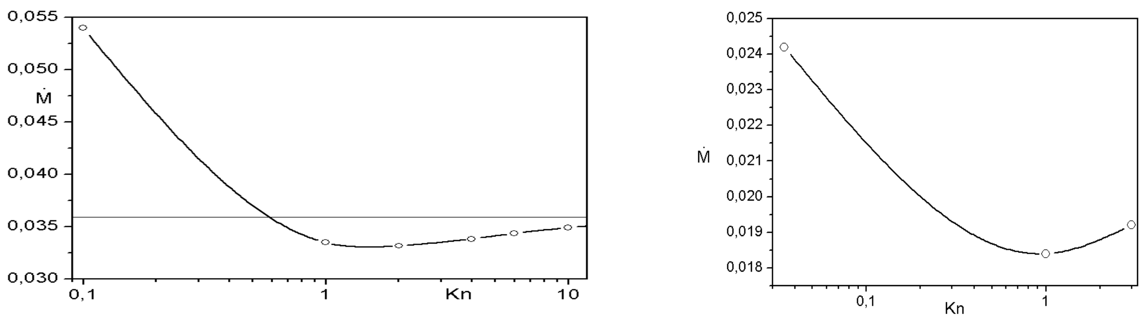

FIGURE 7. The Knudsen effect in a channel with L/d=21 for P0/P1=2 (left) and P0/P1=1.5 (right).

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