# Rarefied Flow between Plates of Finite Length via the Coupling Approach

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**Abstract** The coexistence of rarefied continuum flow regime areas and relatively small elements in which rarefaction effects become important is a typical feature of many complex gas flows micro systems. In rarefied domains, the mean free path of gas molecules is comparable or larger than a characteristic scale of the system. These domains are naturally described by kinetic equation for the velocity distribution function, which involve a considerable effort in terms of CPU time and memory requirements, due to the discretization in both physical and velocity space. The continuum domains are best described by the fluid Navier Stokes (NS) equations in terms of average flow velocity, gas density and temperature. These equations are more efficient, but less accurate in critical rarefied areas. Thus, the development of hybrid solver combining kinetic and continuum models is of great interest especially for applications range from gas flows in micro systems to the aerospace applications, such as high altitude flights. The pressure –driven gas flow of rarified monatomic gas through a two-dimensional short microchannel is considered using hybrid solver. The calculations have been carried out for pressure ratios 0.1, 0.5 and 0.9 and fixed relatively large Knudsen number. The applicability of the solver is discussed via comparison with the kinetic and NS solutions.
**Keywords:** Micro Flow, Hybrid method, model kinetic equation

## 1. Introduction

The coexistence of rarefied and continuum flow regime areas is a typical feature of many complex gas flows micro systems. Rarefied domains, in which the mean free path of gas molecules is comparable or larger than a characteristic scale of the system, are naturally described by kinetic methods, such us the Direct Simulation Monte Carlo (DSMC), or require solutions of the Boltzmann kinetic equation for the velocity distribution function. Unfortunately, realistic kinetic simulations become rapidly too expensive, and often impossible, as the Knudsen number becomes smaller. On the other hand the continuum domains are best described by the continuum (Euler or Navier Stokes) equations in terms of average flow velocity, gas density and temperature. These equations are more efficient, but less accurate in rarefied areas.
The development of hybrid solvers combining kinetic and continuum models has, thus, been an important area of research over the last decade [1, 2]. The key parameter defining the choice of the appropriate physical model is the local Knudsen number, *Kn*. Most references use *Kn* values based on the characteristic size of the system. However, different options are possible: in particular, in a recent paper [3], a more complex criterion based on the difference between the Navier–Stokes stress and Fourier heat flux and the actual values as computed from the molecular solver is proposed. The main challenges in the development of hybrid code are, axtually, the identification of kinetic and continuum domains, as well as the choice of a proper coupling between these domains.

The different methods presented in the open literature can be classified into three categories. The first includes methods employing domain decomposition in physical space. In this category, the computational domain is decomposed into kinetic and continuum sub-domains using appropriate criteria [3-5]. The second category includes methods based on domain decomposition in velocity space where fast and slow particles are treated separately [6]. The third category includes hybrid models. With these methods, one solves both kinetic and fluid equations in

the entire domain and uses the velocity distribution function to compute transport coefficients for the fluid equations [1, 7]. Most of the published works fall into the first category. In [2, 8] particle methods such as DSMC or Molecular Dynamics are used in regions with strong deviations from equilibrium, and a fluid (Euler or NS) solver is used in other regions.

The Direct Numerical Solution (DNS) of kinetic equation is a viable alternative to DSMC [1, 9] and sometimes is preferable to DSMC for coupling kinetic and continuum models because similar numerical techniques are used for solving both the Boltzmann and continuum equations. Recent effort to combine DNS with a NS solver used a priori decomposition of the domain has been done in [5]. In [1] an Unified Flow Solver (UFS) combining the DNS of the Boltzmann equation in rarefied regions with kinetic schemes of continuum fluid dynamics elsewhere was developed. The authors added a Boltzmann solver for one component monatomic gases, compressible Euler and NS solvers based on kinetic scheme, and developed practical criteria for domain decomposition and coupling kinetic and CFD solvers.

In the present approach the computational physical domain is decomposed into kinetic and continuum sub-domains by computing appropriate criteria, based on the local Knudsen number and gradients of macro-parametrs, using a preliminary NS solution throughout the whole physical domain. The hybrid code is the combination of direct numerical solution of the Bhatnagar-Gross-Krook (BGK) model kinetic equation and NS ones. 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 the kinetic and NS domains, taking care of the conservation of momentum, energy and mass through the interface. The accuracy and properties of the proposed method is assessed via the computation of the flow through a short microchannel of the length $L = 0$, 5 and 10. Outlet to inlet pressure ratio of 0.1, 0.5 and 0.9 are considered, for a fixed Knudsen number. The obtained by hybrid solver results are compared with NS and BGK solutions in terms of mass flow and local parameters.

## 2. Statement of the problem

The pressure–driven gas flow between parallel plates of finite length $L$ placed at the distance $H$ from each other and connected two large reservoirs of the size $L_1 \times L_2$ is examined on the basis of three codes: hybrid, kinetic and NS. The gas in the containers far from the plate is in equilibrium at constant pressures $p_0$ and $p_e$, with $p_0 > p_e$, and temperatures $T_0$. The temperature of the walls is equal to the temperature in reservoirs $T_0$. The channel is infinite in $z$ direction and due to the symmetry of the flow only half of the domain will be considered (Fig. 1.).

## 3. Numerical method

### 3.1 Coupling kinetic and Navier-Stokes solvers

The algorithm is based on decomposition of computational domain to kinetic and NS regions using, as switcthing criteria [1, 10], the value of $S_{NS}$:

$$S_{NS} = Kn\sqrt{\left(\frac{\nabla p}{p}\right)^2 + \frac{1}{U^2}\left(\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right)}$$

where all values are given in dimensionless form, and $Kn$ denotes the local Knudsen number, based on the difference between the plates. $S_{NS}$ is derived from the NS solution, and we chose to define the kinetic region as the area where $S_{NS}$ is greater then 0.015. The adequate switching criterion is crucial since a wrong domain decomposition could even lead to a non-positive distribution function when the NS solution is coupled with the kinetic equation solution.

At each time step the kinetic equation is solved on the kinetic domain $\Omega_K$ :

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\frac{\partial f}{\partial \mathbf{x}} = J(f, f), \qquad (1)$$

where $f = f(t, \mathbf{x}, \boldsymbol{\xi})$ is the velocity distribution function, $\mathbf{x} = (x, y, z)$ is the position vector, $\boldsymbol{\xi} = (\xi_x, \xi_y, \xi_z)$ is the velocity vector, $J(f,f)$ is the collision integral. The coupling strategy between kinetic solver and NS one is completely general, and can be applied to the full Boltzmann equation. Nonetheless, for the simplicity, the collision integral $J(f,f)$ is replaced by the BGK model:

$$J_{BGK}(f,f) = \frac{p}{\mu}(M - f)$$

$$M(t,\mathbf{x},\boldsymbol{\xi}) = \frac{n}{(2\pi RT)^{3/2}}\exp[-\frac{(\boldsymbol{\xi}-\mathbf{V})^2}{2RT}]$$

where $M$ is the local Maxwellian distribution function, $n$ is the number density, $p$ is the local pressure and $\mu$ is the gas viscosity at local temperature $T$, $\mathbf{V}$ is the vector of bulk velocity, $R$ is the specific gas constant.

On each time step, molecules come into kinetic domain $\Omega_K$ from the NS one with the Chapman–Enskog distribution function:

$$f(t,\mathbf{x},\boldsymbol{\xi})|_{\Gamma_K} = f_{CE}(M) \quad \text{if} \quad \boldsymbol{\xi}\cdot\boldsymbol{\eta}(\mathbf{x}) < 0$$

$$f_{CE} = M\left(1 + \tau_{ij}\left(\frac{m}{2Tk}\right)c_i c_j - \right.$$

$$\left.\frac{q_i}{p}\left(\frac{m}{kT}\right)\left(1 - \frac{\mathbf{c}^2}{5}\frac{m}{kT}\right)c_i\right), \quad \mathbf{c} = \boldsymbol{\xi} - \mathbf{V}, \; q_i = -\lambda\frac{\partial T}{\partial x_i},$$

$$\tau_{ij} = -\frac{\mu}{p}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right),$$

where $\boldsymbol{\eta}(\mathbf{x})$ is the outward vector normal to the $\Gamma_K$, boundary of $\Omega_K$, $\mathbf{q}$ is the heat flux vector, $\tau_{ij}$ is the shear stress tensor, $\lambda$ is the gas conductivity at local temperature $T$. All macro values are computed in the NS region: in the grid point $x_i$ (if the coupling boundary $\Gamma_K$ is placed in $x_{i+1/2}$) and their gradients in the points $x_{i-1}$, $x_i$, $x_{i+1/2}$.

The Maxwell diffuse reflecting boundary conditions with the full accommodation on walls are applied:

$$f(t,\mathbf{x},\boldsymbol{\xi})|_w = \alpha(\mathbf{x})M(n_w,u_w,T_w) \text{ if } \boldsymbol{\xi}\cdot\boldsymbol{\eta}(\mathbf{x}) < 0,$$

where $n_w$, $T_w$ and $u_w$ are the wall number density, temperature and velocity, respectively. The parameter $\alpha(\mathbf{x})$ is determined to so as to avoid a mass flux across the wall. For all particles coming off the surface it is assumed that molecules are emitted with the Maxwell distribution functions corresponding the zero mean flow velocity, the temperature is equal to the wall temperature $T_w$ and the density calculated from the condition of equality of the fluxes of particles coming on and off the wall. At the symmetry line the specular boundary condition is imposed.

On continuum domain $\Omega_{NS}$ the NS equations are solved, which can be written using the usual abstract conservative form:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

where $U = (\rho, \rho V, \rho e_{tot})$, $e_{tot} = u^2/2 + e_{int}$, $e_{tot}$ is the macroscopic total energy, $e_{int}$ is the macroscopic internal energy. At the inlet total pressure $p_0$ and temperature $T_0$ are defined while the outflow exit pressure $p_e$ is kept constant. The coupling from kinetic solver to the NS one is achieved by imposing the incoming half fluxes $F^-(U)\bullet\eta$, computed by the kinetic solver on the coupling boundary $\Gamma_K$

$$F^-(U)\cdot\boldsymbol{\eta}(\mathbf{x}) = \int\phi(\boldsymbol{\xi})\boldsymbol{\xi}\cdot\boldsymbol{\eta}(\mathbf{x})f_K(t,\boldsymbol{\xi},\mathbf{x})d\boldsymbol{\xi},$$

where $\phi(\boldsymbol{\xi}) = \{1, \boldsymbol{\xi}, \boldsymbol{\xi}^2\}$, $f_K$ is the distribution function, which is solution of kinetic equation for outgoing molecules.

### 3.2 Kinetic solver

In the hybrid solver the same numerical method is applied as for pure kinetic simulations. In the rest of the paper the non-dimensional formulation of the problem is used and for sake of simplicity the dimensionless quantities keep the same designations as the dimensional ones. The scale quantities are the following: $n_0$ is the number density, $T_0$ is the temperature,

$v_0 = \sqrt{2RT_0}$ is the thermal velocity, $H$ is the distance between plates, $\mu_0$ is the gas viscosity at $T_0$. For hard—sphere model the dimensionless viscosity coefficient is $\sqrt{T}$.

In the non-dimensional form collision integral is written as follows:

$$J_{BGK} = \frac{8}{5Kn\sqrt{\pi}} \frac{nT}{\mu}\left(M - f\right), \quad \delta = \frac{8}{5\sqrt{\pi}} \frac{1}{Kn}$$

where $Kn$ is the Knudsen number based on $H$, $\delta$ is the rarefaction parameter. The macroscopic (bulk) distributions of number density, velocity vector and temperature can be written as

$$U = \begin{pmatrix} n \\ \mathbf{V} \\ T \end{pmatrix} = \begin{pmatrix} \int f d\xi \\ \frac{1}{n}\int \xi f d\xi \\ \frac{1}{n}\int (\xi - \mathbf{V})^2 f d\xi \end{pmatrix}$$

Taking advantage of the two-dimensionality of the flow, the z component of the molecular velocity is eliminated by multiplying (1) by 1 and $\xi_z^2$ and integrating on $d\xi_z$. To discretize the obtained system of two equations, the 2D Cartesian grid with equidistant nodes is defined in the velocity space, and the grid $\{x_i, y_j\}$ is defined in the physical space. Introducing of the grid values, the obtained set of equations for $f$ is numerically solved explicit-implicitly in time [11].

The collision part is written on n+1 time level, while macroscopic quantity $U^{n+1}$ can be obtained explicitly, which defines $M^{n+1}$.

The numerical solution of the transport step is treated explicitly and approximated by a standard finite volume scheme with the flux limiter function, provided a second order of the scheme. The time step follows the condition: $\Delta t = CFL/max(V_{max}/\Delta x + V_{max}/\Delta y)$, $CFL = 0.7$ is the Courant - Friedrichs - Lewy number, $V_{max} = 5$ is a boundary of the velocity space and $\Delta x$ and $\Delta y$ are the mesh sizes in the $x$ and $y$ directions, respectively.

The results have been obtained with a non uniform, structured mesh of 280 points in $x$ direction and 40 ones in $y$ (for $L = 5$, $L_1 = 20$, $L_2 = 40$) and $260 \times 40$ (for $L = 10$, $L_1 = 10$, $L_2 = 20$) nodes in physical space. For the slit problem the computational domain is taken in the form of a half circle with radius $L_1 = 100$, kinetic and NS solvers used the mesh of $320 \times 40$ and for the hybrid code mesh was $303 \times 60$ with minimum axial spacing is of the order of $0.02H$. For all calculations $24 \times 24$ mesh in velocity space is used. The iteration process is terminated when a relative convergence criterion of $10^{-7}$ imposed on the dimensionless flow rate is fulfilled.

Parallelization in physical space for kinetic region is adopted in order to improve the efficiency of the algorithm. The software code was written in C++ with the use of MPI (Message Passing Interface). The code run on double processors, quad core systems, using, thus, up to a total of 8 parallel processes.

### 3.3 Navier-Stokes solver

For the solution of the problem the viscous, compressible NS equations for 2D laminar flow are solved by employing a hybrid finite difference-finite volume method. For the time integration implicit, spatially factored ADI scheme proposed by Beam and Warming is used [12]. The program in FORTRAN has been developed by Croce [13] and has already been applied and validated for the simulations of microflows [14].

## 4. Results and discussions

The numerical simulation of 2D gas flow through a short channel of the length $L = 0$, 5 and 10 between two containers for the pressure ratio $p_0/p_e = 0.1$, 0.5 and 0.9 and rarefaction parameter $\delta = 10$ have been carried out using three solvers: kinetic, NS and hybrid.

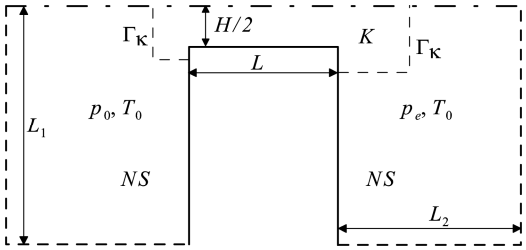



Fig. 1. The computational domain: solid line is the wall, dash- dotted line is symmetry one.

The validation for kinetic solver has been done by comparison with the DSMC results for the case of the flow through the channel of length $L = 0$, 5 and 10 into the vacuum [15]. The dimensionless flow rate $W = m/m_{fm}$ (where $m_{fm} = p_0 H / \sqrt{\pi} v_0$ is the analytically deduced mass flow rate in the free molecular regime) computed by both methods are very close and shown in Fig. 2.

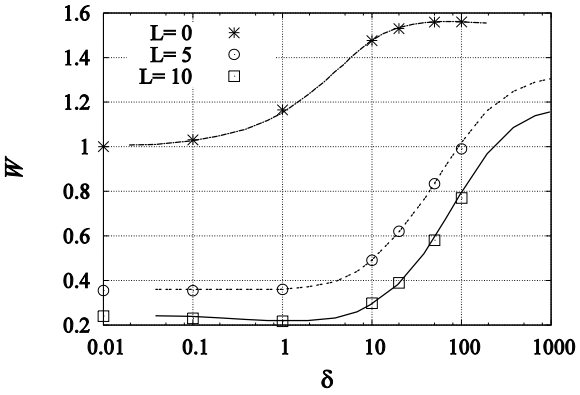


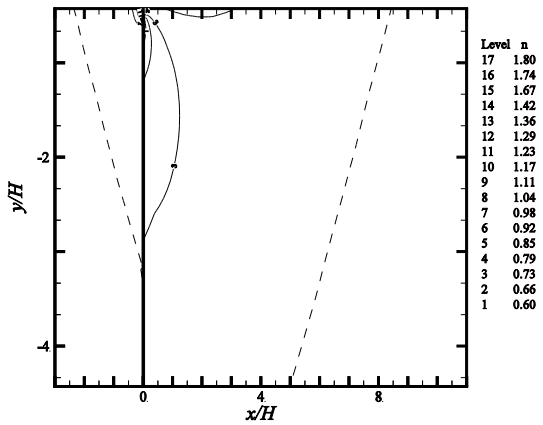

Fig. 2. The dimensionless mass flow rate vs. rarefaction parameter: lines, DSMC results; symbols, BGK ones.

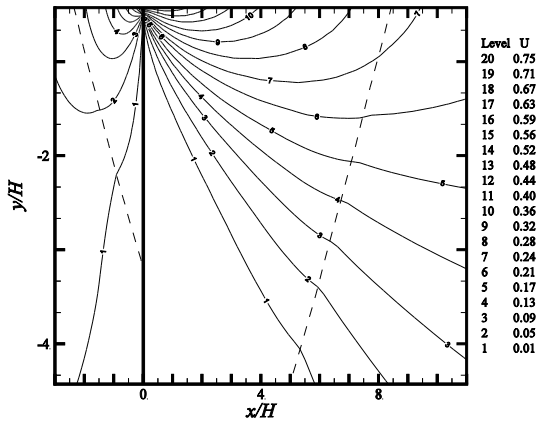
**TABLE 1**. Kinetic domain.

| $p_e/p_0$ | $L$ | $\Omega_K$ |
|---|---|---|
| 0.1 | 0 | $-1.29 < x < 9.84$ |
| | 5 | $-4 < x < 9.28$ |
| | 10 | $-6.61 < x < 8.2$ |
| 0.5 | 0 | $-2.7 < x < 8.75$ |
| | 5 | $-4.25 < x < 7.23$ |
| | 10 | $-6.61 < x < 7.32$ |
| 0.9 | 0 | $-3.64 < x < 4.07$ |
| | 5 | $-3.97 < x < 5.68$ |
| | 10 | $-6.62 < x < 7.3$ |

For hybrid code most of the computational domain is described by the NS model, while a region near the channel is described by the BGK model (see Table 1). To demonstrate the consistency of the hybrid method the contour lines of number density, velocity and temperature for $L = 0$ and pressure ratio $p_e/p_0 = 0.5$ are presented in Fig. 3 (dashed line denotes the domains interface). The coupling between kinetic and NS solutions works well enough, showing a smooth transition along the iso lines crossing the domains interface. It should be noticed that the iso lines of temperature are less smooth. This can be explained by the use of the kinetic BGK model which does not provide correct Prandtl number.

In Fig. 4-6 the variation of the dimensionless number density, velocity and temperature along the symmetry axis are shown for three different length $L = 0$, 5 and 10, and pressure ratio $p_e/p_0 = 0.1$, 0.5 and 0.9.



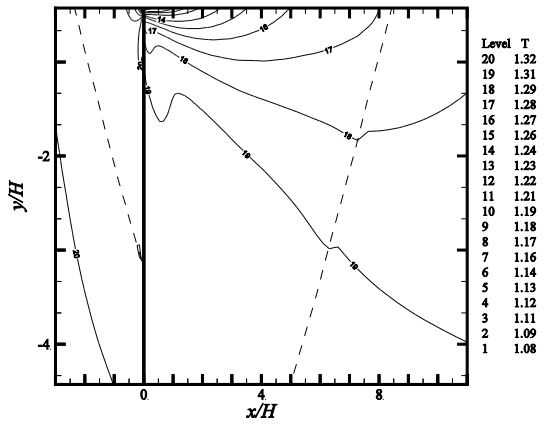



Fig. 3. Contours of number density, velocity and temperature near the slit for $p_e/p_0 = 0.5$.

Coupled solutions are compared with NS and BGK results as a reference. The density (or pressure) variations are qualitatively similar in all cases. In case $L = 0$ (slit flow), before and after the slit density tends to upstream and downstream conditions, while in the slit region it sharply decreases. The axial velocity far upstream is almost zero and it grows in the region around the slit. The temperature decreases near the slit, while at the rest of the domain it remains very close to the reference temperature. The same behavior is observed for the flow through the short channels of length $L = 5$ and 10. Starting from the upstream conditions density and temperature gradually decrease inside the channel while the velocity increases. All values tend to their downstream conditions. The axial velocity, far upstream is equal to zero. It should be noticed that for large pressure ratio $p_e/p_0 = 0.1$, as shown in Fig. 4, the flow demonstrates more complex behavior after the slit due to the transonic flow structures.

It can be seen that coupled results are always closer to NS ones, especially for small pressure ratio 0.1. The largest difference is observed for velocity distribution. It seems that the influence of the NS model on kinetic one by imposing the incoming Chapman–Enskog distribution function $f_{CE}$ on the coupling interface $\Gamma_K$ is dominant and defines the solution of hybrid solver. For moderate and large pressure ratios the results obtained by all solvers are close to each other.

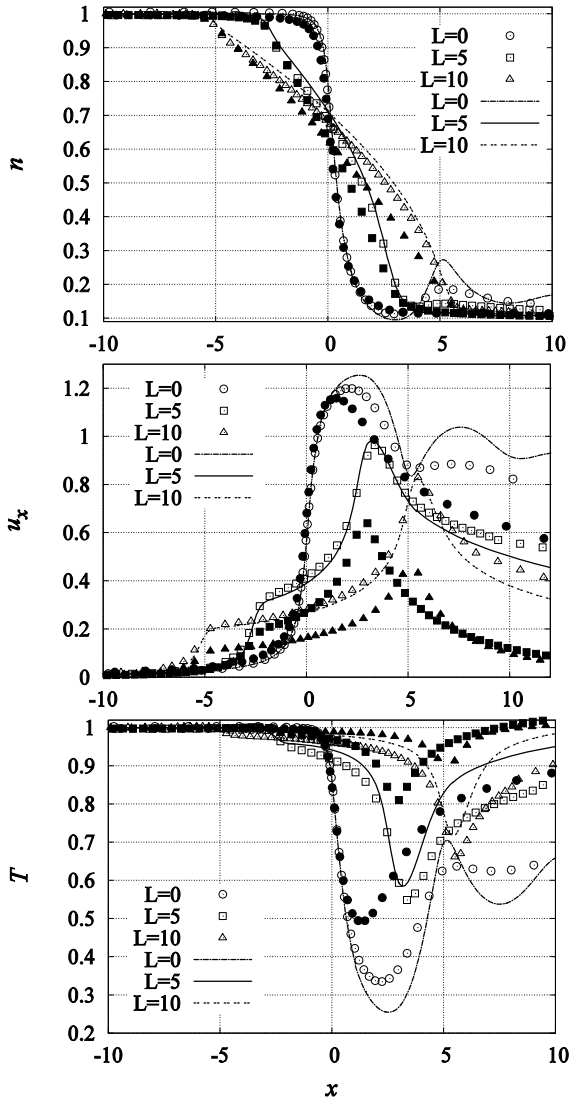
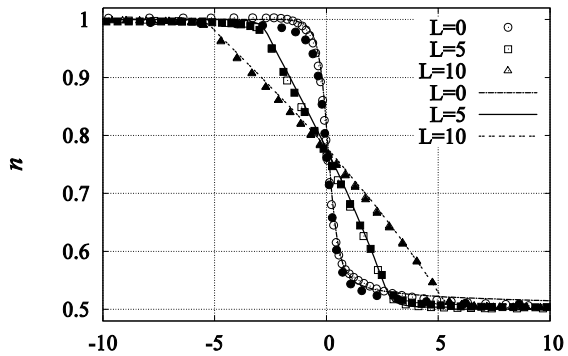



Fig. 4. Distributions of density, velocity and temperature along the symmetry line for $p_e/p_0$=0.1: empty symbols, coupled solutions; filled symbols, BGK ones; lines, NS ones.



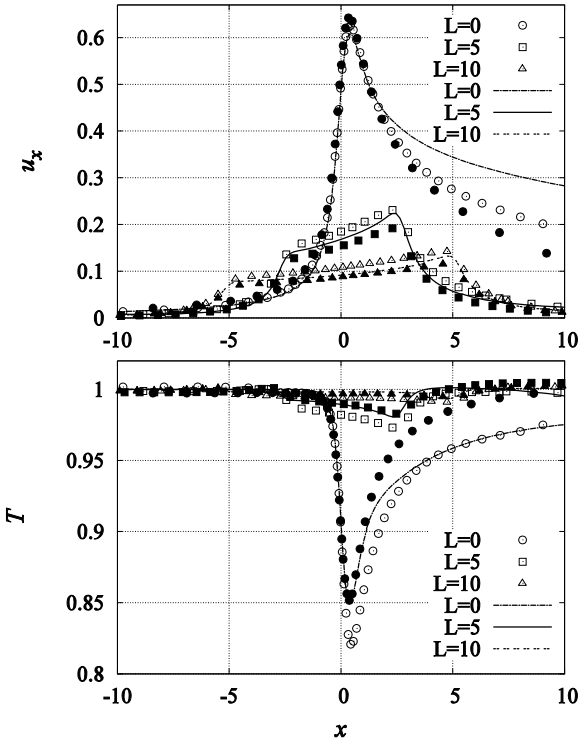
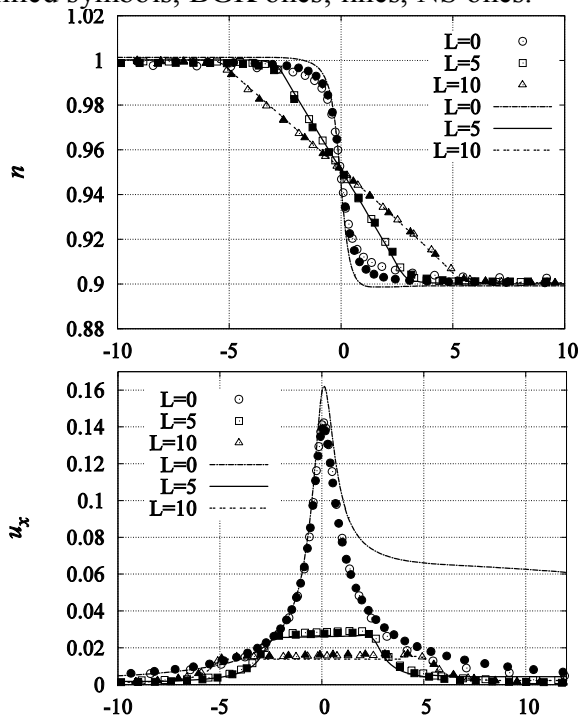



Fig. 5. Distributions of density, axial velocity and temperature along the symmetry line for $p_e/p_0$=0.5: empty symbols, coupled solutions; filled symbols, BGK ones; lines, NS ones.



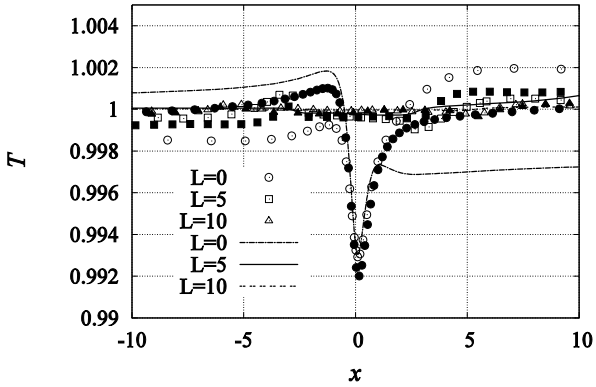




Fig. 6. Distributions of density, axial velocity and temperature along the symmetry line for $p_e/p_0$=0.9: empty symbols, coupled solutions; filled symbols, BGK ones; lines, NS ones.

In case the flow through the slit the mass flow rates obtained by all methods are very close to each other (see Fig. 7). Nevertheless, for smallest pressure ratio 0.1 the maximal difference from NS is 9%, while from BGK the difference is only 3%. The same trend keeps for other cases. For $p_e/p_0 = 0.1$ the difference between coupling and NS remains small, approximately 6%, for both length of the channel but deviation from BGK results drastically increases (50% for $L = 5$, 70% for $L = 10$). For moderate pressure ratio $p_e/p_0 = 0.5$ the NS mass flow rates almost coincide with hybrid ones and the difference with BGK ones is 13%. Under large pressure ratio $p_e/p_0 = 0.9$ all methods give close values.

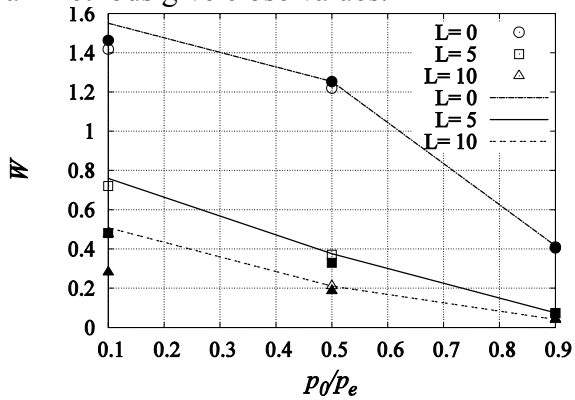



Fig. 7. The dimensionless mass flow rate vs. $p_e/p_0$: empty symbols, coupled solutions; filled symbols, BGK solutions; lines, NS solutions.

## 3. Conclusions

A hybrid algorithm based on the direct numerical solution of the BGK kinetic

equation coupled to a NS model was presented. The coupling was achieved by matching half fluxes at the interface of the kinetic and NS domains, taking care of the conservation of momentum, energy and mass through the interface. We have demonstrated the capability of the hybrid code for pressure driven gas flow through a short microchannel for relatively large rarefaction parameter $\delta = 10$. It was found that influence of NS model on kinetic one via imposing Chapman Enskog distribution function is dominant resulting in hybrid solver results are close to NS one. Thus, further investigation of hybrid cod is necessary.

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