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Numerical Study of Gaseous Flow in Divergent Micro/Nanochannels

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Abstract
The rarefied gas flow through divergent micro/nano channels is numerically studied using a particle-based method, direct simulation Monte-Carlo (DSMC). Simplified Bernoulli-trials (SBT) collision scheme is employed as collision partner selection method. The simulations are performed for nitrogen gas flowing through divergent nanochannels with various divergence angles (0°, 4°, 8°, 12° and 16°). The Knudsen number falls in the slip and early-transition regimes ($0.03 \leq Kn_i \leq 0.2$) and inlet-to-outlet pressure ratio is set to three. The centerline pressure and Mach number distributions are provided for various Knudsen numbers and divergence angles. Additionally, the contours of pressure and Mach number are presented for different divergence angles. The results indicate that the rarefication effects and centerline and slip velocity increase by increasing the divergent angle; while, the centerline pressure decreases by an increase in divergence angle. It is found that there is no reversal flow for rarefied gas flow through divergent micro/nanochannels. These results on rarefied gaseous flow through divergent nanochannels are considerably different than their continuum counterparts.
Keywords: *Micro/Nanoflows; DSMC; Simplified Bernoulli-Trials (SBT); Pressure-Driven Flow; Divergent Micro/Nanochannels.*

Introduction
Studying fluid flow and heat transfer in Micro/Nano systems have become one of modern and active research areas and have attracted many researchers in few past decades. Nowadays, microsystems are widely used in various industries with different applications such as micropumps, microturbines, microvalves and micro-propulsion systems. One of the essential and important component of these systems is micro/nanochannels.

Expansion, which may be sudden or gradual, appears fundamental to Micro/Nano-systems such as micropumps, microturbines, microvalves, gas chromatographs, and micro-propulsion systems. Therefore, study of rarefied gas flow through diverging micro/nanochannel is important for both engineering and scientific applications.

The behavior of gas flow in micro-devices is different than the liquid (or incompressible) flows. Rathakrishnan and Sreekanth [1] studied rarefied gas flow (Kn = 0.0026 – 1.75, Nitrogen) through circular tube with sudden increase in cross sectional area. They noted that in the transition regime, the pressure ratio and length to diameter ratio of the passage strongly influence the discharge through sudden enlargements. In a recent experimental study involving flow through a sudden expansion, Varade et al. [2] observed a discontinuity in the slope of pressure and absence of flow separation at the junction; in the slip regime. These measurements are qualitatively similar to the two-dimensional planar simulations of Agrawal et al. [3]. Lee et al. [4] in an experimental study on gas flow through microchannels connected through diverging section observed that the mass flow rate decreases and the pressure loss increases with increasing included angle of the transition section.

The Direct Simulation Monte-Carlo (DSMC) method is such a particle-based algorithm for simulating rarefied gas flows [5] and is valid for the investigation of gas flows in regimes ranging from continuum to free-molecular conditions. The degree of gas rarefaction is determined by the Knudsen number ($Kn=\lambda/D$), which is defined as the ratio of mean free path (λ) of gas molecules to a characteristic length, D. The rarefaction regimes can be generally categorized as slip ($0.001<Kn<0.1$), transition ($0.1< Kn<10$), and free molecular ($Kn>10$) ones. Recently, Stefanov [6] proposed the simplified Bernoulli trials (SBT) collision scheme as an alternative to NTC scheme that avoids the repeated collision in cells and permits simulations using a much smaller mean number of particles per cell (PPC). It is shown that SBT scheme could obtain an accurate solution even with PPC=2 and even less while the NTC scheme requires a PPC around 15~20 for typical test cases [7]. Detailed information about DSMC method and SBT collision scheme can be found in [5-7]. The DSMC code used in the present work has been implemented in OpenFOAM. This solver, has been validated for a variety of benchmark cases [8]. In our extended DSMC solver the collisions between particles are simulated using Variable Hard Sphere (VHS) collision model and Larsen–Borgnakke internal energy redistribution model [5].

It can be noted that a systematic and detailed analysis for gas flow through divergent nanochannels is not available. The objectives of this work are to investigate the gas flow behavior through divergent nanochannels with different configurations at different rarefication regimes and to highlight significant differences with respect to continuum flow behavior.

Problem Description
The Poiseuille flow of nitrogen gas through a divergent nano-channel is investigated in this paper.

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The schematic diagram of the geometry is shown in figure 1, where the inlet height of channel (H) is 500nm, and the length (L) is 10H. The divergence angle (θ) is considered as a parameter to study and is equal to 0°, 4°, 8°, 12° and 16°. The wall and inlet gas temperatures are all equal at 300 K. The inlet to outlet pressure ratio (PR) is 3. The Knudsen number based on inlet height (H) is set to 0.03, 0.05, 0.1 and 0.2. Only one half of channel is used for simulation due to the symmetry of the channel. A value of 0.926 for the tangential momentum accommodation coefficient, as recommended by Agrawal and Prabhu [9] is employed here. Solution is continued even when the values of mass flow rate at the inlet and outlet become equal to decrease the statistical fluctuations in flow paramters.

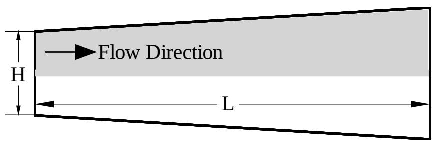

Fig. 1: Schematic diagram of divergent nano-channel

Results and Discussions

To finalize the suitable grid sizes and number of DSMC simulator particles in each cell grid and particle independency tests are performed. A grid with cell sizes of λ/3 in each direction is selected after grid study. Additionally, the simulations are initialized with PPC=5.

To validate our extended DSMC solver a micro-channel Poiseuille flow of nitrogen gas is used. This benchmark includes a channel of height 0.4 µm, and 2 µm length, meshed with 100×60 computational cells. The surface and inlet gas temperatures are set to 300K. The outlet pressure is 101325 Pa, and the inlet to outlet pressure ratio is 2.5. The Knudsen number at the inlet is 0.055 and 0.123 at the exit. These simulations contained two and five DSMC simulator particles in each cell and was solved in parallel on two processors. The results are compared with previous numerical work of the same case from both Liou and Fang [10] and White et al. [11] as well as a first order analytical slip solution and presented in figure 2 and a good agreement is achieved.

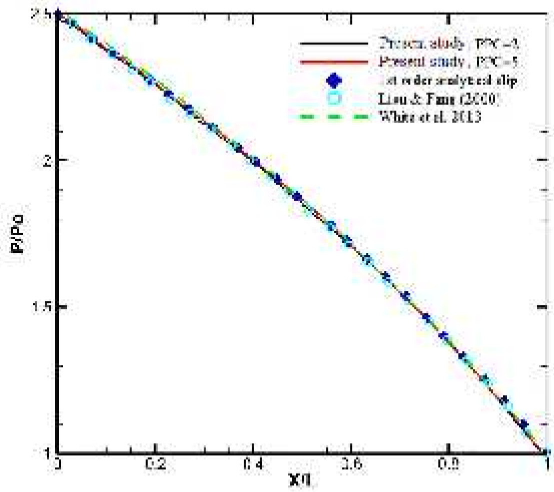

Fig. 2: Comparisons of stream-wise center-line pressure distribution with previous numerical work from [10, 11]

We focus on providing DSMC simulations in the slip and early transition Knudsen number regimes. Pressure and Mach number distributions along the divergent nano-channel center-lines are plotted for a range of Knudsen and divergence angles.

Figure 3 shows the normalized pressure distributions for different channel configurations when Kn_i=0.1. It is observed that an increase in divergence angle would result in a decrease in the slope of pressure distribution. As is seen, the pressure distribution is almost linear for the channel with θ=8°. It should be noted that compressibility increases the pressure nonlinearity while the rarefaction causes more linearity for the pressure distribution. For the divergent channel with θ=8° these two factors balance their impacts. For the divergent channels with θ>8° the rarefication effect becomes more dominant than compressibility effects. Figure 4 represents the local Mach number for different channel configurations when Kn_i=0.1. It is clearly shown indicated that Mach number increases along channel by increasing the divergence angle. It is in consistence with pressure distribution once by decreasing the pressure along the channel the velocity inside the channel will increase.

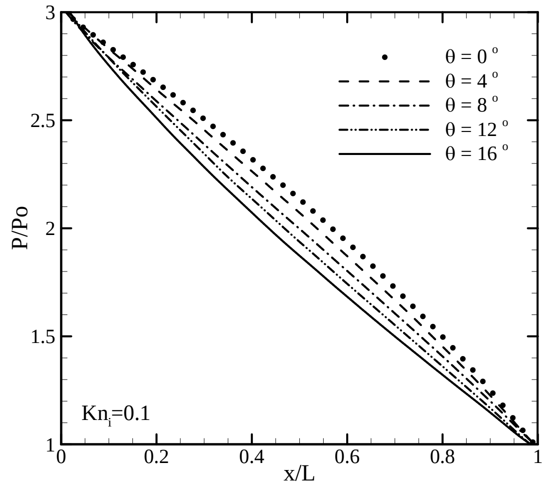

Figure 3. Stream-wise center-line pressure distributions for different divergence angle, Kn_i=0.1

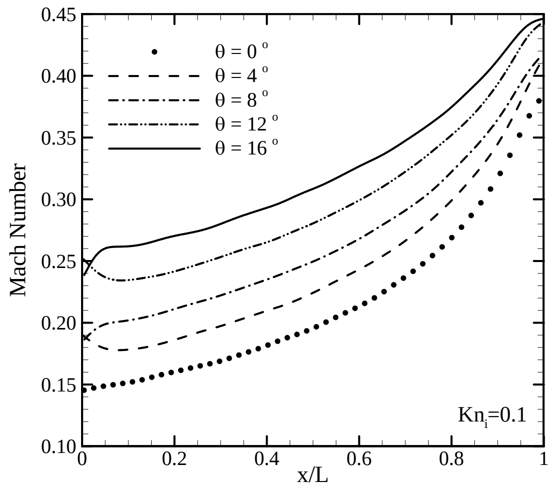

Figure 4. Stream-wise center-line Mach number distributions for different divergence angle, Kn_i=0.1

Figure 5 shows the normalized pressure distributions of the channel with θ=8° for different Knudsen numbers. As expected, non-linear pressure profiles have been found, and the degree of non-linearity decreases with increasing Knudsen number as rarefaction effects begin to dominate the compressibility effects. Figure 6 indicates the local Mach number of the channel with θ=8° for different Knudsen numbers. It is clearly observable that as the Knudsen number increases, the centerline Mach number along the divergent nano-channel decreases. Figure 6 indicates the local Mach number of the divergent nano-channels with θ=8° for different Knudsen numbers. It is clearly observable that as the Knudsen number increases, the centerline velocity along the divergent nano-channel decreases.

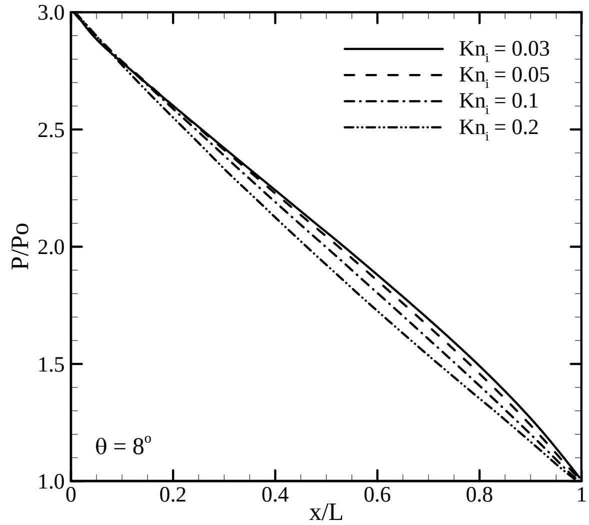

Figure 5. Stream-wise center-line pressure profiles for different Knudsen numbers, θ=8°

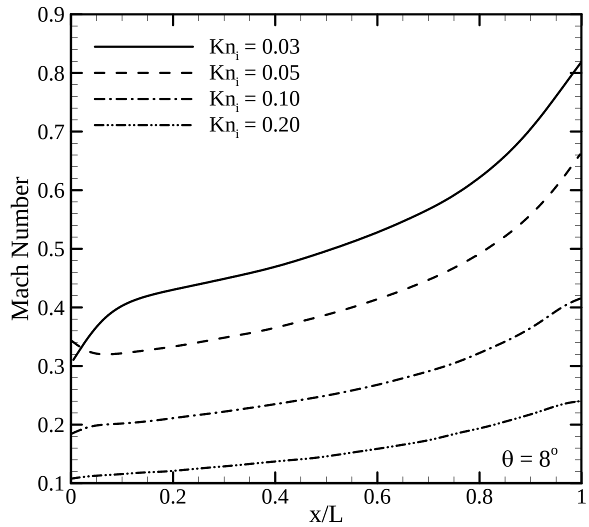

Figure 6. Stream-wise center-line Mach number profiles for different Knudsen numbers, θ=8°

Figure 7 presents the contours of Mach number for divergent nano-channels with θ=0° and 16° at Kn_i=0.1. It is worth mentioning that there is no flow reversal due to slip at the wall. In contrast, White [12] reported flow reversal for incompressible flow through 15° micro-diffuser and Duryodhan et al. [13] noted flow reversal for incompressible flow through 16° diverging microchannel. Additionally, it is clearly seen that the Mach number increases along the channel with an increase in θ.

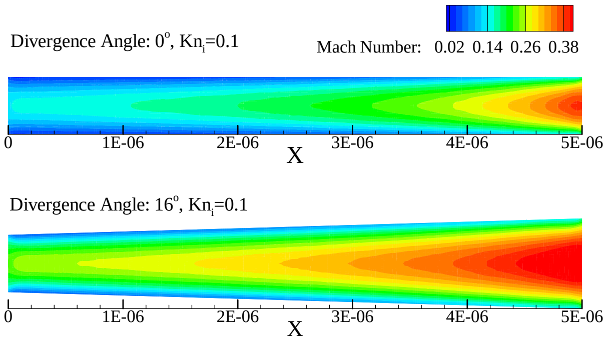

Figure 7. Contours of Mach number for divergent nano-channels with θ=0°, 16°. (Kn_i=0.1)

To investigate the mass flow rate through divergent nano-channels, the mass fluxes are plotted in figure 8. It is observed that the mass flow rate increases by decreasing the Knudsen number. Moreover, the mass flow rate trough divergent nano-channels increases by an increase in divergent angle. The mass flow rate for the divergent nano-channels with divergent angle of 16° is folded up to 1.7 compared to straight nano-channels at same Knudsen number and pressure ratio. It is observed that for a fixed pressure drop, higher divergence angle will result higher mass flow rates.

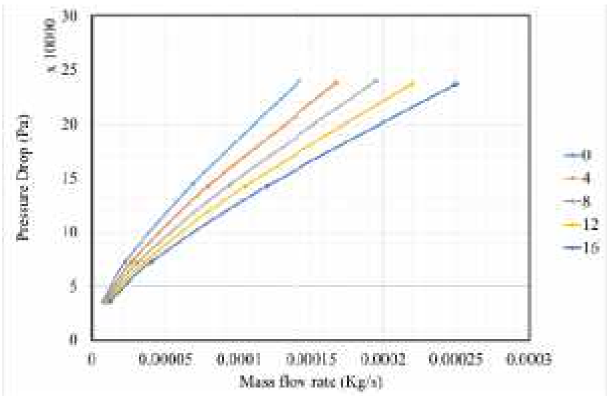

Figure 6. Mass flow rate through divergent nano-channels versus pressure drop.

Conclusions

The DSMC method with SBT collision scheme used to simulate subsonic Poiseuille flow of nitrogen gas through divergent nano-channels. These simulations are implemented in framework of an open-source flow solver, OpenFOAM, and was solved in parallel on two processors. The results presented for different Knudsen numbers and divergence angles at pressure ratio of 3. It is observed that by increasing the divergence angle and Knudsen number the compressibility effect is weakened. Furthermore, it is found that due to slip at the wall of the divergent nano-channels there is no reversal flow. The slip velocity increase as the flow move toward the channel outlet. The mass flow rate of the divergent nano-channels compared with straight nano-channels and it is found that the mass flow rate increases by increasing the divergence angle and decreasing the Knudsen number. Channels with higher divergence angles results higher mass flow rates at a fixed pressure drop.

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