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Parallel DSMC simulation of Nano Cavity Structures

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Abstract: A parallelization strategy is applied to the Direct Simulation Mont Carlo (DSMC) method to improve its efficiency in non-equilibrium regimes. In order to distribute the workload among the processors, we decomposed the physical domain into the subdomains. The Message Passing Interface (MPI) library is used to transfer information between subdomains. We used an intelligent algorithm to specify the physical bounds of subdomains in an order to result in an equivalent computational time for each processor. The effects of domain splitting on the parallel speed up and the idling time of processors are studied. We then investigated a nano lid-driven cavity to investigate the effects of non-equilibrium on the rarefied flow behaviour. As the characteristic length of the driven cavity decreases non-equilibrium effects enlarges, which subsequently reduces the induced moment by the driven lid of the cavity. As a result the center of primary vortex moves toward the physical center of cavity geometry. It is seen that once the characteristic length of the cavity enters the nano scale the center of vortex location changes its trend and move away from the center of cavity. The Knudsen diffusion phenomenon which comes to the play when the frequency of molecule-surface collisions outweighs the intermolecular collision is hold responsible for this behavior.

Keywords: Parallel DSMC; Nano cavity structures; Rarefied flow; Knudsen diffusion; Center of vortex.

Introduction

Micro/Nano-electro-mechanical systems (MEMS/NEMS) are extensively utilized in many application areas including industrial engineering and biomedical devices. The study of gaseous flow in micro and nano scales has been an interesting and appealing topic of researches in recent years. It is well known that the traditional Navier-Stocks-Fourier (NSF) equations lose their promise to describe flow features as characteristic length enters micro range and beyond. Knudsen number, which is defined as the ratio of the mean free path of the fluid to the characteristic length of the flow domain (Kn=λ/L), is the main tool to determine degrees of gas rarefaction. Discrete molecular modelling is the main tool to model flow field in all degrees of rarefaction. In this method, the fluid is modelled as a collection of moving molecules which interact through collisions. The DSMC is known as one of the most successful particle simulation methods in analyzing the rarefied gaseous flows. Roohi et al.[1, 2] used DSMC to simulate the supersonic and subsonic choked flow in the micro/nano channels.

The driven cavity is a common geometry in the industrial application. In spite of the geometrical simplicity, lid-driven cavity can encounter very complex flow features such as compressibility effects and corner eddies. Mohammadzadeh et al [3] utilized DSMC technique to investigate the effectiveness of Navier-Stocks-Fourier equations in prediction of shear stress and heat flux in an isothermal cavity. They claimed that even in the slip regime, existence of rarefaction effects hinder Navier-Stocks-Fourier equations from predicting thermal behavior of the flow accurately. They also showed that the predicted heat flux direction by DSMC is in accordance with the distribution of entropy in the driven cavity. Auld and Lan [4] used a parallelized DSMC code to locate the center of vortex in the micro lid-driven cavity in the Reynolds ranges from 50 to 7500. It was shown that when the Kn number increases the predicted location of the center of vortex by the DSMC method deviates from the NSF results.

DSMC approach

The DSMC method used in this paper follows the scheme proposed by Bird [5]. DSMC is a particle method based on the kinetic theory for simulation of the dilute gases. The method is carried out by modelling the gas flow using many independent simulated molecules. These simulated molecules are representatives of a large number of real gas particles in the flow field. In order to implement DSMC, flow field must be divided into computational cells. The size of each cell should be small enough to result in small changes in thermodynamic properties across each cell. The cells provide geometric boundaries and volumes required for sampling the macroscopic properties. They are also used as a unit where only molecules located within the same cell at a given time are allowed for collision. The cells are then divided into subcells in each direction to facilitate the selection of collision pairs.

The Message Passing Interface (MPI) library is used to extend our basic DSMC solver to a parallel DSMC code. The parallelization is performed according to the Single Program-Multiple Data scheme (SPMD). The parallel implementation of a DSMC algorithm consists of a number of steps, which are briefly described here.

1. Using SPMD, the computational domain is broken into several partitions. Each partition,

including its cells and particles, is attributed to a single processor. Evidently, the DSMC computation should be performed on each partition separately.

2. The global information of the flow field, e.g., number of cells, and number of particles in each partition, are determined. Each processor calculates the primitive required information for the cells and particles located in that partition. Using the ‘‘class’’ feature of the C language, we define three main classes in PDSMC code to collect the relevant data into three packages. These classes are particle properties, cell properties and partition properties.
3. Each processor performs particle movement in the partition.
4. The new cell of each particle is indexed.
5. If any particle crosses the partition boundary, all the related information of that particle such as position, internal energy, rotational energy, and species type are transferred to the buffer memory (sending buffer). They are deleted from the original processor and added into the new processor. The data transfer is performed one-by-one for each of the properties rather than transferring via the packet of arrays.
6. Before starting the communication process, MPI_Barrier function is used to make sure that all the involved processors are ready to exchange data packages. MPI_Send and MPI_Recv commands are used for exchanging the particles information.
7. As soon as the communication is complete, the sending buffer is reset to be used in the next time step.
8. The communication is followed by an additional ‘‘cross-move’’ procedure, where the new particles stored in receiving buffers are directed to their new special locations.
9. Newly moved particles are indexed into their new cells. Moreover, the molecular collision and the flow sampling procedure are fulfilled in the same manner as in a serial DSMC algorithm.

Results and Discussion

In this study the top driven-lid of nano cavity moves in positive x-direction with U_{wall}=100 m/s. The walls temperatures are set to the reference temperature, i.e. $T_w = T_0 = 300$ K. Three grids composed of 100×100, 200×200 and 400×400 cells are used for the grid study. Results of grid study test are shown in Figure 1. In this figure density is non-dimensionalized with respect to a reference density obtained on the driven lid. It is seen that the results are numerically equivalent for 200×200 and 400×400 grids; therefore the grid containing 200×200 cells is selected for the reported results of the parallel DSMC method in this study.

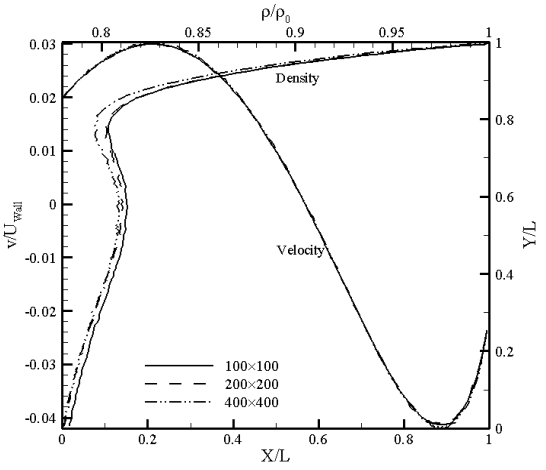

Figure 1: Grid independency test

Figure 2 depicts the distribution of non-dimensional horizontal component of velocity vector in the nano cavity overlaid on the velocity streamlines at Kn=10. As was expected non-equilibrium effects hinders the rarefied flow from sensing the induced velocity by the driven lid of the cavity.

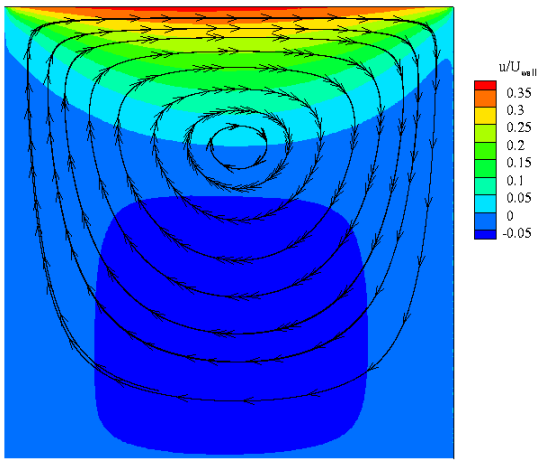

Figure 2: Horizontal velocity distribution overlaid on the velocity streamline, Kn=10

We also define the circulation, Γ of the mean velocity field in order to compare the strength of primarily vortex in the flow field.

$$\Gamma = \oint V.ds = \int rot_n V.dA \approx \sum_{i,j} [\frac{(V_{y\,i+1} - V_{y\,i,j})}{\Delta x} - \frac{(V_{x\,j+1} - V_{x\,i,j})}{\Delta y}] \Delta x \Delta y \qquad (1)$$

where the summation is taken over all cells in the cavity. Figure 3 shows the total circulation in the driven cavity for the Knudsen range. In this figure circulation values are normalized with $\Gamma_0 = U_{wall}.L$. It is seen that increasing non-equilibrium effects, which gradually prevent molecules from sensing the imposed shear stress by the driven lid, reduces the strength of primarily vortex.

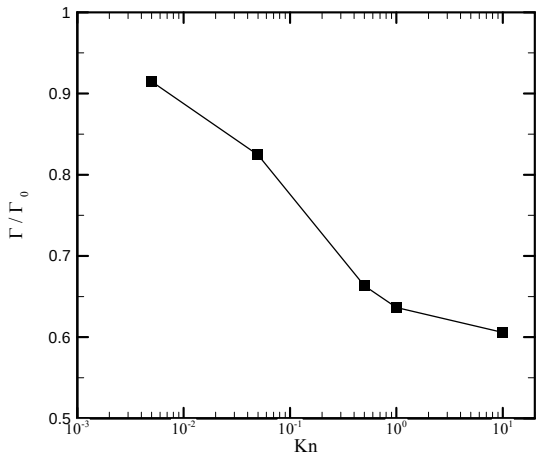

Figure 3: Variation of total circulation by Knudsen number

Variation of centre of vortex location by Knudsen number is shown in Figure 4. As Knudsen number increases Reynolds number decreases, thus viscous dissipation in the flow field enlarges. As a result, the induced kinetic energy from the top lid dissipates more notably in higher Knudsen number, which makes the center of vortex shift toward left to the center of cavity. Figure 4 indicates that there exist a sudden change in the trend of centre of vortex location around Kn=1. Similar to the Knudsen minimum phenomena in microchannels, in which diffusive transport process appear and consequently affect the mass flow rate, such variation in the trend of primary vortex is probably attributed to the effects of Knudsen diffusion. Furthermore, it is seen that as the flow rarefies, centre of vortex moves away from the driven lid of the cavity toward the bottom wall. Reduction of the induced velocity in higher Knudsen regimes forces the center of vortex move toward the bottom wall to compensate the reduction of mass flow rate in the top segments of the cavity.

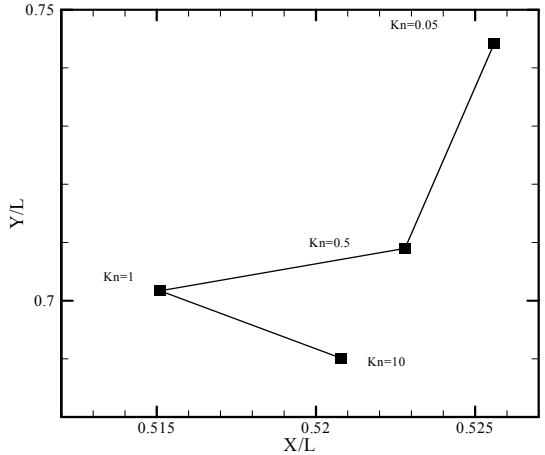

Figure 4: Variation of center of vortex location by Knudsen number

Conclusions

In this paper we implemented parallel DSMC to investigate the nano scale cavity. Our simulation shows that the total circulation in the cavity reduces dramatically once the characteristic length of the cavity enters micro and nano scales. Moreover, as the cavity classifies as nano structured, specific diffusion mechanisms which significantly change the hydrodynamic behavior of the rarefied flow come to the play.

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