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MONTE CARLO ANALYSIS OF GAS FLOW IN CYLINDRICAL MICRO-CHANNEL USING OpenFOAM

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Abstract

Monte Carlo simulations of three-dimensional steady-state rarefied hypersonic flow in cylinder at different Knudsen number are performed by using the direct simulation Monte Carlo (DSMC) method. Direct Stimulation Monte Carlo (DSMC) method is used to solve the problem, which employs a large number of particles in modelling a rarefied gas and where molecular effects are of importance. A control volume analysis is carried out to understand the reason for temperature drop in microchannels. The work focuses on the effects in the aerodynamic surface quantities, such as geometrical parameters, density, shock structure, temperature distribution, and net heat flux on the wall due to variations in Knudsen number. The Knudsen number (Kn) defines the degree of rarefaction. The results show that the presented method can simulate the aerodynamic heating process of a hypersonic vehicle in rarefied flow, during re-entry, and can provide technical support for the design of rarefied-flow hypersonic vehicles in terms of thermal protection systems and aerodynamic heating characteristics analysis. The analysis showed that surface quantities presented at large dependence Knudsen number for the range investigated. An algorithm of the direct simulation Monte Carlo (DSMC) method of the flow of the nitrogen in a cylindrical channel is developed using OpenFOAM. This work presents benchmark trials of a new, open source DSMC code called dsmcFoam. Results for the initial benchmark trials show very good agreement with analytical solutions for a re-entry vehicle.

Index Terms—*3D cylindrical micro-channel, Knudsen number, Heat flux, DSMC method*

Introduction

The Direct Simulation Monte Carlo (DSMC) [1] method allows computation of macroscopic flow field variables of rarefied gas of evolving a number of representing particles in discrete time steps. Each time step consists of decoupled sub-steps, most importantly [2]

I. Convection : Particle position;
II. Collision : Particles collide with each other on a probabilistic basis;
III. Sampling : Macroscopic flow parameters are determined.

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The flow of a gas can either be modeled as Macroscopic or Microscopic. The macroscopic model regards the gas as a continuum medium and the description is in terms of the spatial and temporal variations of the familiar flow properties such as the velocity, pressure, density and temperature. Navier-Stokes equation provides the conventional mathematical model of a gas as a continuum. On the other hand, Microscopic Model recognizes the particulate structure of the gas as a myriad of discrete molecules and ideally provides the information on the position, velocity and state of molecule at all the times. Boltzmann Equation provides the mathematical model for this model.

The macroscopic values are identified as the average values of quantities at any location in a flow. They may therefore be defined as long as there are sufficient numbers of molecules within the smallest significant volume of a flow. This condition is mostly satisfied in ma cases. But, as the density and pressure reduces, the requirement of new method rises. More specifically, the transport terms in the Navier-Stokes Equation of continuum gas dynamics fails when gradients of the macroscopic variables become so steep that their scale length is of the same order as that of the mean free path of the gas (distance travelled between two successive collisions). This leads to the inadequacy of the continuum theory of the fluid, thus particle nature of the fluid/matter is taken explicitly into account. Such flows are characterised by a quantity which gives the degree of rarefaction i.e. *Knudsen Number*, Kn [3]

$$Kn = \frac{\lambda}{L} \qquad \ldots (1)$$

, where λ= Mean Free Path
L=Characteristic Length

The traditional requirement for the Navier-Stokes equation to be valid is that the Kn<0.1. Above, *L* should not be confused with the overall length; the limit can be specified precisely if a local Knudsen Number, Kn is defined with L as the scale length of the macroscopic gradients

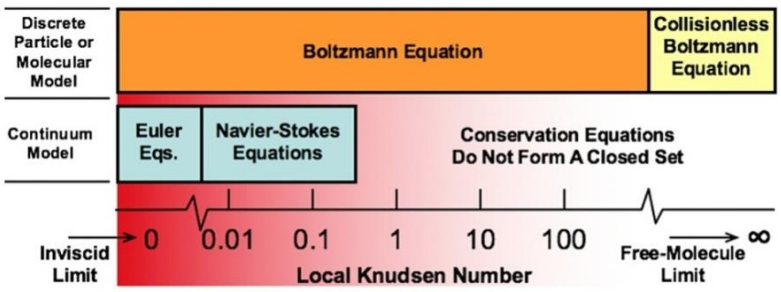

Fig 1. Knudsen Number Limits on different mathematical models

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There has been a recent development in the micro channels, channels/passages whose hydraulic diameter ranges from 10-200 micrometre's, such as *Micro- Electro- Mechanical- Systems (MEMS)* [2]. MEMS is a miniature machine that has both mechanical and electronic components. The physical dimension of a MEMS ranges from a few millimetres to a micrometre[4].

MODELLING

There are various approaches to calculate diffusive and another kinetic properties, one is such where direct tracking is done, i.e. calculation of tracks and collisions of gas molecules. Molecular Dynamics (MD) is an often applied method, where each atom or molecule is individually tracked, however with the expense of very high computational costs if larger problems are considered, to overcome the above case the required computing power and problem size, DSMC can be used[5].

A set of partial differential equation describing these properties (gas molecular properties) that satisfy the Law of Conservation of Mass, Momentum and Energy, Navier-Stokes equation provides a conventional mathematical model for analyzing the flows at macroscopic level, where the Kn < 0.01. Micro flows in the slip flow regime with 0.1> Kn > 0.01 can also use Navier-Stokes equation with slip velocity boundary. Since, Navier-Stokes equation is not valid for Kn > 0.1, to avoid the continuum assumption that breaks down at high Knudsen number, flow can be modelled by microscopic methods.

Another popular Mathematical model at this level is constructed by using the Boltzmann Equation in which the velocity distribution function is the main variable, G. A. Bird (1994) provided us simple derivation of Boltzmann Equation for Mono-atomic with Binary Collision,

$$\frac{\partial}{\partial t}(nf) + \xi_j \frac{\partial}{\partial x_i}(nf) + f_j \frac{\partial}{\partial \xi_j}(nf) = j(f, f^*) \quad \ldots(2)$$

Where n is the number of Density and *f* is the normal velocity distribution function, *xi* and *ξj* are the coordinates and the speeds of molecules. f_j is an external force and *J(f, f*)* is the non-linear collision integral, where the * represents the post-collision values. The Boltzmann equation can be used in all the four Flow Regimes and the Navier-Stokes equation is an approximation of it.

An alternative way to solve the Boltzmann equation is the DSMC, simulates the physical process described by Boltzmann equation using the Gas Dynamics theory and statistical methods. Although molecular dynamics has the advantage of accuracy it is not feasible for micro simulation in Micro- Electro- Mechanical- Systems or MEMS. Hence this becomes the promising numerical method in simulating rarefied gas flows or micro flows. In Dilute gasses, which are the major application of the DSMC method, the probability of a collision including more than 2 particles is so small that only Binary Collisions are considered. The principal requirements for the

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applicability of the method are a dilute gas and molecular chaos. The general definition of a dilute gas is given by

$$\delta \gg d \qquad ..(3)$$

Where, $\delta = n^{-1/3}$, is the mean molecular spacing and the diameter of the molecules.

In addition, if there is a collision between molecules, it is overwhelmingly probable that only two molecules are involved, so binary collisions need to be considered only. Consequently, the DSMC method cannot be used to simulate dense gases or plasmas with a high portion of ionized particles that are affected by long range interactions. In addition, DSMC utilizes models of gas molecules and boundary interactions developed in kinetic theory, which provide only an approximation to real physics. An important difference to the Boltzmann equation is that DSMC does not rely on inverse collisions. Furthermore, the boundary conditions in direct simulations are defined by the behavior of individual molecules rather than by means of a distribution function. This enables the incorporation of complex flow phenomena such as chemical reactions, which cannot be considered in the analytical model [1][3].

SIMULATION

The simulation of the flow of the rarefied gases in micro-channel has been done using the DSMC method in the CFD tool called OpenFOAM[6] using the DSMC solver. The whole work is based on OpenFOAM version 1.7.1. This is a fully parallelized open source C++ library which is freely available under the GNU general
public license from [7]. It is made for Linux operating systems and installation instructions can be found on the same web page1. The source pack is delivered with a user manual [8] and a short programmer's guide [9]. In the present simulation, the flow properties of the fluid are studied in a two dimensional micro channel i.e. rectangular channel.
The geometry of the micro channel is first coded in the OpenFOAM, by entering the spatial co-ordinates of the micro-channel. Later the micro-channel is divided into a finite number of cells. All these cells together constitute to the structure of the considered microchannel. This is called as meshing, and the mesh file for the microchannel is generated. Later the parameters of the fluid are entered (according to the requirements), and the DSMC solver is used to solve the Boltzmann equation in each cell. The solver simultaneously solves the problems at each cell and returns the values at each cell. The intensive properties of the fluid are calculated from the extensive properties.

For the present case study, the simulation of the rarefied gas flowing through cylindrical microchannel is carried out. Here, the flows in micro-channels with Knudsen number 0.031 has been simulated, At the entry gate the velocity (M_i) of the gas particle is 4.15 Mach and the temperature (T_i) 250K. The conditions at which the simulation is carried out are tabulated in Table

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1. The flow conditions and the channel size are given in Table I. The aspect ratio of the channels is set at 5 for all cases and rectangular cells (150x30x30) are used. Shown below are boundary conditions and the flow chart of a typical DSMC program.

Table 1. Boundary Conditions

QUANTITY	VALUE
LENGTH, L (µm)	12 µm
DIAMETER, D (µm)	2.4 µm
ASPECT RATIO (L/D)	5
KNUDSEN No., Kn	0.031
No. of DSMC Particles	2272
INITIAL TEMPERATURE, T_i	250 K
MACH NUMBER, M_i (at inlet)	4.15 Mach; 1423.25m/s
No. DENSITY, n	6.498×10^{23} m^{-3}
MEAN FREE PATH of UNDISTURBED GAS (m)	7.4×10^{-8}

Each computational cell has been divided into two sub-cells in each direction. In the present simulations, the time step has been chosen such that a typical molecule moves about one fourth of the cell dimension in one computational time step. Nitrogen gas is used and the variable hard sphere (VHS) model [1] has been applied
in all the simulations.

For the standard atmospheric condition, the number density is high and the mean collision time is in the order of 10-10 sec. The time step used in the DSMC method, Δt_d, should be less than the mean collision time, so that the particle movement and their collision may be uncoupled, i.e.,

$$\Delta t_d < \Delta x_d / c'_m \quad ...(4)$$

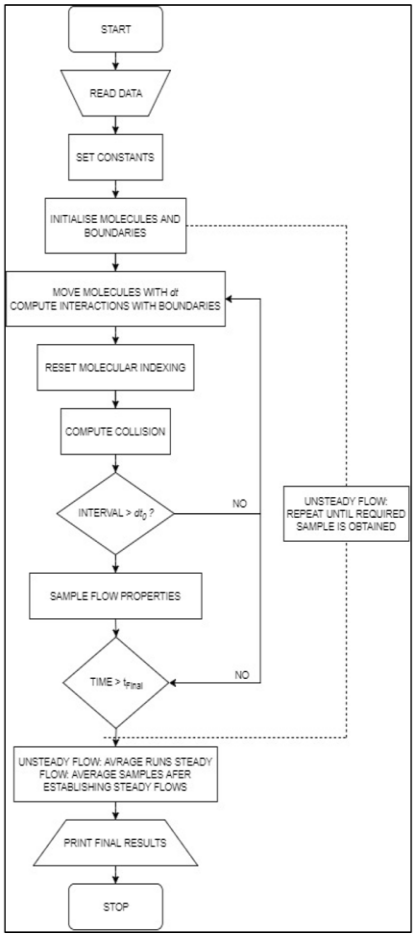

Fig. 2: Flowchart of a typical DSMC program
(Courtesy E. Oram)

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Results and Discussions

During the simulation the mesh was generated and was meshed in the ***SALOME*** software (a meshing tool), later viewed in the ***ParaView*** software. Image below shows the meshed cylinder.

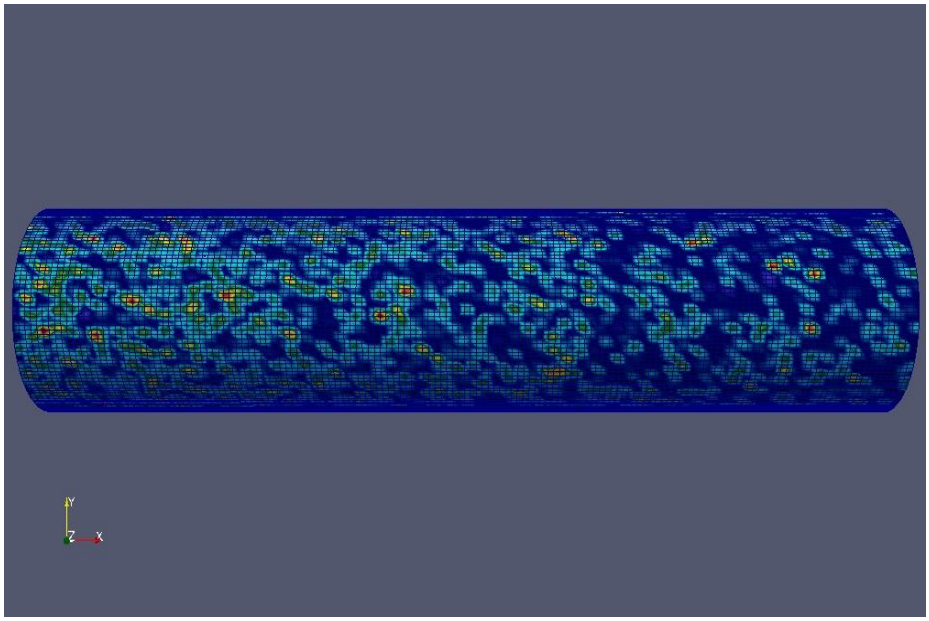

Fig. 3: Cylindrical microchannel with meshes

After mesh generation, the simulation was conducted in OpenFOAM and the following results were obtained:

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1. Mach Number Contour (or Velocity Gradient)

Fig. 4 shows the shock structures for the simulation conducted, it is clear from the figure that in an immediate up-stream of the leading edges, there is a formation of detached bow shocks, which is due to the viscous boundary Layers. The waves resulting from the intersection of the bow shocks diffuse as they separate and extend toward the wall due to the weakening incident shocks. As such, the inter- section of the bow shocks moves upstream.

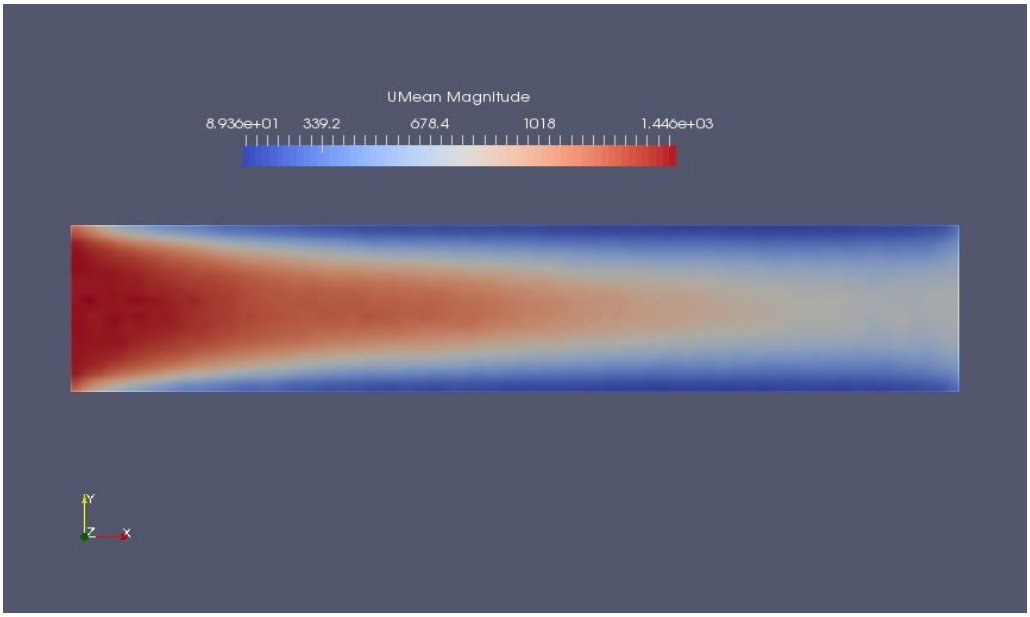

Fig. 4: Mach number Contour

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2. Temperature Contour

Fig.5 shows the temperature contours. This figure shows the incident bow shock and the strong temperature gradients across the bow shocks near the leading edges. It is also apparent that an island of high temperature is formed as the Knudsen number increases and the location of the high-temperature island moves upstream as the Knudsen number increases. The formation of the high-temperature island is, as was mentioned above, accompanied by the deceleration of the flow. Also, the thickness of the thermal boundary layers in both the cases can be observed to increase with Knudsen number.

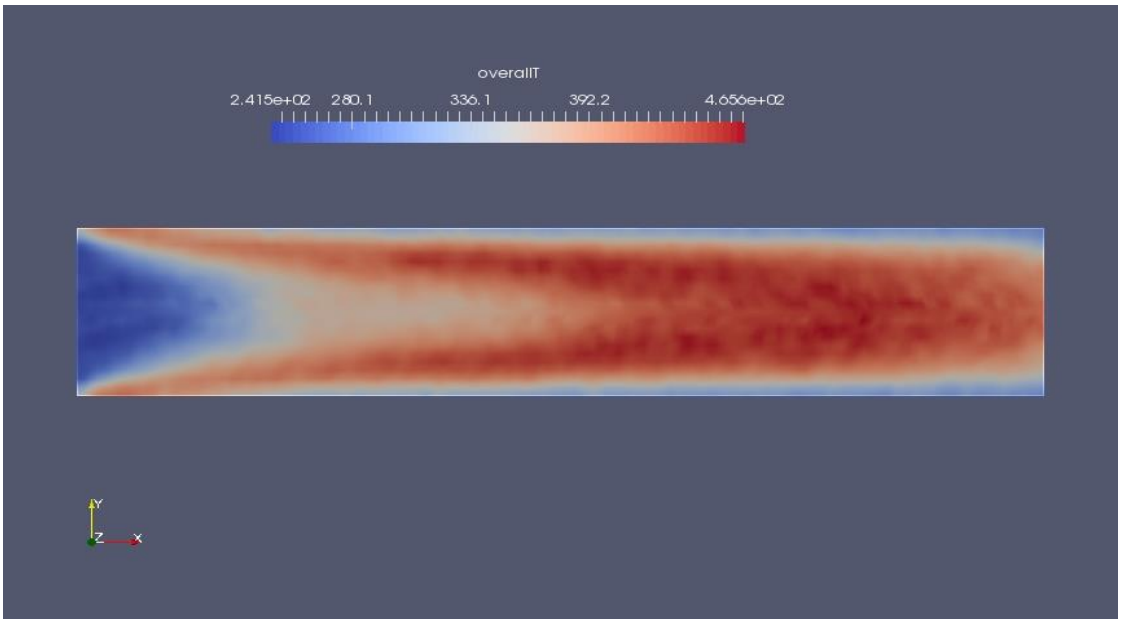

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Fig.5: Temperature Contour

3. Number Density

As shown in Figure 6, below we can observe that due to slow moving particles/molecules (at roughly 3 x 10^{-6} m) there is accumulation of molecules and thus there is increase in the number density of the paticles. This is so because of the molecular collision dominance and later accompanied by deceleration in the flow this trend can also be observerved in Mach Number contour

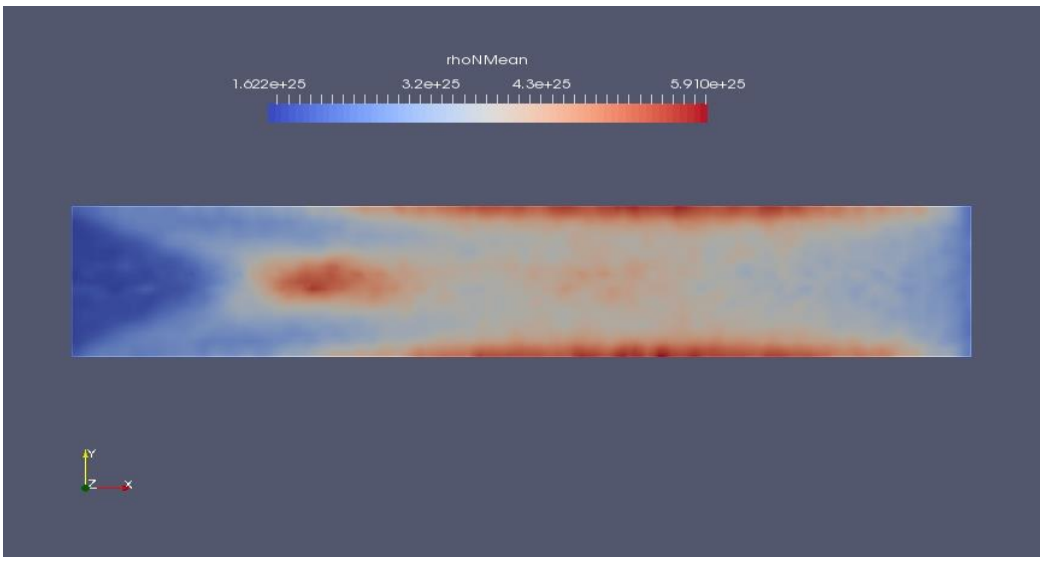

Fig. 6 Variations in Number Density

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4. Pressure Variatio

As the flow inside the microchannel is flowing in the constriction, so according to Bernoulli's theorem the reduction in the speed shoild be acccompanied by the rise in the pressure, which can be seen in here. At 3 x 10^{-6} m, there is sudden rise in the pressure, due to more amount of collisions happening at the centre of the microchannel. As the flow disperse the pressure also reduces, but stays comparativly high throughouty the flow.

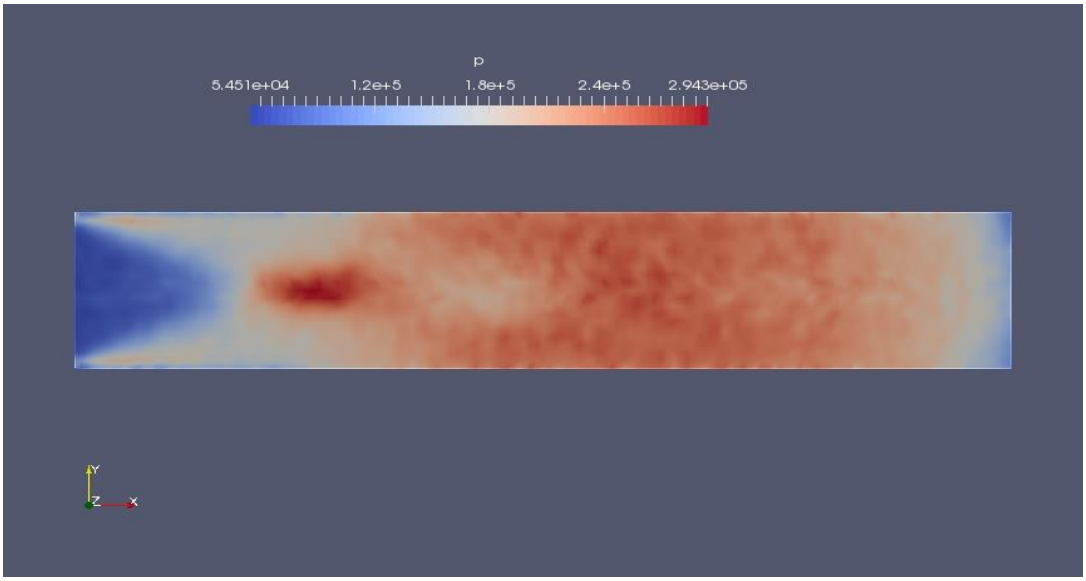

Fig. 7 Pressure Contour

Conclusion and Future Scope

We have presented benchmark trials of a new, open source DSMC code called dsmcFoam. The code has been written within the framework of the open source CFD toolbox OpenFOAM. Distinguishing features of the dsmcFoam code include its modular C++ construction with easy

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implementation of new user coding, unlimited parallel processing capabilities and an ability to handle complex, 3D geometries.

Short term future work for dsmcFoam will include the implementation of more sophisticated collision models (e.g. VSS), the inclusion of vibrational energy exchange leading to chemically reacting flows and the implementation of pressure driven boundary conditions for low-speed, in microchannel heat sinks, rarefied gas flows. Longer term objectives may include transient adaptive schemes in space and time.

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