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Direct Simulation Monte Carlo (DSMC) Algorithm – A Comparison of Mathematica Code with FLUENT 6.2 for Low Knudsen Number

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***Abstract*—**A code has been developed in Mathematica using Direct Simulation Monte Carlo (DSMC) technique. The code was tested for 2-D air flow around a circular cylinder. Same geometry and flow properties were used in FLUENT 6.2 for comparison. The results obtained from Mathematica simulation indicated significant agreement with FLUENT calculations, hence providing insight into particle nature of fluid flows.

***Keywords*—**DSMC algorithm, non continuum gas flows, Monte Carlo methods

I. Introduction

DIRECT Simulation Monte Carlo (DSMC) [1] technique is a numerical method which employs the concepts of probability theory and statistics to analyze non continuum gas flows. The gas is modeled as a collection of numerous particles. Position and velocity of every particle is determined during each time step.

A general DSMC technique comprises of five steps:-

1) Initial conditions
2) Movement of particles and interaction with walls
3) Simulation of molecular collisions
4) Indexation of particles
5) Sampling of macroscopic properties

Steps 2 – 5 are repeated for each time step.

The number of particles used, may range from few thousands to several millions, to increase the accuracy of simulation results.

Knudsen number is a parameter defined as ratio of mean free path (λ) to the characteristic length of the domain. When Knudsen number exceeds 0.3, continuum model of gas is not able to provide accurate results [1]. Therefore, molecular approach must be adopted instead. DSMC technique is one such method.

It should, however, be noted that if the Knudsen number is very low, i.e. continuum model of gases is still applicable; the molecular model must also validate the results achieved from continuum model. There are two main methods of analyzing fluid flows, firstly, Euler approach (particle tracking), and secondly, Lagrangian approach (approximating fluid as a continuum). The motivation behind current study is that at low Knudsen numbers, particle tracking approach is comparable with continuum model of fluids.

A lot of research has been undertaken to improve and propose modifications to original idea presented by Bird [1]. Cheng and Liao [2] studied the flow over a rectangular cylinder successfully for Mach numbers ranging from 0.85 to 8, and Knudsen number ranging from 0.01 to 1.0.

Ewart *et al.* [3] developed DSMC software in C++ and parallelized it using message passing interface (MPI) and OpenMP application. The authors were able to validate their results successfully.

DSMC technique has been successfully implemented in Mathematica before [4] and [5]. FLUENT is general purpose software which has been used for CFD simulations of different research areas such as turbo machinery, compressor designs and analysis, drag reduction of motor vehicles and other aerodynamic related phenomena.

In the present study, 2D flow over circular cylinder was studied at low Knudsen number using Mathematica. Air was used as the working fluid. Same geometry was used for CFD simulations in FLUENT 6.2. A comparison of results is presented here.

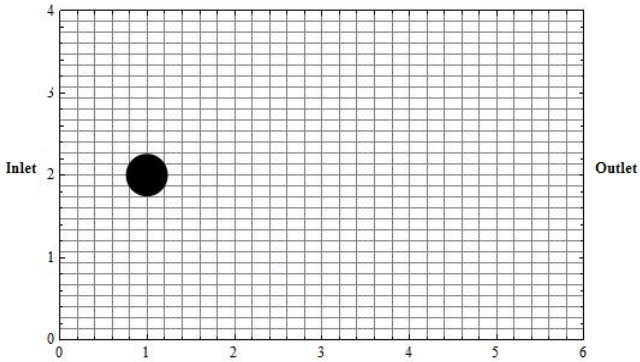

Fig. 1 Geometry of problem. Center of cylinder lies at (2.0, 1.0)

II. Methodology

A. Initial Conditions – Step 1

The domain of study, (Fig. 1) was divided into 30×30 cells. Number of particles was chosen to be 30,000. So that, each cell may contain, on the average, approximately 33 particles. To initialize particle positions, random numbers were generated with uniform probability distribution between range of x and y values of the domain. The velocities of particles are initialized according to Maxwell velocity distribution using acceptance and rejection method [6]. To determine whether the generated random numbers followed Maxwell speed distribution, speed was calculated from the equation $s = \sqrt{v_x^{\,2} + v_y^{\,2}}$.

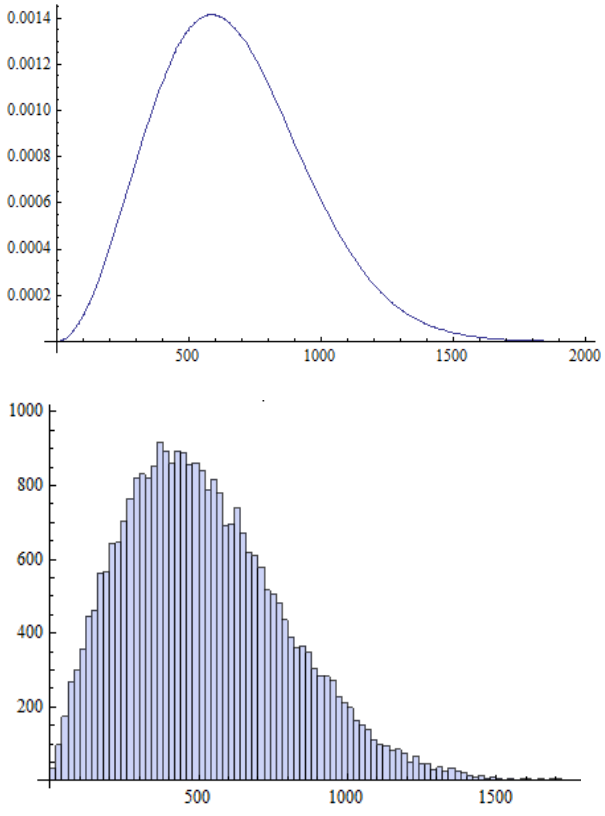

Fig. 2 (above) Probability density function, (below) Histogram of speed

Histogram of speed indicated that random numbers follow the required speed distribution, as depicted in Fig. 2.

B. Movement of particles and Wall interactions – Step 2

Motion of molecules was simulated in this step. Reflections of particles from solid boundaries were simulated using specular reflection from [1]. The particles leaving the domain were introduced back through the inlet with new velocities.

C. Simulation of molecular collisions – Step 3

The "no time counter" (NTC) method [1] was adopted to simulate the collision among molecules. Hard sphere (HS) model [1] was implemented.

D. Indexation of Particles – Step 4

As particles move to different cells during motion and collision, therefore, a particle indexation technique was developed for this purpose.

E. Sampling of molecular properties

During this step, x and y components of velocities of particles in each cell were averaged.

III. CFD Simulations in FLUENT 6.2

Pre processing of the selected geometry for study was done in Gambit. Simulations were performed in FLUENT 6.2. Table 1 presents the properties of air. The physical and geometric conditions used for study are given in Table 2.

TABLE I PROPERTIES OF AIR

m [kg]	T [K]	d [m]	P [Pa]	Ma
4.81×10^{-26}	273	4.19×10^{-10}	0.0885	2.0

IV. Results and Comments

The average velocities computed for each cell in Mathematica code were saved into 30×30 matrix for visualization. Fig. 3 shows the velocity vectors. Cells which did not contain any molecule were given velocity equal to zero, so as to reduce complications in the simulation.

TABLE II PHYSICAL AND GEOMETRICAL PROPERTIES

L [m]	H [m]	r [0.2]	λ [m]	Kn = λ/r
6.0	4.0	0.2	0.0546	0.273

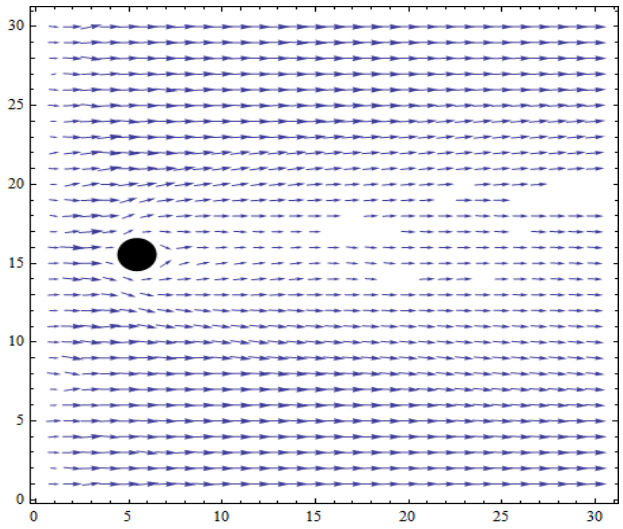

Fig. 3 Velocity vectors for average velocity for each cell

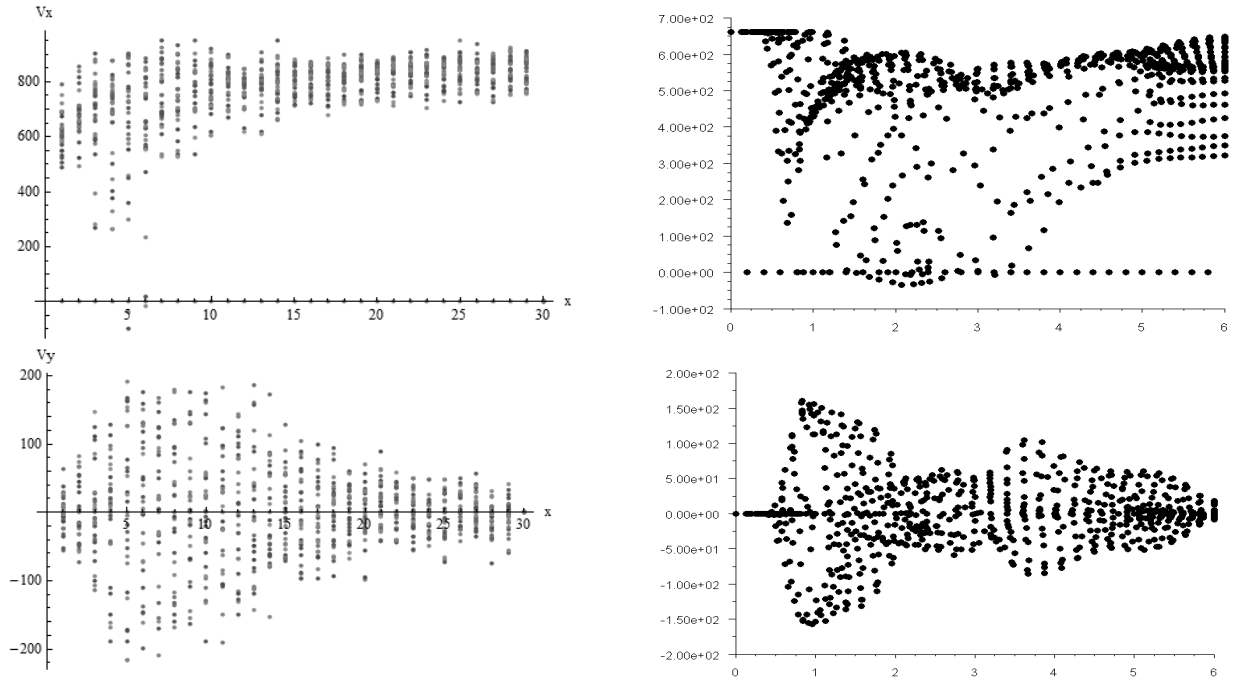

Fig. 4 List plots of Vx and Vy with respect to x axis. (Left) DSMC, (Right) FLUENT calculations

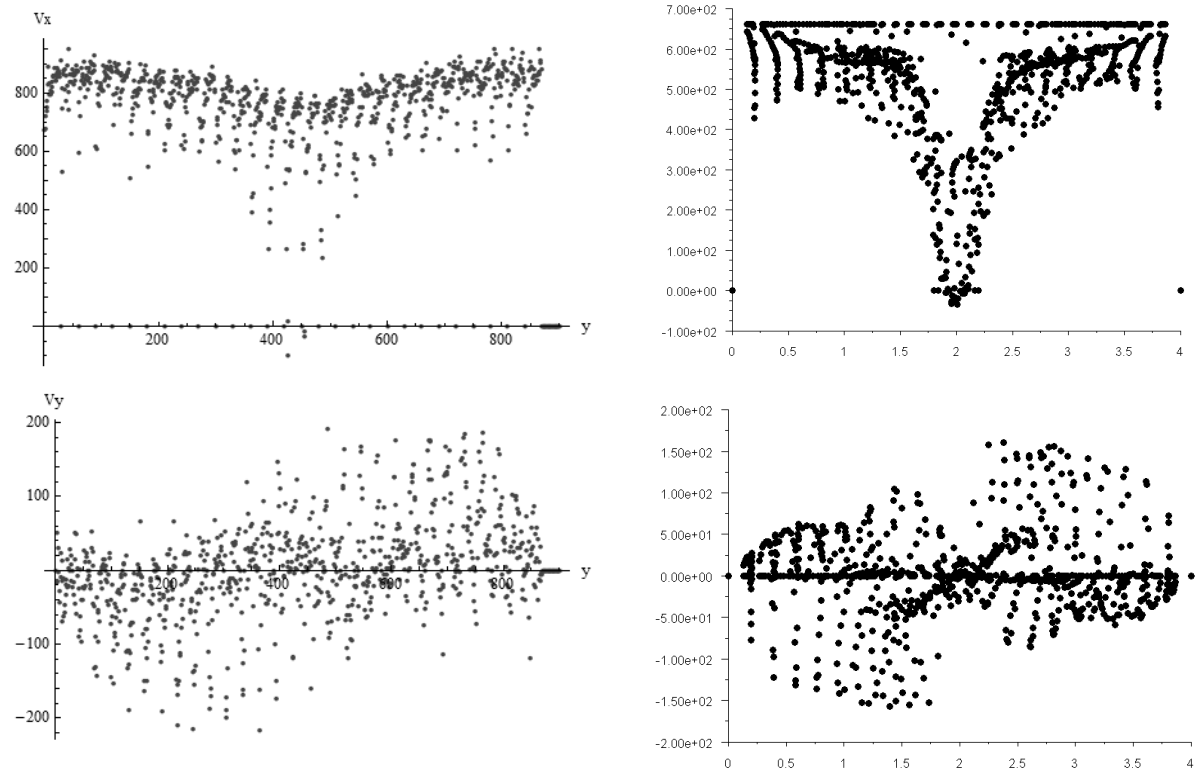

Fig. 5 List plots of Vx and Vy with respect to y axis. (Left) DSMC, (Right) FLUENT calculations

Fig. 4 and 5 present the comparison of results between Mathematica DSMC code calculations and CFD simulation run on FLUENT. Upon visual inspection, significant agreement between DSMC based code and FLUENT can be observed.

V. Conclusion And Future Work

DSMC code was developed in Mathematica. Air flow over a circular cylinder was studied. Same geometry was modeled in Gambit. CFD Simulation was run on FLUENT. It was observed that the values obtained from DSMC based code calculations follow the same pattern and are in significant agreement with results obtained from FLUENT. Although, due to choosing only HS model of molecules, and only specular reflection for boundary interactions, the values do not exactly match the values as that of CFD simulations.

For future work, it is proposed that other molecular models, which incorporate rotational energies and diffuse specular interaction with solid boundaries, can be introduced in DSMC algorithm. This would provide better insight into concerned research.

VI. Nomenclature

m = molecular mass

T = temperature

D = diameter

P = pressure

Ma = Mach number

L = length

H = height

r = radius of cylinder

λ = Mean free path

Kn = Knudsen number

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