Enhancement of Computational Performance of DSMC Code

BACHELOR OF TECHNOLOGY
IN
MECHANICAL ENGINEERING

Submitted by:

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CERTIFICATE

TO WHOM IT MAY CONCERN

This is to certify that, Mr. Jheel Nikulkumar Patel student of Mechanical engineering, 6th Semester of Nirma University, Institute of Technology, School of Engineering has satisfactorily completed the Mini project report titled Enhancement of Computational Performance of DSMC Code.

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Approval Sheet

The Project entitled **Enhancement of Computational Performance of DSMC Code** by **Jheel Nikulkumar Patel(17BME044)** is approved for the course **MINI PROJECT II** in Mechanical Engineering.

Examiners

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The success and final outcome of this project required a lot of guidance and assistance from many people and I am extremely privileged to have got this all along the completion of my project. All that I have done is only due to such supervision and assistance and I would not forget to thank them.

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ABSTRACT

Continuum mechanics is used for studying and formulating fluid mechanics problems, when Knudsen number (Kn, ratio of the mean free path length of the molecules of a fluid to a characteristic length) is less than 0.01. Macroscopic properties are calculated without considering the statistical fluctuations (negligible) in continuum flows. But when rarefied gas flows (Kn > 0.1) are to be studied then continuum hypothesis in no longer valid and statistical mechanics is to be invoked. Boltzmann transport equation plays a central role in rarefied gas flows. Numerous methods are formulated to solve and apply Boltzmann equation in practical cases. One such method is Direct Simulation Monte Carlo (DSMC). DSMC is a direct simulation method, where flow is simulated at the molecular level but in a probabilistic manner to make it practical and efficient. In this project, DSMC method is explored and it is studied how to implement it on CUDA framework to exploit the power of parallel processing.

Key words: Direct Simulation Monte Carlo, DSMC, Statistical methods, Boltzmann transport equation, CUDA.

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Abbreviation and Notations

$n = number\ desity$

$\mu = mean$

$\sigma = standard\ deviation$

$\lambda = mean\ free\ path$

$k_B = Boltzmann\ equation$

$Z_M = collision\ frequency\ per\ unit\ volume$

$z_M = collision\ frequency\ of\ single\ molecule$

$\tau_M = mean\ free\ time$

$C_a = mean\ velocity\ of\ chaotic\ motion$

CHAPTER 1

Introduction

Primary goal of physics is to develop and test a theory or formulations put forward to describe Natural phenomena. One such domain of study is Thermodynamics. Thermodynamics, if seen at microscopic level, is formulated using laws of statistical mechanics. At microscopic level, thermodynamics is simply the statistical or collective behavior of large number of particles governed by Newtonian mechanics, if formulated classically, or Quantum mechanics, if quantum effects are significant.

Some basic definitions

- **Thermodynamics:** It is a phenomenological description of properties of macroscopic systems in thermodynamic equilibrium. (Mehran Kardar)
- **Statistical Mechanics:** It is an inherently *probabilistic* description of the system, where collective behavior of an ensemble (system of many identical particles) is studied.
- **Kinetic Theory of Gases:** It is a part of statistical physics where flows of gases are considered on the molecular level, i.e. on the level of individual molecules, and described in terms of changes of probabilities of various states of gas molecules in space and time based on known laws of interaction between individual molecules.
- **Rarefied gas dynamics (RGD)** is often used as a synonymous of the kinetic theory of gases. In the narrow sense, the kinetic theory focuses on the general methods of statistical description of gas flows, while the rarefied gas dynamics focuses on solutions of practical gas dynamics problems based on methods of kinetic theory.
- **Non-equilibrium gas dynamics** combines methods of rarefied gas dynamics and continuum gas dynamics for description of non-equilibrium gas flows.
- **Direct simulation Monte Carlo (DSMC)** method is a stochastic Monte Carlo method for simulation of dilute gas flows on the molecular level. To date, DSMC is the state-of-the-art numerical tool for the majority of applications in the kinetic theory of gases and rarefied gas dynamics.
- **Monte Carlo (MC)** method is a general numerical method for a variety of mathematical problems based on computer generation of (pseudo) random numbers and probability theory.

CHAPTER 2

Mathematical Prerequisites

Before studying statistical mechanics, some mathematical terms are to be introduced, like phase space, distribution functions, etc.

Phase Space: Phase space is the set of all possible states of a system. Take for e.g., a particle which can take 100 discrete positions and 100 discrete speeds. Then the phase space for this system is set of all $100 \times 100 = 10000$ possible states of the particle.

Further, we can define a map from phase space to real line such that it assigns with each point (state) in phase space with a real value called the probability of the particle to be in that state. We call this map a **probability distribution function** and let it be denoted by $p(\tilde{x})$. Where, $\tilde{x}$ is vector in phase space.

Hence, $p(\tilde{x})$ have following properties:

$$0 \leq p(\tilde{x}) \leq 1 \qquad 2.1a$$

$$\int_{space} p(\tilde{x}) = 1 \qquad 2.1b$$

If total number of molecules in a system is n then, $\mathrm{f}(\tilde{x}) = np(\tilde{x})$ denotes the number of molecules in state $\tilde{x}$. $\mathrm{f}(\tilde{x})$ is called the distribution function.

For thermodynamic system:

$$n(x,t) = \frac{\text{Number of molecules in the cell } \Delta x \text{ of the physical space}}{\Delta x} \qquad 2.2a$$

$$f(x, v_x, t) = \frac{\text{Number of molecules in the cell } \Delta x \Delta v_x \text{ of the phase space}}{\Delta x \Delta v_x} \qquad 2.2b$$

Distribution function $f(x,\ v_x,\ t)$ is equal to the average number of molecules in a unit "volume" of a phase space, i.e. $f(x,\ v_x,\ t)$ is *the number density of molecules in the phase space*.

If we chose infinitely small phase volume $dxdv_x$, then

$$dN = f(x, v_x, t)dxdv_x \qquad 2.3$$

is equal to the average number of molecules whose phase coordinates x_i and v_{ix} at time t satisfy the conditions,

$$x < x_i < x + dx, \qquad v_x < v_{ix} < v_x + dv_x, \tag{2.4}$$

2.2. Standard Probability Distribution Functions

In statistical mechanics much of the formulation is done in terms of probabilistic distribution of states. Hence, it is necessary to study some of the standard probability distribution function. Distribution can be discrete or continuous. In discrete distribution, the random variable can take only discrete values. Whereas in continuous distribution, the random variable can take any values with the property that infinitely many values are there between any two numbers, how close they are, which can be taken by the random variable.

a. Discrete

1) **Uniform distribution:** We say that a discrete variable has uniform distribution if it accepts finite number n of values with equal probabilities

$$p_k = \frac{1}{n}, \qquad k = 1,2, \dots n. \tag{2.5a}$$

$$\mu = \sum_{k=1,2,\dots} x_k p_k = \sum_{k=1}^{n} \frac{k-1}{n} = \frac{n-1}{2}, \tag{2.5b}$$

$$\sigma^2 = \sum_{k=1,2,\dots} x_k^2 p_k - \mu^2 = \sum_{k=1}^{n} \frac{(k-1)^2}{n} - \mu^2 = \frac{n^2-1}{12}. \tag{2.5c}$$

2) **Poisson distribution** with parameter a is the distribution of a random variable K that takes arbitrary positive integer values and 0 with probabilities

$$p_k = P(K = k) = \frac{a^k}{k!} e^{-a}, \qquad k = 0,1,2, \dots. \tag{2.6a}$$

$$\mu = \sum_{k=0}^{\infty} k p_k = a, \qquad \sigma^2 = \sum_{k=0}^{\infty} k^2 p_k - \mu^2 = a. \tag{2.6b}$$

b. Continuous

1) **Uniform distribution:** We say that a continuous variable X has uniform distribution in an interval $[a,\ b]$ if

$$f(x) = \begin{cases} 1/(b-a), & a \le x \le b; \\ 0, & x < a \text{ or } x > b. \end{cases} \qquad 2.7$$

2) **The standard random variable** γ is the variable with uniform distribution in the interval [0,1]

$$f(x) = \begin{cases} 1, & 0 \le x \le 1; \\ 0, & x < 0 \text{ or } x > 1, \end{cases} \qquad F(x) = \begin{cases} 0, & x < 0; \\ x, & 0 \le x \le 1; \\ 1, & x > 0. \end{cases} \qquad 2.8$$

3) **Normal or Gaussian:** We say that a continuous variable X has normal or Gaussian distribution if

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \qquad 2.9$$

Parameters of this distribution, μ and σ, are equal to the mean and standard deviation of variable X.

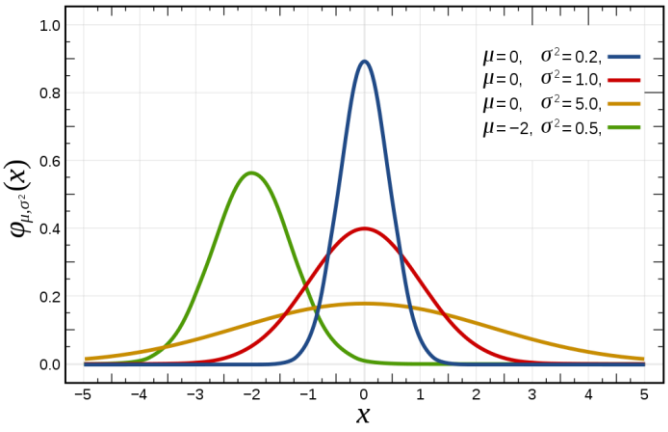


Fig. 2.1. Gaussian Distribution

4) **Rayleigh distribution:** We say that a non-negative continuous variable has the Rayleigh distribution with parameter σ if its PDF at $x \ge 0$ is equal to

$$f(x) = \frac{x}{\sigma^2} \exp\left(-\frac{x^2}{2\sigma^2}\right). \qquad 2.10$$

2.2. Random Number Generators

When working with computer simulations, it becomes necessary to find a way to generate random numbers with required probability distribution. Some of the methods to generate random numbers is given in this section. Numbers having standard random variable distribution can be generated using standard library functions.

Let the **standard random variable** γ.

1) **Poisson distribution**

$$K = \min\left\{k = 1,2, \ldots \left| \prod_{i=1}^{k} \gamma_i < e^{-a} \right.\right\} - 1. \qquad 2.11$$

2) **Uniform distribution** in a finite interval [a, b]

$$X = a + (b - a)\gamma. \qquad 2.12$$

3) **Rayleigh distribution** with parameter σ

$$X = \sigma\sqrt{-2\log\gamma}\,. \qquad 2.13$$

4) **Gaussian distribution**

$$\mathcal{R} = \sqrt{-2\log\gamma_1}\,, \qquad E = 2\pi\gamma_2, \qquad 2.14a$$

$$x = \mathcal{R}\cos E\,, \qquad y = \mathcal{R}\sin E\,. \qquad 2.14b$$

These equations allow one to obtain two independent samples of variable X simultaneously. One can use both or only one of them as needed. Here mean and standard deviation of generated numbers is 0 and 1 respectively.
A Gaussian random variable Y with mean μ and standard deviation σ can be obtained from random variable X, which has a Gaussian distribution with mean 0 and standard deviation 1 as follows:

$$Y = \mu + \sigma X. \qquad 2.15$$

CHAPTER 3

Statistical Mechanics

3.1. Need for Statistical Description

The degree of rarefaction of a gas is generally expressed through the *Knudsen number (Kn)* which is the ratio of the mean free path λ to the characteristic dimension *L*.

$$Kn = \frac{\lambda}{L} \tag{3.1}$$

Kn number shows the applicability of continuum hypothesis. For $Kn < 0.1$ continuum hypothesis i.e. Navier-Stokes equations are applicable. If $Kn > 0.1$ then continuum hypothesis is no longer applicable and statistical fluctuations are prevalent.

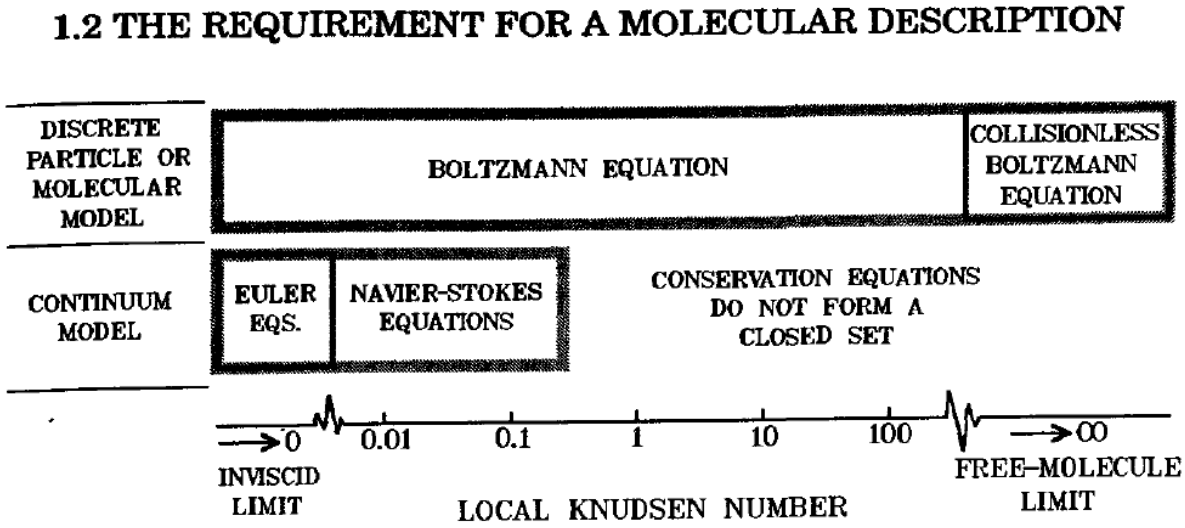


Fig. 3.1. The requirement for a Molecular Description (G. A. Bird, Molecular Gas Dynamics)

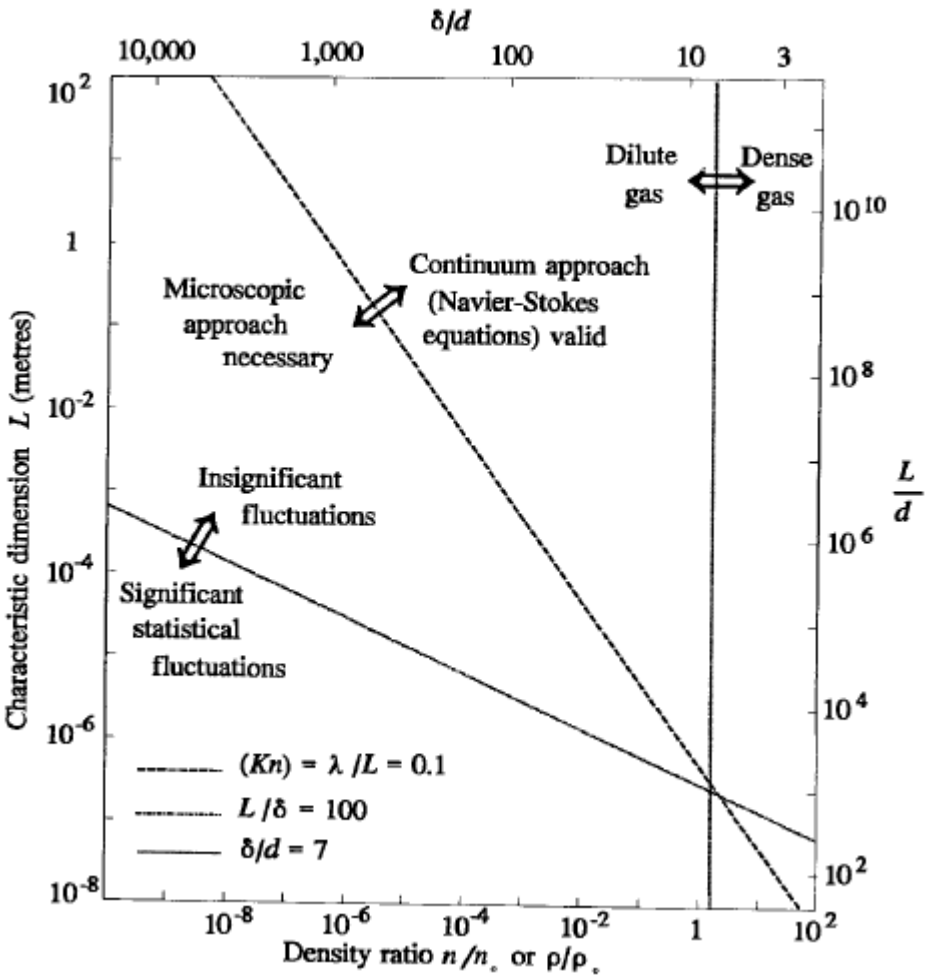


Fig. 3.2. Effective limits of major approximations (G. A. Bird, Molecular Gas Dynamics)

Where, $\delta = mean\ molecular\ spacing,\ d = molecular\ diameter$

3.2. Origin of Statistical Mechanics

Statistical mechanics was first primarily studied by Ludwig Eduard Boltzmann. In his study he derived what is called Boltzmann transport equation, which gives time evolution of probabilistic distribution of states of molecules in phase space. Before studying what is phase space just think of thermodynamic system as collection of molecules exhibiting a collective motion.

3.3. Boltzmann Equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int_0^{2\pi} \int_0^{r_{max}} (f' f'_1 - f f_1) c_r b db d\varepsilon d\mathbf{v}_1 . \qquad 3.2$$

Above equation is called Boltzmann equation which is truncated equation of BBGKY hierarchy. It governs the variation of distribution function with time and space.
Note: Above equation is applicable for rarefied gases where only binary collisions are significant. As the denseness of gas increases more terms of the BBGKY hierarchy are required to incorporate tertiary and higher collisions.

3.4. Maxwell Distribution

For steady state homogeneous system, Maxwell obtained analytical solution for velocity distribution function.

$$f_M(\mathbf{v}) = \frac{n}{(2\pi RT)^{3/2}} \exp\left[-\frac{(\mathbf{v}-\mathbf{u})^2}{2RT}\right]. \qquad 3.3$$

Where, **u** is mean velocity or stream velocity, T is temperature, $R = {k_B}/{m}$ is gas constant. Above distribution function is known as Maxwell-Boltzmann velocity distribution function.

In terms of velocities of chaotic motion $\boldsymbol{c} = \boldsymbol{v} - \boldsymbol{u}$, the Maxwell-Boltzmann distribution function can be written as follows

$$f_M(\mathbf{c}) = \frac{n}{(2\pi RT)^{3/2}} \exp\left[-\frac{\mathbf{c}^2}{2RT}\right] \qquad 3.4$$

We can use it in order to characterize the distribution of absolute chaotic velocity $c = |\boldsymbol{c}|$

The **mean square velocity of chaotic motion** C

$$C = \left(\frac{1}{n}\int \mathbf{c}^2 f_M(\mathbf{c}) d\mathbf{c}\right)^{1/2} = \sqrt{3RT}. \qquad 3.5$$

The **mean velocity of chaotic motion** C_a

$$C_a = \frac{1}{n}\int_0^\infty c\, f_M(c)dc = \sqrt{\frac{8}{\pi}RT}. \qquad 3.6$$

The **most probable chaotic velocity** $C_m = \sqrt{(2RT)}$

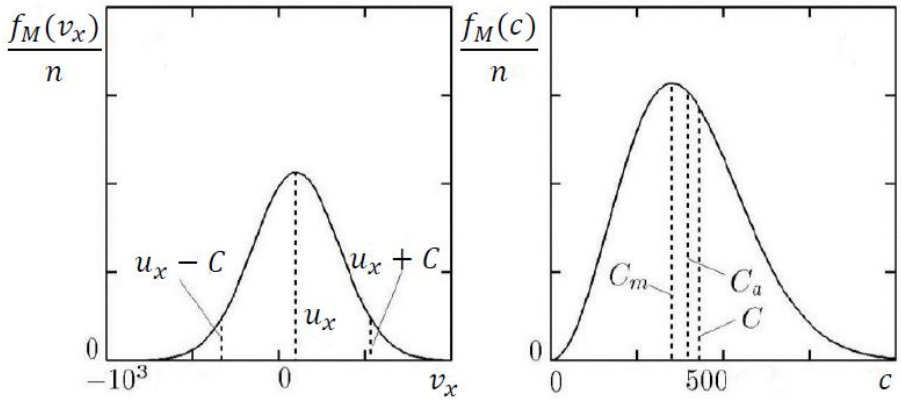


Fig. 3.3. Maxwell Distribution, (a) Velocity, (b) Chaotic Velocity

3.5. Chapman-Enskog Theory

Further, Chapman-Enskog obtained distribution function for small deviations from equilibrium flow by taking perturbations of Maxwellian distribution and obtained following distribution.

$$f = f_0\left[1 - C\beta v'\left\{3\left(\beta^2 c'^2 - \frac{5}{2}\right)\frac{\lambda}{T}\frac{\partial T}{\partial y} + 4\beta u's\,\frac{\lambda}{u_0}\frac{\partial u_0}{\partial y}\right\}\right], \qquad 3.7$$

Above equation is for the special case of a flow in the x-direction with gradients only in the y-direction. This theory authenticated the assumption, inherent in the Navier-Stokes formulation, that the shear stresses, heat fluxes, and diffusion velocities are linear functions of the gradients in velocity, temperature, and species concentration.

Analytical solutions for Boltzmann equation are available for few special cases. For flows with complicated geometries and non-equilibrium flows, it is quite difficult (or impossible with current mathematical tools) to obtain analytical solution. So, we resort of some indirect/direct methods for solutions. Some examples of such methods are:

1. Finite element methods (FEM)
2. Lattice Boltzmann method (LBM)
3. Direct Simulation Monte Carlo (DSMC)
4. Particle in Cell (PIC)

In this study, we are going to implement DSMC method for finding solutions to Boltzmann equation.

CHAPTER 4

Molecular Models

In a gas, at molecular level, there is chaotic motion and collisions between molecules. The collisions can be described using proper collision potentials between two or more molecules. Describing collisions using potential forces can be very difficult and computationally very costly. A frame of collision between two molecules is shown below (in different reference frames).

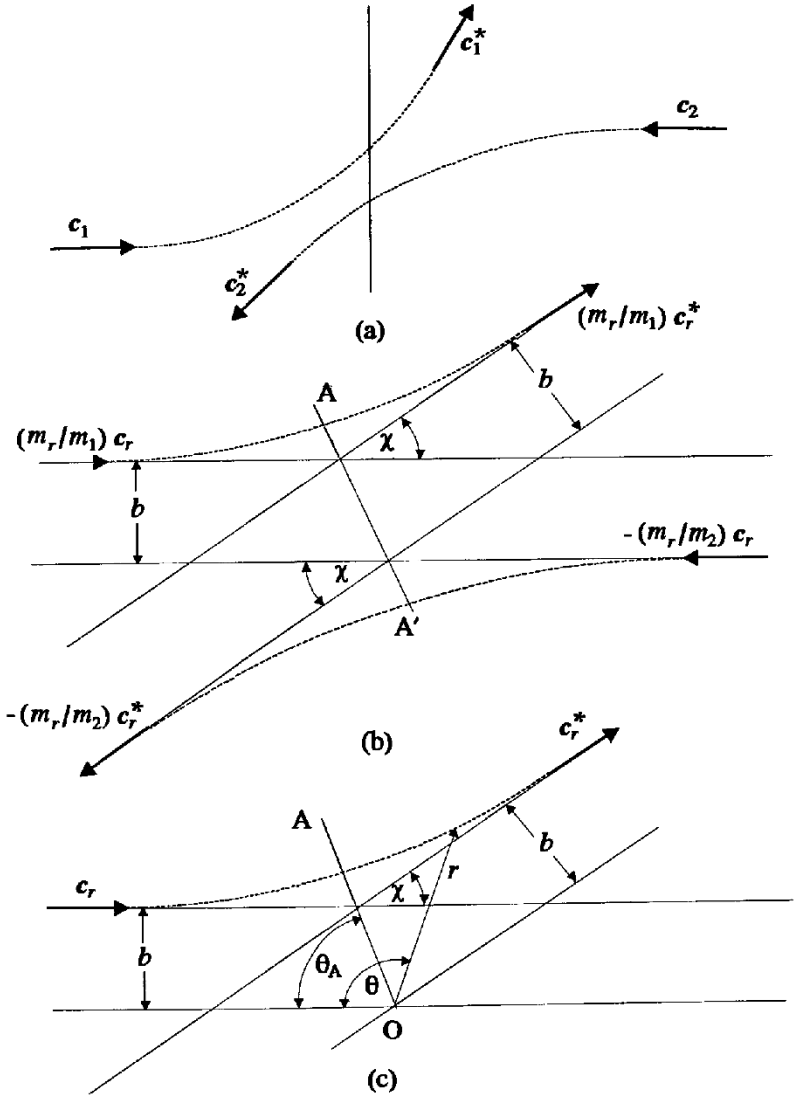


Fig. 4.1. Collision between two molecules, (a) In stationary reference frame, (b) In center of mass reference frame, (c) In center of force reference frame (G. A. Bird, Molecular Gas Dynamics)

Considering collision dynamics, the collision trajectories are governed by intermolecular force potential φ, as given below in polar coordinates,

$$\theta_A = \int_0^{W_1} \{1 - W^2 - \phi/(\tfrac{1}{2} m_r c_r^2)\}^{-\frac{1}{2}} dW, \tag{4.1}$$

Where,

$$W = b/r, \tag{4.2}$$

And, W_1 is the root of the equation,

$$1 - W^2 - \phi/(\tfrac{1}{2} m_r c_r^2) = 0. \tag{4.3}$$

$$c_r = \textit{relative velocity}, \quad m_r = \frac{m_1 m_2}{m_1 + m_2} \textit{ is the reduced mass} \tag{4.4}$$

Finally, the deflection angle of velocity is,

$$\chi = \pi - 2\theta_A. \tag{4.5}$$

4.1. Inverse Power Law Model

For inverse power law model of force potentials,

$$F = \kappa/r^{\eta} \tag{4.6}$$

$$\phi = \kappa/[(\eta - 1) r^{\eta - 1}]. \tag{4.7}$$

trajectory is given by,

$$\chi = \pi - 2 \int_0^{W_1} [1 - W^2 - \{2/(\eta - 1)\}(W/W_0)^{\eta - 1}]^{-\frac{1}{2}} dW \tag{4.8}$$

Where,

$$W_0 = b(m_r c_r^2/\kappa)^{1/(\eta - 1)}. \tag{4.9}$$

And W_1 is the positive root of the equation,

$$1 - W^2 - \{2/(\eta - 1)\}(W/W_0)^{\eta - 1} = 0. \tag{4.10}$$

Total collision cross-section is given by,

$$\sigma_T = 2\pi \int_0^{\pi} \sigma \sin\chi \, d\chi \, . \qquad 4.11$$

Where,

$$\sigma = (b/\sin\chi) \, | \, db/d\chi \, | \, . \qquad 4.12$$

As the force in inverse power law models extends to infinity, many times, it happens that the above integrals diverge when infinitely large distances are considered. Hence, it becomes necessary to introduce cut-off distances after which it is assumed that the forces vanish. Other two cross-sections are **viscosity cross-section σ_μ** and **momentum/diffusion cross-section σ_M** governing the viscosity and momentum transport properties respectively.

As can be see above, using generalized collision mechanics with generalized potentials can make the solution very time consuming and computationally costly. Hence, we try to describe collisions by considering variations in hard sphere model. In deriving Maxwell equation, it is inherently assumed that the molecule has spherical structure with constant diameter. Hence, this model is known as hard sphere model. In hard sphere model, the molecules after collision attain velocities based on scattering law. The value of diameter (called kinetic diameter) is taken based on correlation of experimental results with collision cross-section.

4.2. Hard Sphere Model

For hard sphere model, total collision cross-section is given by,

$$\sigma_T = \pi d^2 \qquad 4.13a$$

$$Z_M = \frac{\sigma_T n^2}{\sqrt{2}} C_a, \qquad z_M = \sqrt{2}\sigma_T n C_a, \qquad \tau_M = \frac{1}{\sqrt{2}\sigma_T n C_a}, \qquad \lambda_M = \frac{1}{\sqrt{2}\sigma_T n}. \qquad 4.13b$$

Where, Z_M is collision frequency per unit volume, z_M collision frequency of single molecule, τ_M is mean free time, λ_M is mean free path and C_a is mean velocity of chaotic motion.

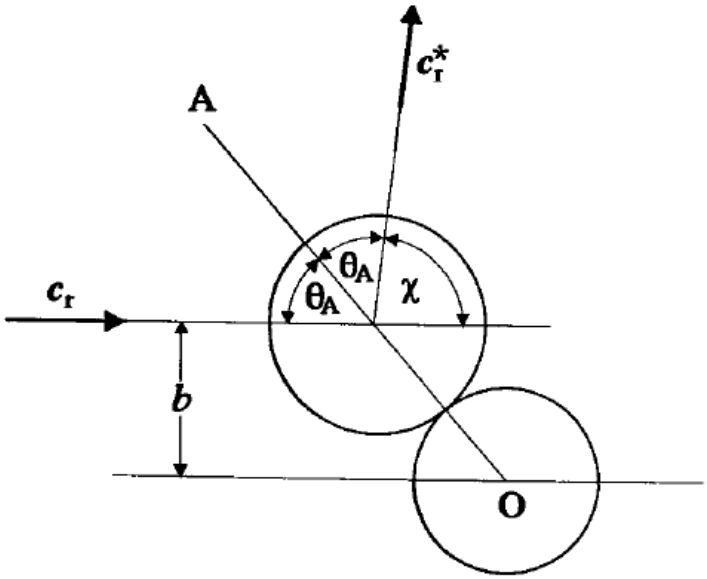


Fig. 4.2. Collision trajectory for hard sphere model (G. A. Bird, Molecular Gas Dynamics)

And viscosity and momentum cross-sections are given by,

$$\sigma_\mu = \frac{2}{3}\sigma_T. \qquad \sigma_M = \sigma_T. \tag{4.14}$$

As can be inferred, the hard sphere model is oversimplified. In general, viscosity and diffusion both depends on temperature of the gas, hence viscosity and momentum cross-section shouldn't be constant but depend of relative velocities of molecules. To take care of variation of cross-sections with temperature Variable Hard Sphere (VHS) model is introduced.

4.3. Variable Hard Sphere (VHS) Model

In VHS model the diameter is no longer constant but changes with temperature (or in other words mean chaotic velocity) to match with experimental changes of viscosity with temperature. The molecular diameter is given by,

$$d = d_{ref}(c_{r,ref}/c_r)^{\upsilon}, \tag{4.15}$$

$$\chi = 2\cos^{-1}(b/d) \tag{4.16}$$

Where, υ is the power of inverse power model with which the VHS model can be compared. Other parameters are

$$Z_M = \frac{\sigma_{T,Ref} n^2}{\sqrt{2}} \Gamma\left(\frac{4-\varpi}{2}\right)\left(\frac{c_{r,Ref}}{\sqrt{4RT}}\right)^{\varpi} C_a, \tag{4.17}$$

$$\lambda_M = \tau_M C_a = \frac{1}{\sqrt{2}\sigma_{T,Ref} n \Gamma\left(\frac{4-\varpi}{2}\right)}\left(\frac{\sqrt{4RT}}{c_{r,Ref}}\right)^{\varpi} \tag{4.18}$$

$$z_M = \frac{2Z_M}{n} = \sqrt{2}\sigma_{T,Ref} n \Gamma\left(\frac{4-\varpi}{2}\right)\left(\frac{c_{r,Ref}}{\sqrt{4RT}}\right)^{\varpi} C_a, \qquad \tau_M = \frac{1}{z_M}. \tag{4.19}$$

VHS model account for the variation of mean free path and Knudsen number with the real gas temperature exponent of viscosity. However, the viscosity and momentum cross-sections are still given by eqs. 4.14 This is the limitation of VHS model and to overcome this limitation Variable Soft Sphere (VSS) model was introduced.

4.4. Variable Soft Sphere (VSS) Model

In VSS model, molecular diameter is given by,

$$d = d_{ref}(c_{r,ref}/c_r)^{v}, \tag{4.20}$$

Which is same as the VHS model. But the deflection angle is different and is given by,

$$\chi = 2\cos^{-1}\{(b/d)^{1/\alpha}\}. \tag{4.21}$$

for some parameter α. And the viscosity and momentum cross-sections become,

$$\sigma_\mu = \frac{4\alpha}{(\alpha+1)(\alpha+2)}\sigma_T. \tag{4.22}$$

$$\sigma_M = \frac{2}{(\alpha+1)}\sigma_T. \tag{4.23}$$

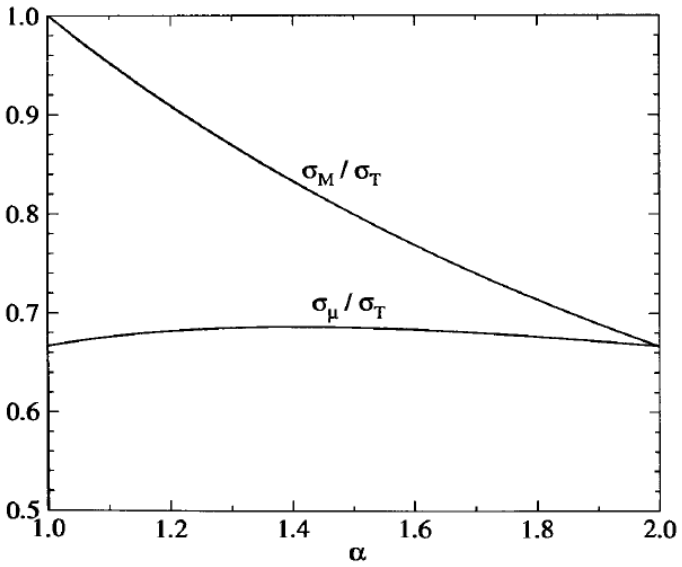


Fig. 4.3. Variation of σ_μ and σ_M with parameter α (G. A. Bird, Molecular Gas Dynamics)

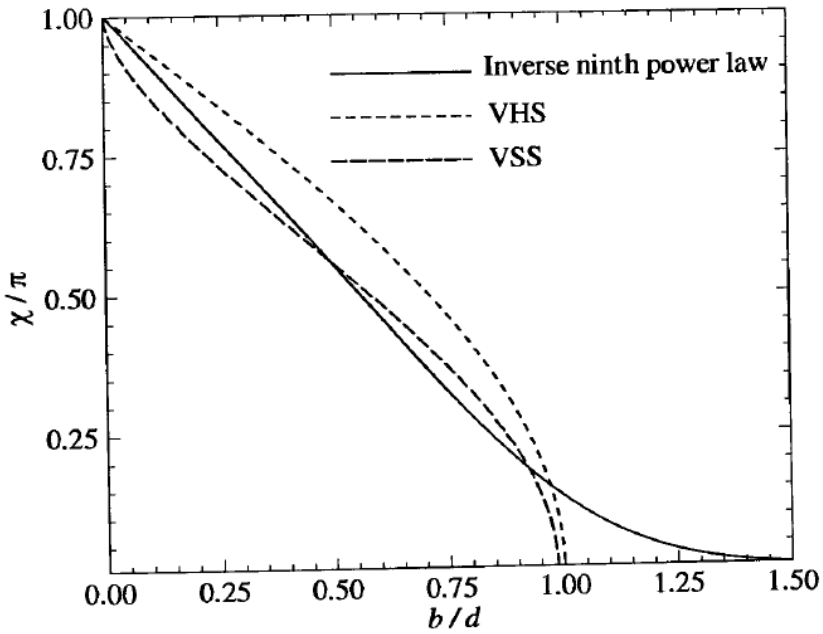


Fig. 4.4. Change in deflection angle with miss distance (G. A. Bird, Molecular Gas Dynamics)

In this study VHS model is employed, though it is not a very general model but it satisfies most of the required real gas conditions.

CHAPTER 5

Direct Simulation Monte Carlo

In this study, we are going to implement DSMC method for finding solutions to Boltzmann equation. In DSMC method instead of finding direct solution of Boltzmann equation we try to obtain statistical average of various quantities by directly simulating the dynamics of flow at molecular level. Here, we try to follow motion of molecules. But instead of simulating each and every molecule, we simulate representative molecules were each representative molecule is equivalent to several molecules. Hence, we invoke **criteria of similarity of flows** to scale the parameters.

5.1. Criteria of Similarity of flows

Two flows (physical phenomena) are called similar if numerical properties of such flows are identical in reduced units. In application to the rarefied gas flows, it means that two similar flow correspond to the same solution of the Boltzmann equation in reduced units. Two solutions are similar if they correspond to the same Sh, Fe, and Kn. These non-dimensional numbers (parameters) are called the criteria of similarity.

$$Sh = \frac{L_*}{t_* v_*}, \qquad Fr = \frac{m v_*^2}{F_* L_*}, \qquad Kn = \frac{\lambda_*}{L_*} = \frac{1}{\pi d_{Ref}^2 n_* L_*}, \qquad \lambda_* = \frac{1}{\pi d_{Ref}^2 n_*}. \tag{5.1}$$

Thus, one can simulate a real gas flow with characteristic number density $n_{*(r)}$ composed of molecules with characteristic cross section $\sigma_{*(r)} = \pi d_{Ref}^2$ by a flow with another characteristic number density $n_{*(s)}$ and composed of simulated molecules of another size $\sigma_{*(s)}$. The real and simulated flows are similar, if the Knudsen number is the same in both flows:

$$Kn = \frac{1}{\sigma_{*(r)} n_{*(r)} L_*} = \frac{1}{\sigma_{*(s)} n_{*(s)} L_*}. \tag{5.2}$$

In the DSMC method, the ratio

$$W = \frac{n_{*(r)}}{n_{*(s)}} \tag{5.3}$$

is called the **statistical weight** of a simulated particle. Practically, *one can say that every simulated particle represents W particles in the real gas flow*.

Hence,

$$\sigma_{*(s)} = W\sigma_{*(r)}. \qquad 5.4$$

5.2. Outline of DSMC

First flow domain is divided into cells. The dimensions of cell are of the order of mean free path. Then, initially, simulated molecules are distributed over the phase space covering the flow domain according to assumed distribution function. Here, the number of simulated molecules a quite less than the original number of molecules. Hence, each simulated molecule represents several real molecules according to the statistical weight. Generally, for rarefied gas, in each cell, 30 simulated molecules are taken.

Basic idea in DSMC method is to divide the simulation time step into two parts. In one part, position of simulated molecules is (deterministically) incremented according to their velocities. In this step collisions are not taken into account. In second part of the time step only collisions are taken into account. Collisions are considered to be instantaneous, i.e. the transition from pre-collision velocities to post-collision velocities is instantaneous.

Here, not every pair is considered for collision but a probabilistic estimate is considered based on the collision cross-section and relative velocity. The probability of a collision between two molecules in a homogenous gas is proportional to the product of their relative speed and total collision cross-section.

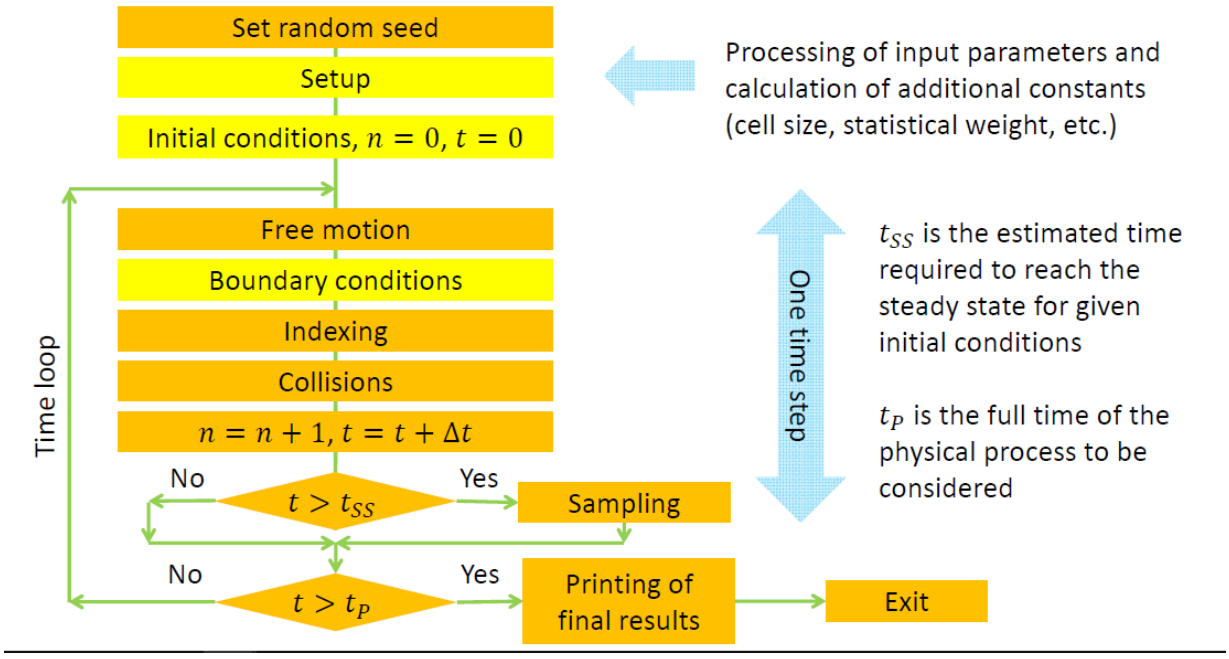
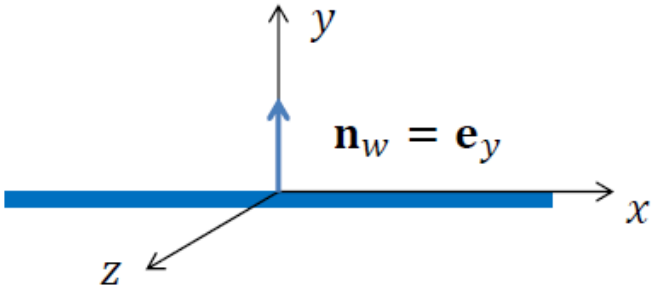


Fig. 5.1. DSMC Flowchart

Physics of Boundary collisions and Binary collisions is as follows:
Boundary collisions – Diffuse Scattering
Binary collisions – Isotropic scattering after collision

5.3. Boundary Collisions

Let us take one example of boundary collision. Take a surface with normal in positive direction.



Then distribution of velocities after surface collisions is given by,

$$S(\mathbf{v}|\mathbf{n}_w) = \frac{|\mathbf{v}\cdot\mathbf{n}_w|}{2\pi(RT_w)^2}\exp\left[-\frac{\mathbf{v}^2}{2RT_w}\right]. \qquad 5.5$$

$\boldsymbol{n}_w = (0,\ 1,\ 0)$, hence,

$$S(\mathbf{v}|\mathbf{n}_w) = \frac{v_y}{2\pi(RT_w)^2}\exp\left[-\frac{v_x^2+v_y^2+v_z^2}{2RT_w}\right] = S_t(v_x)S_n(v_y)S_t(v_z)\,. \qquad 5.6a$$

$$S_n(v) = \frac{v}{RT_w}\exp\left[-\frac{v^2}{2RT_w}\right], \qquad S_t(v) = \frac{1}{\sqrt{2\pi RT_w}}\exp\left[-\frac{v^2}{2RT_w}\right]. \qquad 5.6b$$

Rayleigh distribution Gaussian distribution

5.4. Binary Collisions

In the case of VHS model, post-collisional velocities after a binary collisions of molecules i and j are given by

$$\mathbf{v}'_i = \mathbf{v}_c - \frac{1}{2}\mathbf{c}'_r, \qquad \mathbf{v}'_j = \mathbf{v}_c + \frac{1}{2}\mathbf{c}'_r, \qquad \mathbf{v}_c = \frac{\mathbf{v}_i+\mathbf{v}_j}{2}, \qquad \mathbf{c}'_r = |\mathbf{v}_j-\mathbf{v}_i|\mathbf{e}'_{cr}. \qquad 5.7$$

where the unit vector $\boldsymbol{e}'_{cr}$ defines the direction of relative velocity $\boldsymbol{c}'_r$ after the collision. Distribution of directions of $\boldsymbol{e}'_{cr}$ is given by the differential collision cross section $\sigma = \sigma(C_r)$. $\boldsymbol{e}'_{cr}$ is an *isotropic random vector* given by,

$$\cos T = 1 - 2\gamma_1, \qquad E = 2\pi\gamma_2, \tag{5.8a}$$

$$\sin T = \sqrt{1 - \cos^2 T}\,, \tag{5.8b}$$

$$X = \cos T\,, \qquad Y = \sin T \cos E\,, \qquad Z = \sin T \sin E\,. \tag{5.8c}$$

5.5. NTC Scheme

Selection of collision pairs is based on a technique devised by Bird. If probability of collisions between all possible pairs is calculated then computation cost is of the order of N^2. But Bird found that it is not necessary to calculate all collision pairs.

Bird introduced No Time Counter (NTC) scheme which gives the number of pairs to be calculated. The **NTC scheme** by Bird utilizes the acceptance and rejection Monte Carlo method and is based on the introduction of a **majorant** $[\sigma_T C_r]_{max}$, i.e. such quantity that

$$[\sigma_T C_r]_{max} \geq \sigma_{T(ij)} c_{r(ij)} \text{ for every pair of molecules i, j in a cell.}$$

Majorant collision frequency in the cell:

$$Z_{max} = \frac{W}{V} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} [\sigma_T C_r]_{\max} = \frac{N(N-1)}{2} \frac{W}{V} [\sigma_T C_r]_{\max} \tag{5.9}$$

In the NTC scheme, $N_{pair} = Z_{max} \Delta t$ random pairs (i, j) of molecules is selected, but for every pair collision happens with probability $P_{collision} = \sigma_{T(ij)} c_{r(ij)} / [\sigma_T C_r]_{max}$. In this case, the number of arithmetic operations is proportional to $N \log N$ and grows with N. Majorant $[\sigma_T C_r]_{max}$ is important **numerical parameter** of the NTC scheme.

$N_{pair} = Z_{max} \Delta t$ collisions are sampled during time step. **Real** collision (accepted collision) occurs with probability $P_{coll} = \sigma_{T(ij)} c_{r(ij)} / [\sigma_T C_r]_{max}$. All other collisions are **fictitious** (rejected collisions).

The *simplified* flowchart of the NTC scheme can be formulated as follows:

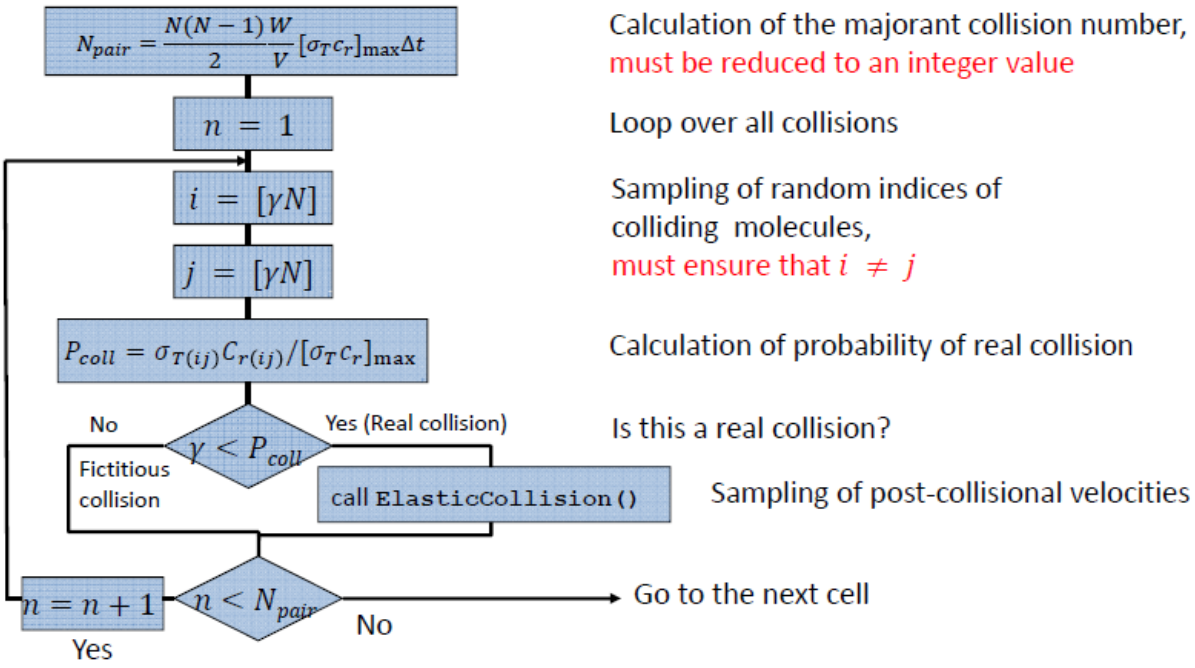


Fig. 5.2. NTC Scheme Flowchart

CHAPTER 6

Coding Scheme

6.1. Parallelization

As can be inferred, in Direct simulation of molecules lot of computational power is required. Even though criteria of similarity of flow is invoked to decrease the number of simulated molecules, but still a huge amount of computational power is required to simulate complex flows. If serial computing is employed then the time taken for simulation may become impractical. In present scenario and based on the ongoing trend, there is and will be a lot of advancement in parallel computing using GPUs or Vector processors.

In this study, parallel processing is used to carry out DSMC simulation. But before going further into parallel computing some basics of serial and parallel computing is outlined. Let us take a simple example. Addition of two arrays with 1000 elements. In serial computing it is simple. A loop is invoked and in each loop cycle one element is added. Now in parallel computing, we use multiple cores of GPU. So that on each core one element is added and all the cores work simultaneously.

Hence, in serial computing same calculation (i.e. addition) is carried out 1000 times **one after other**. Whereas in parallel computing, calculation is carried out 1000 times only, but here all 1000 calculations occur **simultaneously**.

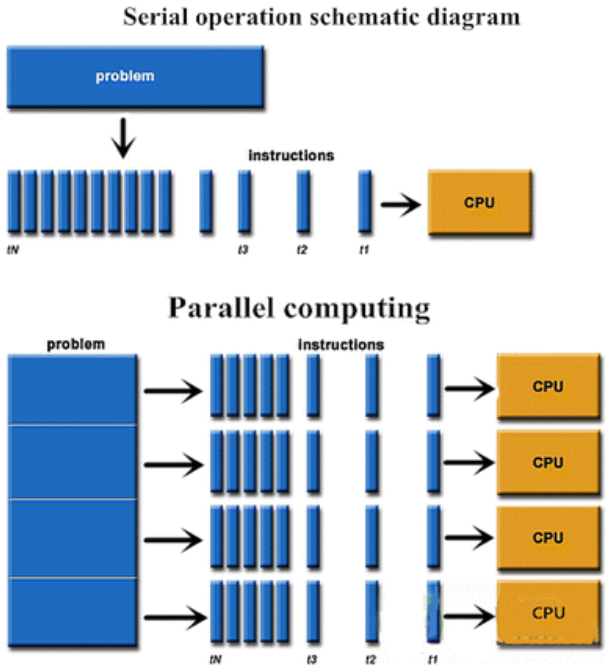


Fig. 6.1. Comparing Parallel and Serial Computing

6.2. CUDA Framework

If we want to use GPU it requires certain framework to communicate and give instructions to GPU hardware. Take for example high graphic games. For the games to use the vector processors for rendering the graphics it requires certain libraries and APIs to compile and communicate instructions the GPU. One such library is Microsoft's DirectX.

Hence in order to compile and give arithmetic instructions to GPU, certain libraries and APIs are required. One such framework is provided by Nvidia called CUDA which is a parallel computing platform and application programming interface model. It enables the user to write and compile programs for CUDA compatible devices.

A CUDA sample C code written in Visual Studio IDE is given below,

```
#define N 10000000

__global__ void vector_add(float *out, float *a, float *b, int n) {
        int i = threadIdx.x;
        int k = n/256 + 1;
        for(int j = 0; j < k; j++){
                if((i + k * 256) < n){
                        out[i + k * 256] = a[i + k * 256] + b[i + k * 256];
                }
        }
}

int main(){
        float *h_a, *h_b, *h_out, *d_a, *d_b, *d_out;
        h_a   = (int*)malloc(sizeof(int) * N);
        h_b   = (int*)malloc(sizeof(int) * N);
        h_out = (int*)malloc(sizeof(int) * N);
        cudaMalloc(*d_a, sizof(int) * N);
        cudaMalloc(*d_b, sizof(int) * N);
        cudaMalloc(*d_out, sizof(int) * N);
        cudaMemcpy(d_a, h_a, sizof(int) * N, cudaMemcpyHostToDevice);
        cudaMemcpy(d_b, h_b, sizof(int) * N, cudaMemcpyHostToDevice);
        cudaMemcpy(d_out, h_out, sizof(int) * N, cudaMemcpyHostToDevice);

        vector_add<<<1, 256>>>(d_out, d_a, d_b, N);

        cudaMemcpy(h_out, d_out, sizof(int) * N, cudaMemcpyDeviceToHost);
        cudaFree(d_a);
        cudaFree(d_b);
        cudaFree(d_out);
        return 0;
}
```

Description of the code:

This code takes two vectors, performs elementwise addition and stores the values in a third vector. In CUDA, DEVICE refers to the GPU and HOST refers to the main unit. Hence, device

memory is the GPU memory and host memory is the system RAM. Any CUDA code consists of two parts: Main program and Kernel program. Main program is executed on CPU and Kernel is executed on GPU. Most of the code is same as simple C code. The new is CUDA memory processing modules and the Kernel. For GPU memory allocation, first a pointer is declared (here d_a, d_b, d_out) and cudaMalloc is called. cudaMalloc allocates memory area in GPU memory and the arguments are pointer to the pointer and size in bytes. Then cudaMemcpy is called. It copies data from host memory to device memory and vice versa and the direction is determined by the last argument. Finally, the kernel is called. The calling method is,

function_name<<<gridDim, blockDim>>>(arguments);

Here, the gridDim and blockDim determines the grid dimensions and block dimensions respectively. Block dimension decides the number of threads in each grid block. When the kernel is called, it executes the instructions of kernel on all the threads (which is equal to the product of number of grid blocks and number of threads in each block) of GPU simultaneously. In the example code, there is one grid block with 256 threads in it. Note grid and grid blocks can have more than one dimensions (up to 3 dimensions).

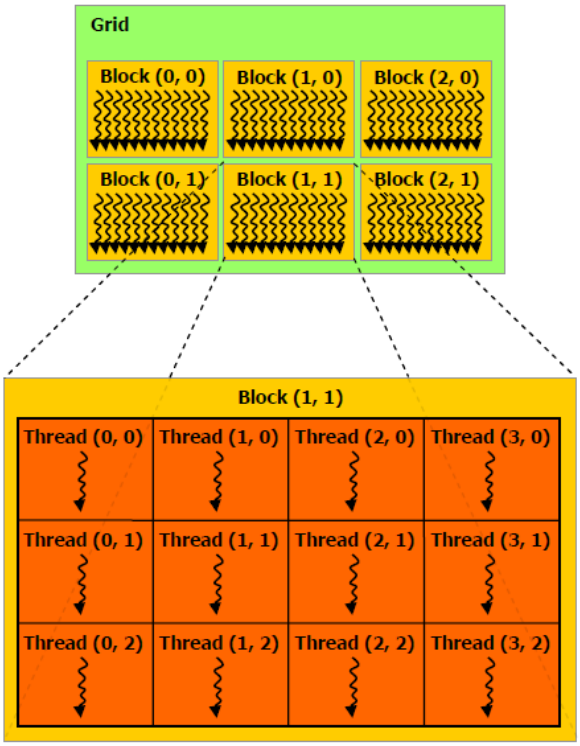


Fig. 6.2. Two-dimensional Grid with two-dimensional grid blocks (CUDA programming guide)

Now, execution threads are 256 and total elements in vectors are 10000000. Hence, addition is looped (10000000/256 + 1) times in the kernel. Then final step is to get the values from device memory back to the host memory. This is done by calling cudaMemcpy function but this time with the argument cudaMemcpyDeviceToHost. Lastly, cudaFree is called to free the device memory.

Summary and Conclusion

In this study the outline of Statistical mechanics was studied. Behavior of gas was studied at the molecular levels. The inverse power law model was used to study the intermolecular collisions. It was noted that inverse power law model, though much accurate, are very difficult and computationally costly to work with and so, certain molecular models are introduced to simulate the real gas flows. First, hard sphere model is introduced to approximate the inverse power law model but it was found that it doesn't comply with the experimental results. So, a more refined model with variable molecular diameter is introduced which is called Variable Hard Sphere (VHS) model. It was found that VHS model satisfies the result of variation of viscosity with temperature. But, still there are some limitations of VHS model. To overcome the limitations of VHS model, Variable Soft Sphere (VSS) model is introduced which is much accurate model for molecular simulations. VHS model though less accurate then VSS, VHS model is generally used in real gas flow simulation as it satisfies the required experimental results and it computationally more efficient. Then a powerful method called Direct Simulation Monte Carlo (DSMC) was explored and its implementation in simulation of rarefied gases was studied. It can be employed with any of the above discussed molecular models. Then the use of parallel computing in DSMC was explored and a code was written in CUDA framework. For future work code can be written is CUDA for simulation of real gas flows.

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Continuum mechanics is used for studying and formulating fluid mechanics problems, when Knudsen number (Kn, ratio of the mean free path length of the molecules of a fluid to a characteristic length) is less than 0.01. Macroscopic properties are calculated without considering the statistical fluctuations (negligible) in continuum flows. But when rarefied gas flows (Kn > 0.1) are to be studied then continuum hypothesis in no longer valid and statistical mechanics is to be invoked. Boltzmann transport equation plays a central role in rarefied gas flows. Numerous methods are formulated to solve and apply Boltzmann equation in practical cases. One such method is Direct Simulation Monte Carlo (DSMC). DSMC is a direct simulation method, where flow is simulated at the molecular level but in a probabilistic manner to make it practical and efficient. In this project, DSMC method is explored and it is studied how to implement it on CUDA framework to exploit the power of parallel processing. In this study the outline of Statistical mechanics was studied. Behavior of gas was studied at the molecular levels. The inverse power law model was used to study the intermolecular collisions. It was noted that inverse power law model, though much accurate, are very difficult and computationally costly to work with and so, certain molecular models are introduced to simulate the real gas flows. First, hard sphere model is introduced to approximate the inverse power law model but it was found that it doesn't comply with the experimental results. So, a more refined model with variable molecular diameter is introduced which is called Variable Hard Sphere (VHS) model. It was found that VHS model satisfies the result of variation of viscosity with temperature. But, still there are some limitations of VHS model. To overcome the limitations of VHS model, Variable Soft Sphere (VSS) model is introduced which is much accurate model for molecular simulations. VHS model though less accurate then VSS, VHS model is generally used in real gas flow simulation as it satisfies the required experimental results and it computationally more efficient. Then a powerful method called Direct Simulation Monte Carlo (DSMC) was explored and its implementation in simulation of rarefied gases was studied. It can be employed with any of the above discussed molecular models. Then the use of parallel computing in DSMC was explored and a code was written in CUDA framework. For future work code can be written is CUDA for simulation of real gas flows.

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Primary goal of physics is to develop and test a theory or formulations put forward to describe Natural phenomena. One such domain of study is Thermodynamics. Thermodynamics, if seen at microscopic level, is formulated using laws of statistical mechanics. At microscopic level, thermodynamics is simply the statistical or collective behavior of large number of particles governed by Newtonian mechanics, if formulated classically, or Quantum mechanics, if quantum effects are significant. Some basic definitions Thermodynamics: It is a phenomenological description of properties of macroscopic systems in thermodynamic equilibrium. (Mehran Kardar) Statistical Mechanics: It is an inherently probabilistic description of the system, where collective behavior of an ensemble (system of many identical particles) is studied. Kinetic Theory of Gases: It is a part of statistical physics where flows of gases are considered on the molecular level, i.e. on the level of individual molecules, and described in terms of changes of probabilities of various states of gas molecules in space and time based on known laws of interaction between individual molecules. Rarefied gas dynamics (RGD) is often used as a synonymous of the kinetic theory of gases. In the narrow sense, the kinetic theory focuses on the general methods of statistical description of gas flows, while the rarefied gas dynamics focuses on solutions of practical gas dynamics problems based on methods of kinetic theory. Non?equilibrium gas dynamics combines methods of rarefied gas dynamics and continuum gas dynamics for description of non?equilibrium gas flows. Direct simulation Monte Carlo (DSMC) method is a stochastic Monte Carlo method for simulation of dilute gas flows on the molecular level. To date, DSMC is the state?of?the?art numerical tool for the majority of applications in the kinetic theory of gases and rarefied gas dynamics. Monte Carlo (MC) method is a general numerical method for a variety of mathematical problems based on computer generation of (pseudo) random numbers and probability theory. Before studying statistical mechanics, some mathematical terms are to be introduced, like phase space, distribution functions, etc. Phase Space: Phase space is the set of all possible states of a system. Take for e.g., a particle which can take 100 discrete positions and 100 discrete speeds. Then the phase space for this system is set of all 100×100=10000 possible states of the particle. Further, we can define a map from phase space to real line such that it assigns with each point (state) in phase space with a real value called the probability of the particle to be in that state. We call this map a probability distribution function and let it be denoted by p(x ?). Where, x ? is vector in phase space. Distribution function f(x, v_x, t) is equal to the average number of molecules in a unit “volume” of a phase space, i.e. f(x, v_x, t) is the number density of molecules in the phase space. is equal to the average number of molecules whose phase coordinates x_i and v_ix at time t satisfy the conditions, In statistical mechanics much of the formulation is done in terms of probabilistic distribution of states. Hence, it is necessary to study some of the standard probability distribution function. Distribution can be discrete or continuous. In discrete distribution, the random variable can take only discrete values. Whereas in continuous distribution, the random variable can take any values with the property that infinitely many values are there between any two numbers, how close they are, which can be taken by the random variable. Discrete Uniform distribution: We say that a discrete variable has uniform distribution if it accepts finite number n of values with equal probabilities Poisson distribution with parameter a is the distribution of a random variable K that takes arbitrary positive integer values and 0 with probabilities Continuous Uniform distribution: We say that a continuous variable X has uniform distribution in an interval [a, b] if The standard random variable ? is the variable with uniform distribution in the interval [0,1] Normal or Gaussian: We say that a continuous variable X has normal or Gaussian distribution if Parameters of this distribution, μ and ?, are equal to the mean and standard deviation of variable X. When working with computer simulations, it becomes necessary to find a way to generate random numbers with required probability distribution. Some of the methods to generate random numbers is given in this section. Numbers having standard random variable distribution can be generated using standard library functions. These equations allow one to obtain two independent samples of variable X simultaneously. One

can use both or only one of them as needed. Here mean and standard deviation of generated numbers is 0 and 1 respectively. A Gaussian random variable Y with mean μ and standard deviation ? can be obtained from random variable X, which has a Gaussian distribution with mean 0 and standard deviation 1 as follows: The degree of rarefaction of a gas is generally expressed through the Knudsen number (Kn) which is the ratio of the mean free path ? to the characteristic dimension L. Kn number shows the applicability of continuum hypothesis. For Kn<0.1 continuum hypothesis i.e. Navier-Stokes equations are applicable. If Kn>0.1 then continuum hypothesis is no longer applicable and statistical fluctuations are prevalent. Statistical mechanics was first primarily studied by Ludwig Eduard Boltzmann. In his study he derived what is called Boltzmann transport equation, which gives time evolution of probabilistic distribution of states of molecules in phase space. Before studying what is phase space just think of thermodynamic system as collection of molecules exhibiting a collective motion. Above equation is called Boltzmann equation which is truncated equation of BBGKY hierarchy. It governs the variation of distribution function with time and space. Note: Above equation is applicable for rarefied gases where only binary collisions are significant. As the denseness of gas increases more terms of the BBGKY hierarchy are required to incorporate tertiary and higher collisions.

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For steady state homogeneous system, Maxwell obtained analytical solution for velocity distribution function. Where, u is mean velocity or stream velocity, T is temperature, R=k_B?m is gas constant. Above distribution function is known as Maxwell-Boltzmann velocity distribution function. In terms of velocities of chaotic motion c=v-u, the Maxwell?Boltzmann distribution function can be written as follows Further, Chapman-Enskog obtained distribution function for small deviations from equilibrium flow by taking perturbations of Maxwellian distribution and obtained following distribution. Above equation is for the special case of a flow in the x-direction with gradients only in the y-direction. This theory authenticated the assumption, inherent in the Navier-Stokes formulation, that the shear stresses, heat fluxes, and diffusion velocities are linear functions of the gradients in velocity, temperature, and species concentration. Analytical solutions for Boltzmann equation are available for few special cases. For flows with complicated geometries and non-equilibrium flows, it is quite difficult (or impossible with current mathematical tools) to obtain analytical solution. So, we resort of some indirect/direct methods for solutions. Some examples of such methods are: Finite element methods (FEM) Lattice Boltzmann method (LBM) Direct Simulation Monte Carlo (DSMC) Particle in Cell (PIC) In a gas, at molecular level, there is chaotic motion and collisions between molecules. The collisions can be described using proper collision potentials between two or more molecules. Describing collisions using potential forces can be very difficult and computationally very costly. A frame of collision between two molecules is shown below (in different reference frames). Considering collision dynamics, the collision trajectories are governed by intermolecular force potential ?, as given below in polar coordinates, As the force in inverse power law models extends to infinity, many times, it happens that the above integrals diverge when infinitely large distances are considered. Hence, it becomes necessary to introduce cut-off distances after which it is assumed that the forces vanish. Other two cross-sections are viscosity cross-section ?_? and momentum/diffusion cross-section ?_M governing the viscosity and momentum transport properties respectively. As can be see above, using generalized collision mechanics with generalized potentials can make the solution very time consuming and computationally costly. Hence, we try to describe collisions by considering variations in hard sphere model. In deriving Maxwell equation, it is inherently assumed that the molecule has spherical structure with constant diameter. Hence, this model is known as hard sphere model. In hard sphere model, the molecules after collision attain velocities based on scattering law. The value of diameter (called kinetic diameter) is taken based on correlation of experimental results with collision cross-section. Where, Z_M is collision frequency per unit volume, z_M collision frequency of single molecule, ?_M is mean free time, ?_M is mean free path and C_a is mean velocity of chaotic motion. As can be inferred, the hard sphere model is oversimplified. In general, viscosity and diffusion both depends on temperature of the gas, hence viscosity and momentum cross-section shouldn’t be constant but depend of relative velocities of molecules. To take care of variation of cross-sections with temperature Variable Hard Sphere (VHS) model is introduced. In VHS model the diameter is no longer constant but changes with temperature (or in other words mean chaotic velocity) to match with experimental changes of viscosity with temperature. The molecular diameter is given by, VHS model account for the variation of mean free path and Knudsen number with the real gas temperature exponent of viscosity. However, the viscosity and momentum cross-sections are still given by eqs. 4.14 This is the limitation of VHS model and to overcome this limitation Variable Soft Sphere (VSS) model was introduced. In this study VHS model is employed, though it is not a very general model but it satisfies most of the required real gas conditions. In this study, we are going to implement DSMC method for finding solutions to Boltzmann equation. In DSMC method instead of finding direct solution of Boltzmann equation we try to obtain statistical average of various quantities by directly simulating the dynamics of flow at molecular level. Here, we try to follow motion of molecules. But instead of simulating each and every molecule, we simulate representative molecules were each representative molecule is equivalent to several molecules. Hence, we invoke criteria of

similarity of flows to scale the parameters. Two flows (physical phenomena) are called similar if numerical properties of such flows are identical in reduced units. In application to the rarefied gas flows, it means that two similar flow correspond to the same solution of the Boltzmann equation in reduced units. Two solutions are similar if they correspond to the same Sh, Fe, and Kn. These non?dimensional numbers (parameters) are called the criteria of similarity. Thus, one can simulate a real gas flow with characteristic number density n_(*(r)) composed of molecules with characteristic cross section ?_(*(r))=?d_Ref^2 by a flow with another characteristic number density n_(*(s)) and composed of simulated molecules of another size ?_(*(s)). The real and simulated flows are similar, if the Knudsen number is the same in both flows: is called the statistical weight of a simulated particle. Practically, one can say that every simulated particle represents W particles in the real gas flow. First flow domain is divided into cells. The dimensions of cell are of the order of mean free path. Then, initially, simulated molecules are distributed over the phase space covering the flow domain according to assumed distribution function. Here, the number of simulated molecules a quite less than the original number of molecules. Hence, each simulated molecule represents several real molecules according to the statistical weight. Generally, for rarefied gas, in each cell, 30 simulated molecules are taken. Basic idea in DSMC method is to divide the simulation time step into two parts. In one part, position of simulated molecules is (deterministically) incremented according to their velocities. In this step collisions are not taken into account. In second part of the time step only collisions are taken into account. Collisions are considered to be instantaneous, i.e. the transition from pre-collision velocities to post-collision velocities is instantaneous.

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Here, not every pair is considered for collision but a probabilistic estimate is considered based on the collision cross-section and relative velocity. The probability of a collision between two molecules in a homogenous gas is proportional to the product of their relative speed and total collision cross-section. Physics of Boundary collisions and Binary collisions is as follows: Boundary collisions – Diffuse Scattering Binary collisions – Isotropic scattering after collision In the case of VHS model, post?collisional velocities after a binary collisions of molecules i and j are given by where the unit vector e_cr^' defines the direction of relative velocity c_r^' after the collision. Distribution of directions of e_cr^' is given by the differential collision cross section ?=?(C_r). e_cr^' is an isotropic random vector given by, Selection of collision pairs is based on a technique devised by Bird. If probability of collisions between all possible pairs is calculated then computation cost is of the order of N2. But Bird found that it is not necessary to calculate all collision pairs. Bird introduced No Time Counter (NTC) scheme which gives the number of pairs to be calculated. The NTC scheme by Bird utilizes the acceptance and rejection Monte Carlo method and is based on the introduction of a majorant [?_T C_r]_max, i.e. such quantity that In the NTC scheme, N_pair=Z_max ?t random pairs (i, j) of molecules is selected, but for every pair collision happens with probability P_collision=(?_(T(ij)) c_(r(ij)))?[?_T C_r]_max . In this case, the number of arithmetic operations is proportional to N log?N and grows with N. Majorant [?_T C_r]_max is important numerical parameter of the NTC scheme. N_pair=Z_max ?t collisions are sampled during time step. Real collision (accepted collision) occurs with probability P_coll=(?_(T(ij)) c_(r(ij)))?[?_T C_r]_max . All other collisions are fictitious (rejected collisions). As can be inferred, in Direct simulation of molecules lot of computational power is required. Even though criteria of similarity of flow is invoked to decrease the number of simulated molecules, but still a huge amount of computational power is required to simulate complex flows. If serial computing is employed then the time taken for simulation may become impractical. In present scenario and based on the ongoing trend, there is and will be a lot of advancement in parallel computing using GPUs or Vector processors. In this study, parallel processing is used to carry out DSMC simulation. But before going further into parallel computing some basics of serial and parallel computing is outlined. Let us take a simple example. Addition of two arrays with 1000 elements. In serial computing it is simple. A loop is invoked and in each loop cycle one element is added. Now in parallel computing, we use multiple cores of GPU. So that on each core one element is added and all the cores work simultaneously. Hence, in serial computing same calculation (i.e. addition) is carried out 1000 times one after other. Whereas in parallel computing, calculation is carried out 1000 times only, but here all 1000 calculations occur simultaneously. If we want to use GPU it requires certain framework to communicate and give instructions to GPU hardware. Take for example high graphic games. For the games to use the vector processors for rendering the graphics it requires certain libraries and APIs to compile and communicate instructions the GPU. One such library is Microsoft's DirectX. Hence in order to compile and give arithmetic instructions to GPU, certain libraries and APIs are required. One such framework is provided by Nvidia called CUDA which is a parallel computing platform and application programming interface model. It enables the user to write and compile programs for CUDA compatible devices. This code takes two vectors, performs elementwise addition and stores the values in a third vector. In CUDA, DEVICE refers to the GPU and HOST refers to the main unit. Hence, device memory is the GPU memory and host memory is the system RAM. Any CUDA code consists of two parts: Main program and Kernel program. Main program is executed on CPU and Kernel is executed on GPU. Most of the code is same as simple C code. The new is CUDA memory processing modules and the Kernel. For GPU memory allocation, first a pointer is declared (here d_a, d_b, d_out) and cudaMalloc is called. cudaMalloc allocates memory area in GPU memory and the arguments are pointer to the pointer and size in bytes. Then cudaMemcpy is called. It copies data from host memory to device memory and vice versa and the direction is determined by the last argument. Finally, the kernel is called. The calling method is, Here, the gridDim and blockDim

determines the grid dimensions and block dimensions respectively. Block dimension decides the number of threads in each grid block. When the kernel is called, it executes the instructions of kernel on all the threads (which is equal to the product of number of grid blocks and number of threads in each block) of GPU simultaneously. In the example code, there is one grid block with 256 threads in it. Note grid and grid blocks can have more than one dimensions (up to 3 dimensions). Now, execution threads are 256 and total elements in vectors are 10000000. Hence, addition is looped (10000000/256 + 1) times in the kernel. Then final step is to get the values from device memory back to the host memory. This is done by calling cudaMemcpy function but this time with the argument cudaMemcpyDeviceToHost. Lastly, cudaFree is called to free the device memory.

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c 1 , respectively, , is the collision cross-section, t represents time, r the physical space, anddirect simulation monte carlo (dsmc) 171 in a gas mixture consisting of a total of sif two particular species are represented by subscripts p and q, the boltzmann equation for species p of...

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