

**GIAN Course on
Rarefied & Microscale Gases and Viscoelastic Fluids:
a Unified Framework**

**Lecture 6
Gas Kinetic Theory and Boltzmann Equation**

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Content

I. Gas kinetic theory

II. Boltzmann equation

III. V & V of DSMC

I. Gas kinetic theory

- Hypersonic rarefied regime: $Kn = O(10^{-3} \sim 10^{-1})$, $N_\delta = O(10^{-1} \sim 1)$
- Low-speed microscale creeping regime: $Kn = O(10^{-2} \sim 1)$, $N_\delta = O(10^{-5} \sim 10^{-2})$
- High-speed free-molecular regime: $Kn = O(1 \sim 10)$, $N_\delta = O(1 \sim 10)$
- **Local Equilibrium**
 - Global thermal equilibrium exists when all parts of a system are at the same temperature and this temperature is the same as that of the surroundings.
 - Global thermodynamic equilibrium (GTE) means that the intensive parameters are *homogeneous throughout* the whole system
 - **Local thermodynamic equilibrium** (LTE) means that the intensive parameters are *varying in space and time*, but are *varying so slowly* that for any point, one can assume *thermodynamic equilibrium in some neighborhood about that point*.
 - **Translational, rotational, vibrational modes**

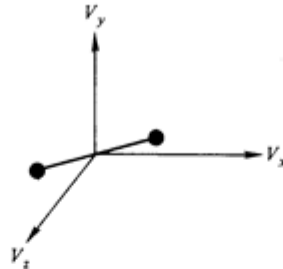
I. Gas kinetic theory

(a) Diatomic molecule



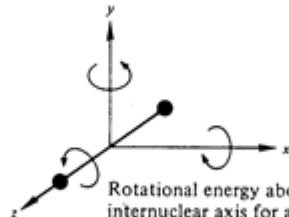
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(b) Translational energy ϵ'_{trans}



Translational kinetic energy of the center of mass (thermal degrees of freedom-3)

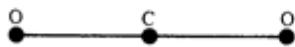
(c) Rotational energy ϵ'_{rot}



Rotational kinetic energy; (thermal degrees of freedom-2 for diatomic; 2 for linear polyatomic; and 3 for nonlinear polyatomic)

Rotational energy about the internuclear axis for a diatomic molecule is negligibly small.

(d)

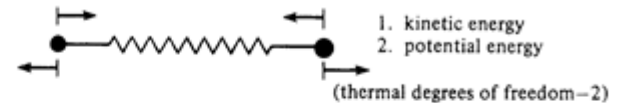


CO₂; linear polyatomic molecule

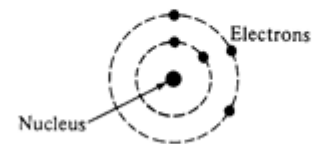


H₂O; nonlinear polyatomic molecule

Vibrational energy ϵ'_{vib}



Electronic energy ϵ'_{el}

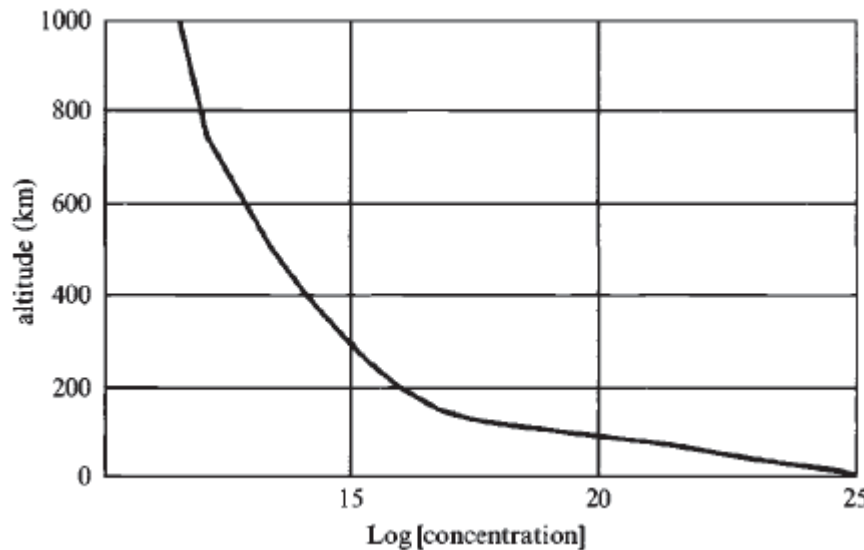


1. Kinetic energy of electrons in orbit
2. Potential energy of electrons in orbit

Modes of molecular energy.

I. Gas kinetic theory

- The gas kinetic theory aims to explain and compute the macroscopic properties of gases such as conserved and non-conserved variables and transport coefficients from the properties of their microscopic constituents.
- There are about 10^{20} molecules in a cubic meter at the altitude of 100 km.



I. Gas kinetic theory: Distribution function

- Let us consider the number of cars whose weights lie within a certain interval Δw . Then the fraction of cars per unit interval of weight can be written as

$$f_k = \frac{\Delta N_k}{N \Delta w} \text{ where } \Delta N_k \text{ the number of cars with weights in } k \text{ interval}$$

- When Δw becomes infinitesimally small, the function becomes a continuous function, referring to as the normalized distribution of car weights

$$f(w) = \lim_{\Delta w \rightarrow 0} f_k = \lim_{\Delta w \rightarrow 0} \frac{\Delta N_k}{N \Delta w} \quad \text{and} \quad \int_0^\infty f(w) dw = \lim_{\Delta w \rightarrow 0} \sum_{k=0}^\infty f_k \Delta w = 1$$

- This distribution function can be interpreted as a probability density function.
- One can calculate the average weight of a car in the community

$$\bar{w} = \lim_{\Delta w \rightarrow 0} \left\{ \sum_{k=0}^\infty \left(\frac{w_k + w_{k+1}}{2} \right) \frac{\Delta N_k}{N} \right\} = \int_0^\infty w f(w) dw \Rightarrow \bar{Q} = \int_0^\infty Q(w) f(w) dw$$

I. Gas kinetic theory

- The normalized phase space distribution function is the probability density of finding a particle at the velocity space point \mathbf{v} at the configuration space location \mathbf{r} .

$$f(\mathbf{r}, \mathbf{v}) = \frac{F(\mathbf{r}, \mathbf{v})}{n(\mathbf{r})} \text{ where } n(\mathbf{r}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(\mathbf{r}, \mathbf{v}) dv_x dv_y dv_z$$

- Macroscopic physical parameters are averages of quantities that depend on molecular velocities (velocity space averages).

$$\bar{Q} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Q(\mathbf{v}) f(\mathbf{r}, \mathbf{v}) dv_x dv_y dv_z \text{ or simply } \int Q(\mathbf{v}) f(\mathbf{r}, \mathbf{v}) d\mathbf{v}$$

- J. C. Maxwell derived a velocity distribution for spatially uniformly distributed molecules in the gas

$$f(\mathbf{v}) = \left(\frac{\beta}{2\pi} \right)^{3/2} e^{-\beta \frac{\mathbf{v} \cdot \mathbf{v}}{2}}$$

I. Gas kinetic theory

- Until this stage, no explicit mention of what the distribution function actually means is given; anything like molecules in a gas or probability density function of agents with wealth in open market economy is possible in principle.
- In fact, it turned out that the determination of another unknown β provides the connection necessary to assign a physical meaning to the distribution function, otherwise, a pure mathematical object.
- In gas kinetic theory, thermodynamics plays such a role.
- Local equilibrium Maxwell-Boltzmann distribution

$$\beta = \frac{m}{k_B T} \Rightarrow f(\mathbf{v}) = \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-\frac{m}{k_B T} \frac{(\mathbf{v}-\mathbf{u})^2}{2}}$$

I. Gas kinetic theory

- Worldwide poll among mathematicians: What do you think is the most beautiful mathematical equation?



- Worldwide poll among every human being: What do you think is the most beautiful or amazing number?

Memo

II. Boltzmann equation

- Let us assume that the gas density is low enough to ensure that the mean free path is large in comparison with the effective range of the intermolecular forces. The velocities of the colliding particles are uncorrelated, that is, particles which have already collided with each other will have many encounters with other particles before they meet again. (Molecular chaos and break of time reversal)
- Assume time, location and particle velocity are independent variables of the phase space distribution function. We have a first-order partial differential equation in space and time.

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}, \mathbf{v}) = C[f, f_2]$$

Movement

Collision (or Interaction)

Kinematic

Dissipation

II. Boltzmann equation

- Let us assume the molecules and their intermolecular forces are assumed to be spherically symmetric. This assumption is sometimes questionable for real gases.
- Assume also effects of the external forces on the magnitude of the collision cross section are neglected.
- Boltzmann collision integral

$$C[f, f_2] = \text{Gain (scattered into)} - \text{Loss (scattered out)}$$

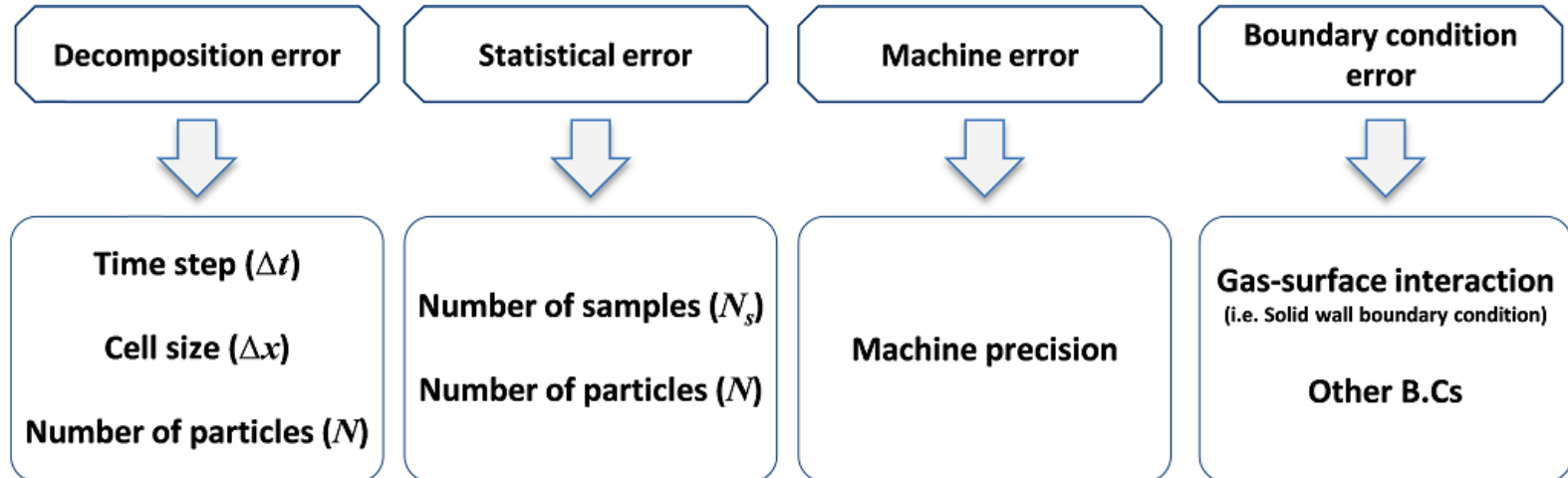
$$= \left(\frac{\delta f}{\delta t} \right)^+ - \left(\frac{\delta f}{\delta t} \right)^-$$

$$\sim \int |\mathbf{v} - \mathbf{v}_2| (f^* f_2^* - f f_2) d\mathbf{v}_2$$



III. V & V of DSMC

- Background: why we care about the verification of pure simulation methods
- There always exist computational errors in any simulation methods so that we may need a tool to verify them.
- But, it is impossible to find exact solutions free from computational errors for pure simulation methods like the DSMC, hindering further refinement of the method.



III. V & V of DSMC

- A **verification is possible** based on the following property [C&F 15]

$$\nabla \cdot \left(\rho \mathbf{u} \mathbf{u} + \frac{1}{\gamma M^2} p \mathbf{I} + \frac{1}{\text{Re}} \mathbf{\Pi} \right) = 0 \quad \text{or} \quad \oint_S \mathbf{F} \cdot \mathbf{n} dS = 0 \quad \text{at steady-state}$$

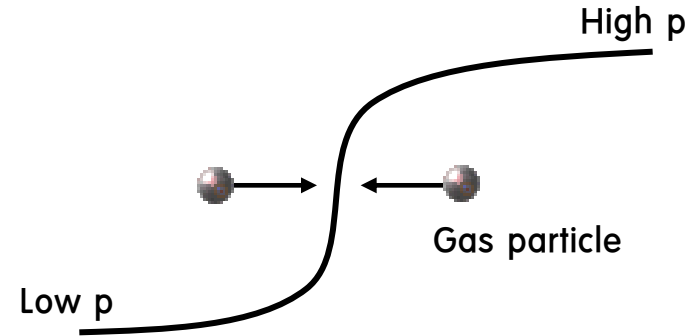
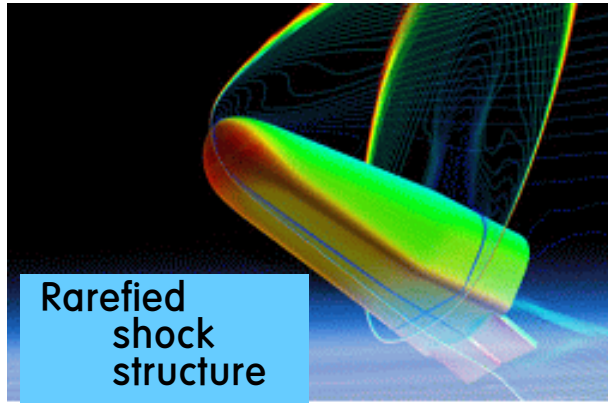
- A challenge is the statement of C. Villani (2004):

*“The conservation laws should hold true when there are no boundaries. In presence of boundaries, however, conservation laws may be violated: **momentum is not preserved by specular reflection.**”*

- In conservative PDE-based schemes, the nearest cell to the wall always satisfies the conservation laws via $\mathbf{U}_{i,j}^{n+1} = \mathbf{U}_{i,j}^n - \frac{\Delta t}{A_{i,j}} \sum_{k=1}^4 \mathbf{F}_k \Delta L_k$ but **it may not be true in the case of non-PDE schemes.**

III. V & V of DSMC

First benchmark problem: Gaseous compressive shock structure



$$\text{error}_{mass} \equiv \rho u - \overline{\rho u}$$

$$\text{error}_{x\text{-momentum}} \equiv \rho u^2 + p - \Pi_{xx} - \left\{ \overline{\rho u^2 + p - \Pi_{xx}} \right\}$$

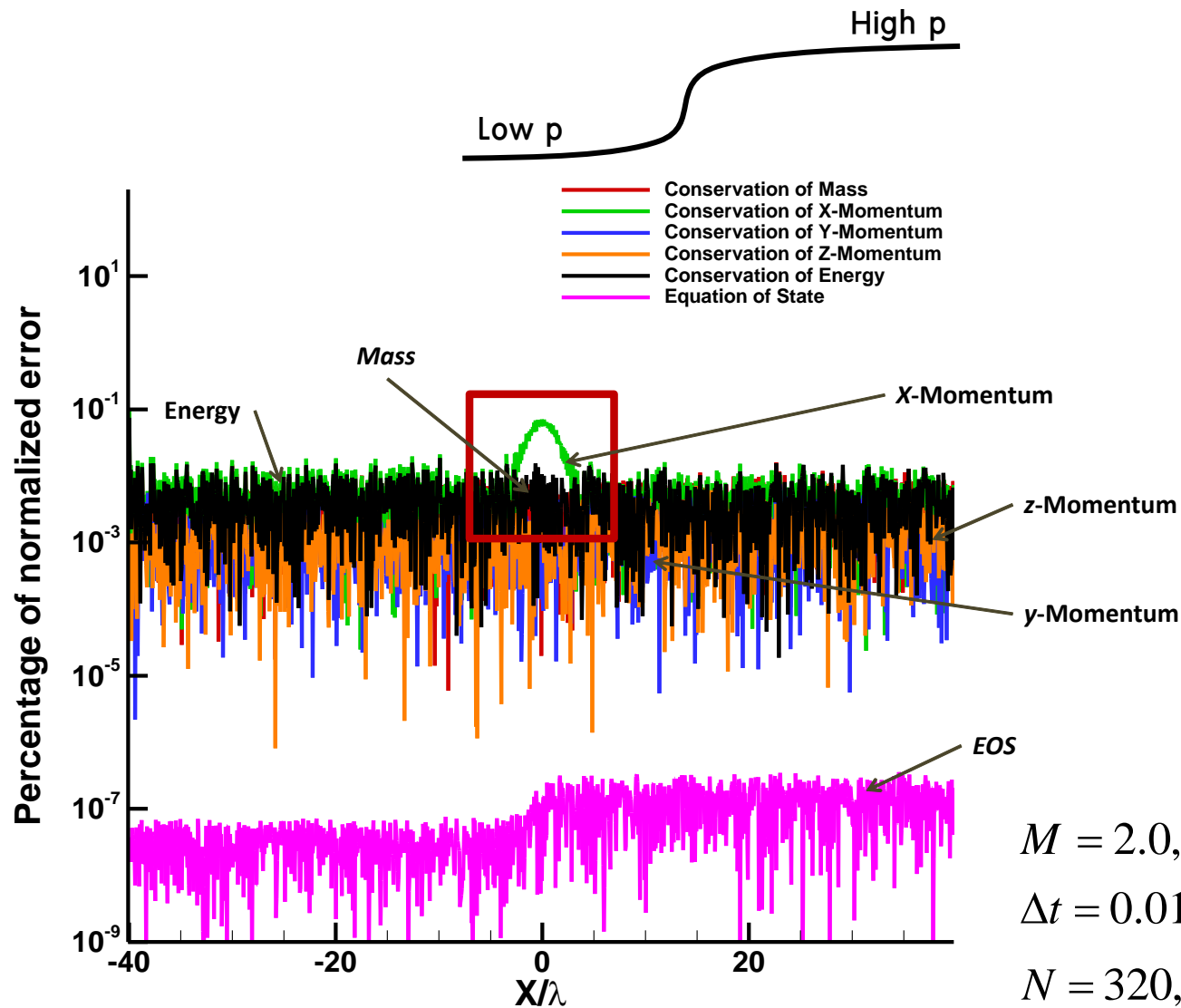
$$\text{error}_{y\text{-momentum}} \equiv -\Pi_{xy} + \overline{\Pi_{xy}}$$

$$\text{error}_{z\text{-momentum}} \equiv -\Pi_{xz} + \overline{\Pi_{xz}}$$

$$\text{error}_{energy} \equiv (\rho E + p)u - \Pi_{xx}u + Q_x - \left\{ \overline{(\rho E + p)u - \Pi_{xx}u + Q_x} \right\}$$

$$\text{error}_{EOS} \equiv p - \rho RT \quad \Rightarrow \quad \text{Round-off error}$$

III. V & V of DSMC

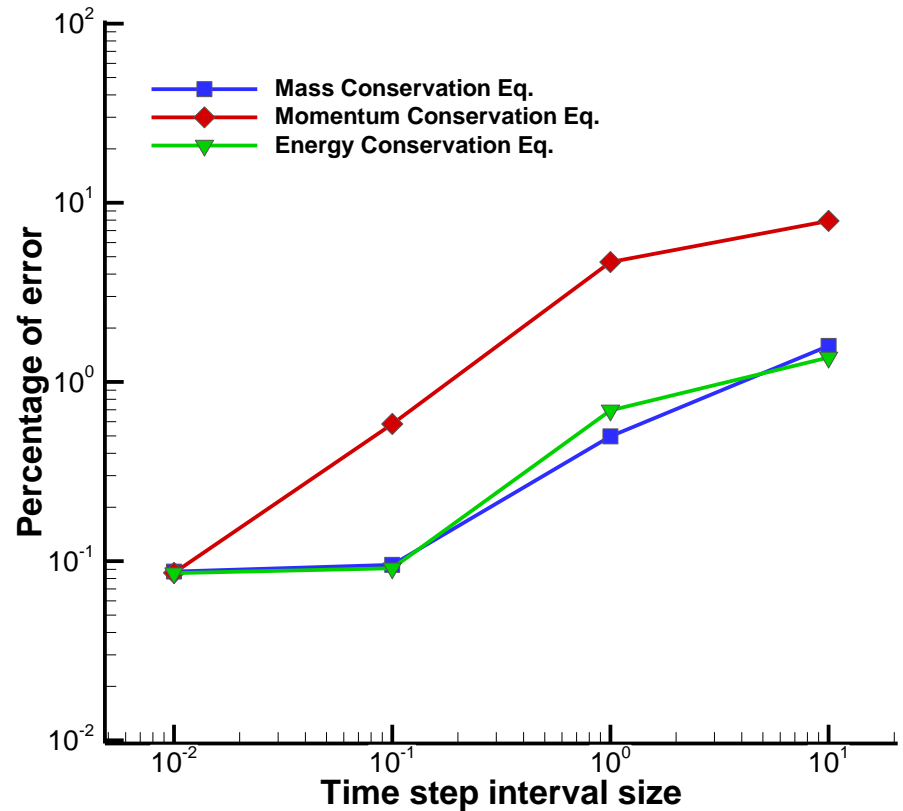
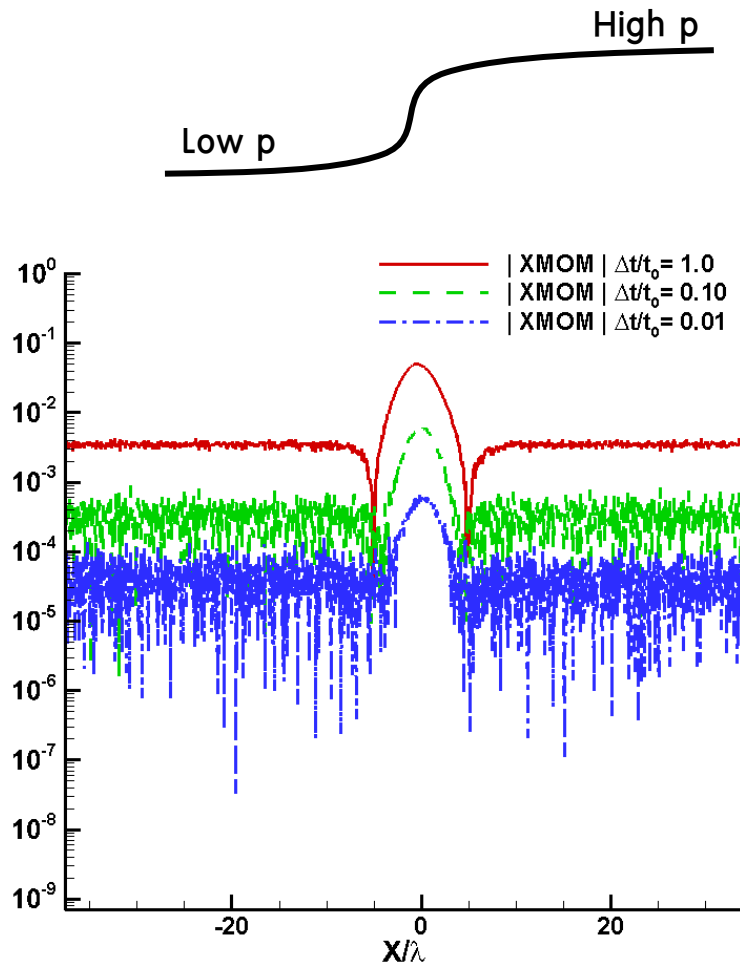


$$M = 2.0, \text{Kn} = 1.0,$$

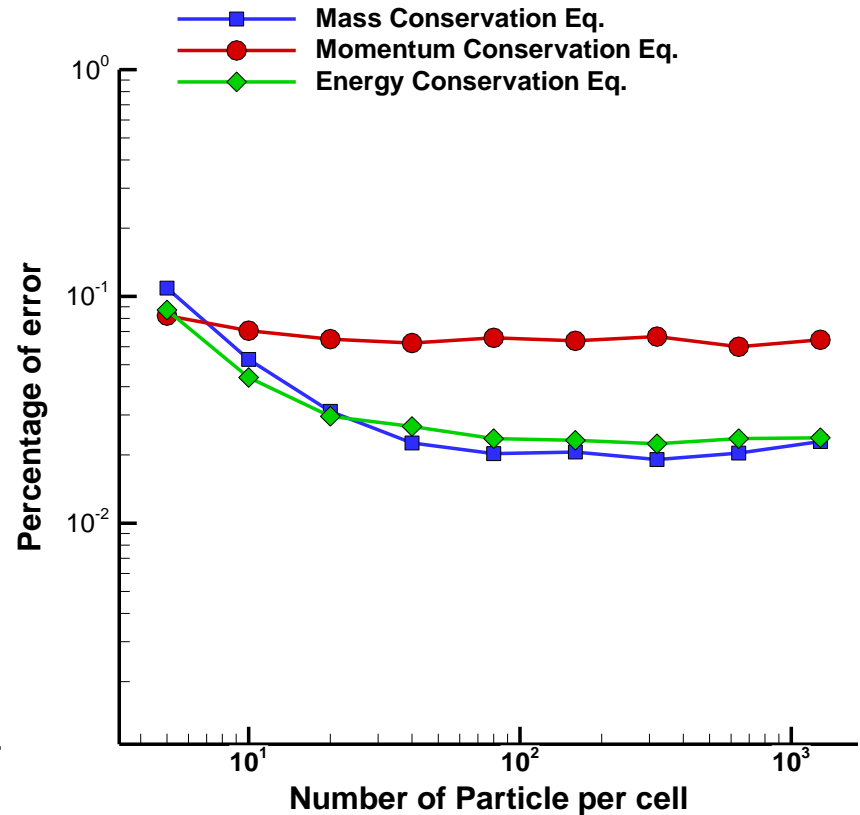
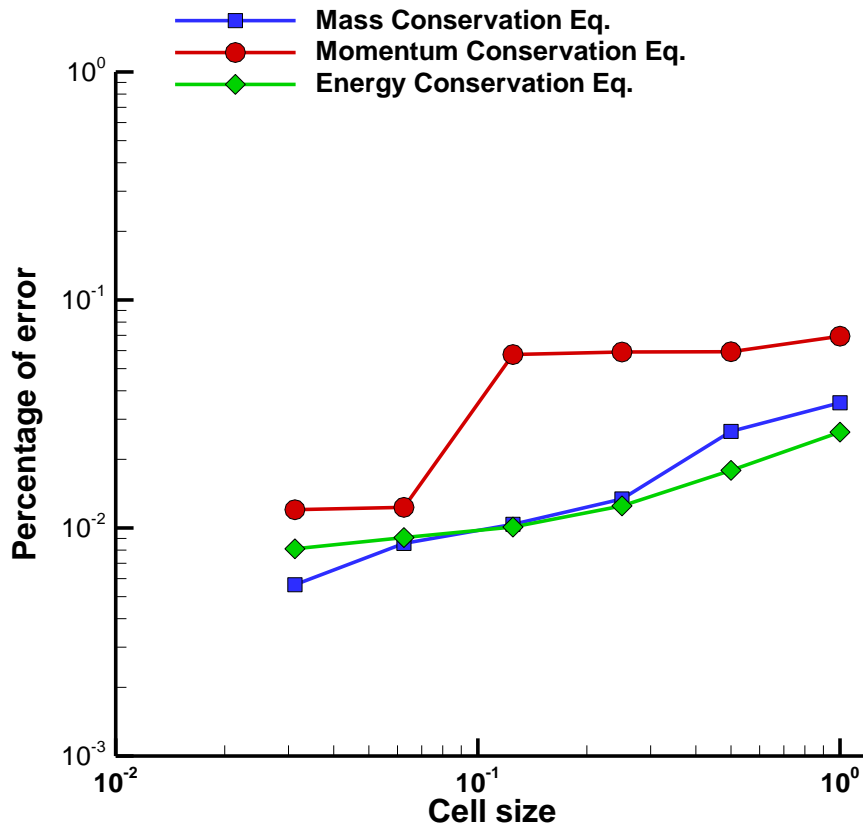
$$\Delta t = 0.01\tau_{\infty}, \Delta x = 1/32\lambda_{\infty},$$

$$N = 320, N_s = 10^8$$

III. V & V of DSMC

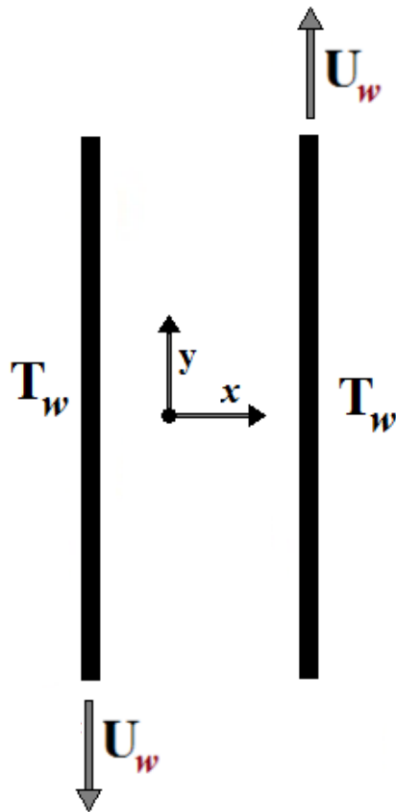


III. V & V of DSMC



III. V & V of DSMC

Second benchmark problem: Wall-driven Couette flow



$$\text{error}_{x\text{-momentum}} \equiv p - \Pi_{xx} - \left[\overline{P - \Pi_{xx}} \right]$$

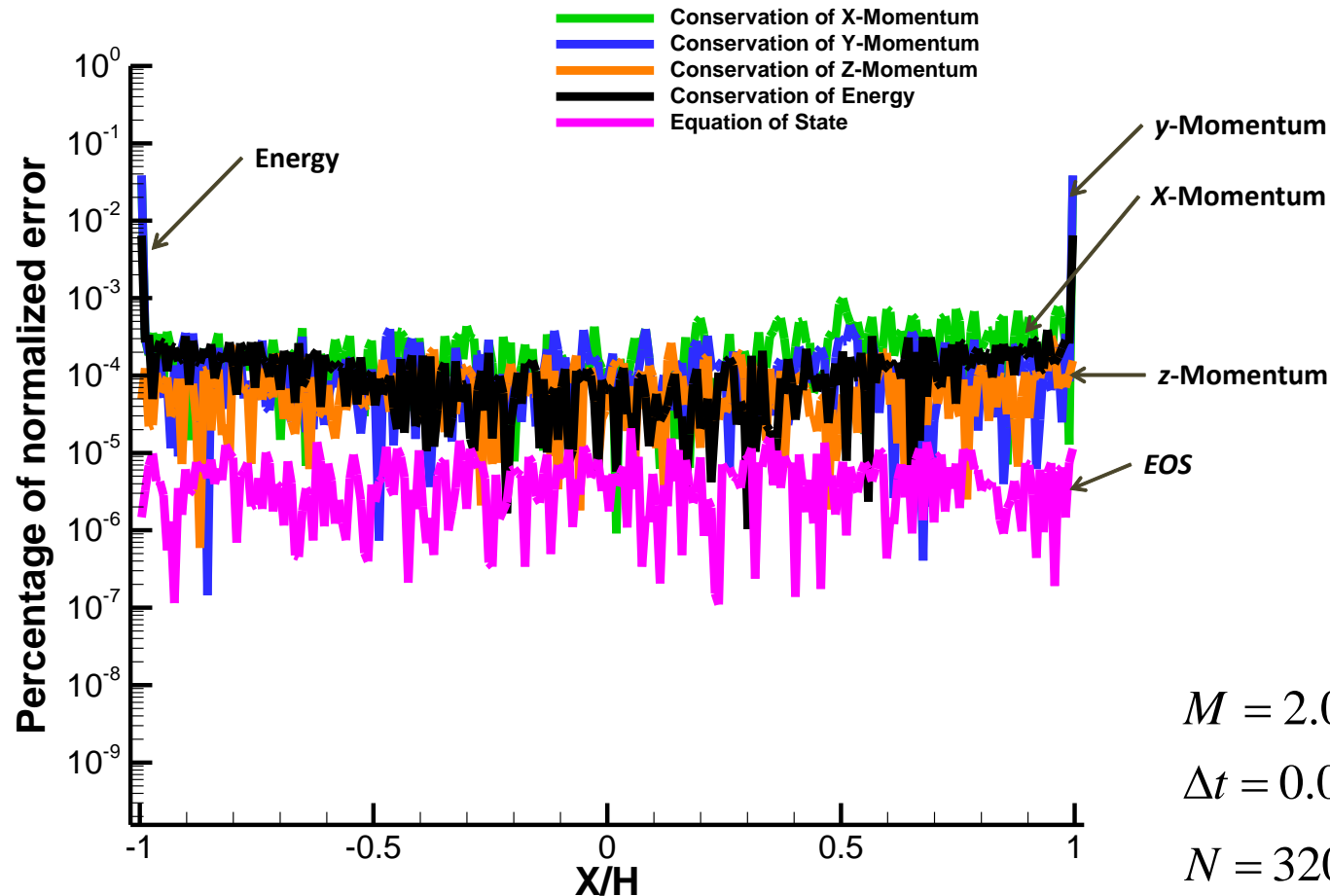
$$\text{error}_{y\text{-momentum}} \equiv \Pi_{xy} - \overline{\Pi_{xy}}$$

$$\text{error}_{z\text{-momentum}} \equiv \Pi_{xz} - \overline{\Pi_{xz}}$$

$$\text{error}_{\text{energy}} \equiv -\Pi_{xy}v + Q_x - \left[\overline{-\Pi_{xy}v + Q_x} \right]$$

$$\text{error}_{EOS} \equiv p - \rho RT \quad \Rightarrow \quad \text{Round-off error}$$

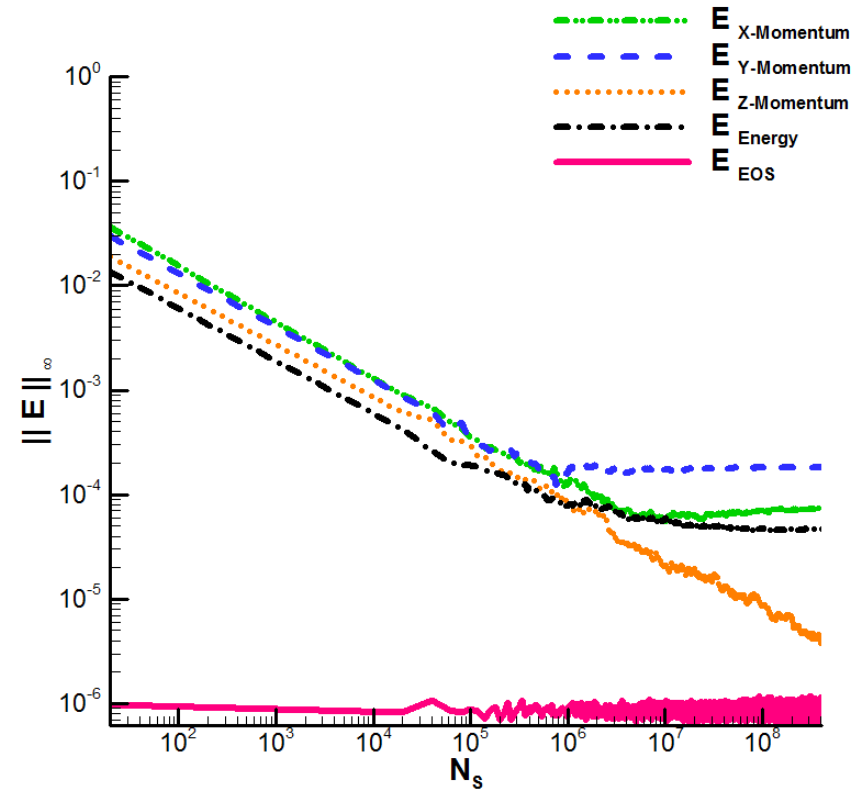
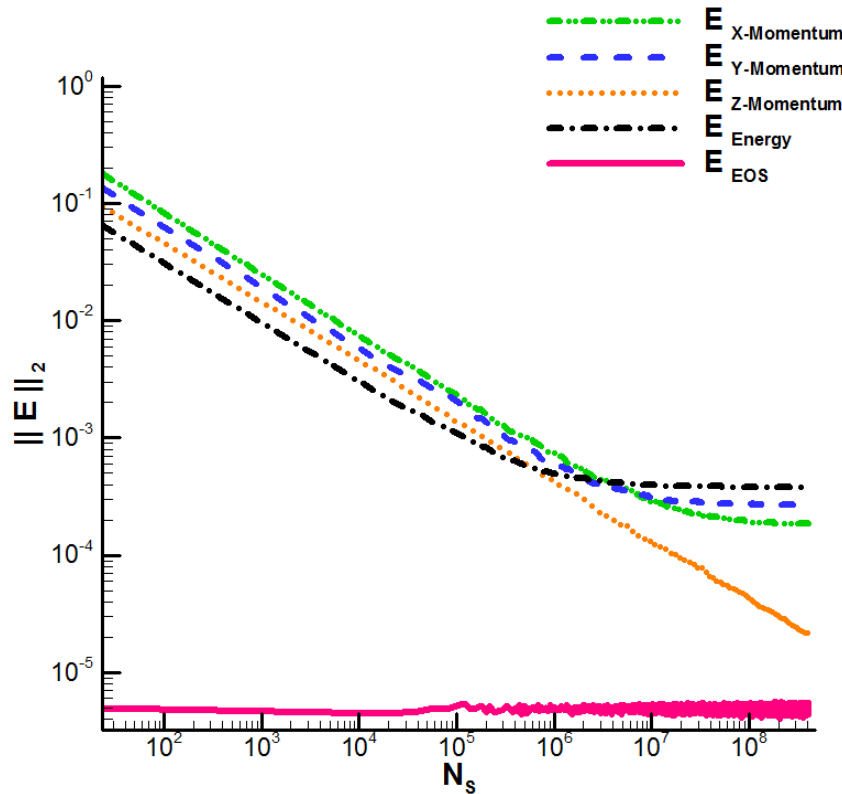
III. V & V of DSMC



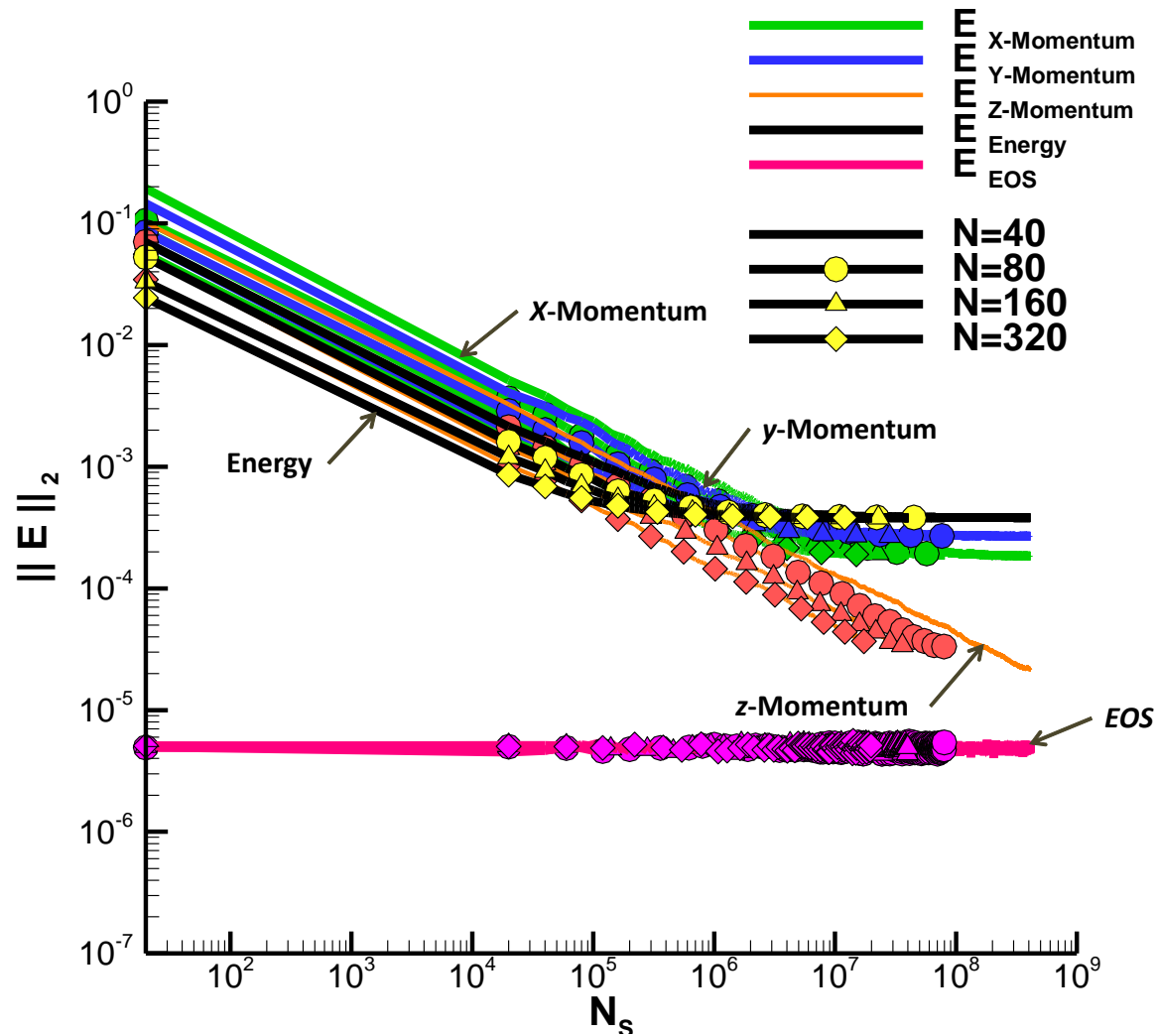
$$M = 2.0, \text{Kn} = 1.0,$$
$$\Delta t = 0.01\tau_{\infty}, \Delta x = 1/32\lambda_{\infty},$$
$$N = 320, N_s = 10^8$$

III. V & V of DSMC

Convergence history of DSMC simulation



III. V & V of DSMC



Q & A
