Introduction to Molecular Aerodynamics and Direct Simulation Monte Carlo Method

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Ludwig Eduard Boltzmann

Ludwig Eduard Boltzmann was born in Wien on February 20th, 1844. He is one of the most important theoretical physicists in history for his founding contributions in the field of: gas kinetic theory, statistical mechanics, and statistical thermodynamics. He is also one of the most important advocates for atomic theory. In 1869, at the age of 25, he was appointed full Professor in Mathematical Physics at the University of Graz. In 1869, he spent several months in Heidelberg, working with Robert Bunsen and Leo Königsberger and then, in 1871, he worked with Gustav Kirchhoff and Hermann von Helmholtz in Berlin. In 1872, he obtained his famous equation, and in 1873 he joined the University of Wien as a Professor in Mathematics where he stayed until 1876. He died by suicide in Duino on September 5th, 1906, succumbing to the pain he felt after the premature death of one of his children. He was buried in Vienna in the Zentralfriedhof. The epigraph, engraved on his tomb, is:

$$S = k \ln(\Omega)$$

with S: the entropy, k: the Boltzmann constant, and Ω: the number of microstates of the thermodynamic system, or the number of ways in which the particles constituting the system are distributed over the energy levels E_1, E_2, E_3,…E_j.

CONTENTS

LIST OF SYMBOLS

A_i, i=1, 2, 3 : Functions of C
a : Laplacian speed of sound
a_1, b_1, e_i, i=1, 8 : Parameters in the Burnett boundary conditions
B_i, i=1, 2, 3 : Functions of C
C : Thermal velocity
C_L, C_D, C_{Mz} : Lift, drag, pitching moment coefficients
C_x, C_y, C_z : Thermal velocity components along x-, y-, z-axis
c : Most probable thermal velocity
c_p, c_v : Constant pressure, constant volume specific heats
D_{pq} : Diffusivity of molecular species p and q
D_s : Satellite diameter or satellite aerodynamic drag
d : Diameter of a molecule
dp : Probability
dr : Volume element in the position space (dr=dxdydz)
dS_r, dS_V : Elements of S_r, S_V
dV : Volume element in the velocity space (dV=dudvdw)
E : Energy of a molecule
e : Specific energy per unit mass
e_r : Unit vector normal to an element in the position space
e_v : Unit vector normal to an element in the velocity space
e* : Internal energy for unit of volume
F : Force per unit mass
F_a : Friction force for unit surface
F_N : Number of real molecules represented by each simulated molecule
f : Distribution function
f_e, f_n, f_t : Accommodation coefficients of energy, normal momentum, tangential momentum
f_M : Maxwell distribution function
G : Generic quantity of a molecule
h, H : Altitude
J : Jacobian operator

K : Kernel function or thermal conductivity or super/hypersonic similarity parameter or a constant

Kn : Knudsen number

K_r^2 : Cheng-Chang rarefaction parameter

k : Boltzmann constant or number of parameters

L : Characteristic linear dimension

Ma : Mach number

m : Mass of a molecule

N : Number of simulated molecules

n : Number density or local normal to the body surface or number of degrees of freedom of a molecule

P : Continuum break-down parameter of Bird

P_E : Electrical power provided to the heater of an arc wind tunnel

Pr : Prandtl number

p : Probability density function or pressure

q : Dynamic pressure

$\dot{q}$: Heat flux

R : Gas constant

Re : Reynolds number

r : Position vector or linear coordinate in a spherical coordinate system

S : Speed ratio or surface

S_r : Surface of a volume in the position space

St : Stanton number

S_V : Surface of a volume in the velocity space

t : Time

T : Temperature or tether tension

$\underline{\underline{U}}$: Unit tensor

u, v, w : Components of the total velocity along the x-, y- and z-axis

V : Total velocity ($V=V_0+C$)

V_r : Relative velocity between two molecules

V_0 : Stream velocity

W_s : Apparent weight of the satellite

X : Generic stochastic variable or molar fraction

x, y, z : Space coordinates

X, Y, Z : Dimensions of the calculation domain

z, Z : Altitude

Greek symbols

α	: Fraction of molecules re-emitted in a diffuse way or angle of attack
β	: Shock wave angle or supersonic similarity parameter
δ	: Molecular spacing
γ	: Ratio of constant pressure and constant volume specific heats or angle of the tether with respect to horizontal
Φ	: Dissipation function
φ	: Disturbance or angle in a spherical coordinate system
λ	: Mean free path
μ	: Viscosity
ν	: Collision frequency
ρ	: Density
σ	: Total collision cross section
ϑ	: Local angle of incidence with surface
θ	: Burnett constant
$\underline{\underline{\tau}}$	: Tangential stress tensor
ω	: Viscosity temperature index or angle in a spherical coordinate system or Burnett constant
Ω	: Solid angle or number of microstates of the thermodynamic system

Subscripts and superscripts

CG	: Center of Gravity
c	: Collision
d	: Dissipative
dif	: Diffusive
inc	: Incident
rem	: Re-emitted
w	: Wall
*	: Per unit volume or post-collision
$(\ )_s^0$	: Symmetric (s) and non-divergent (0)
$\overline{G}$	: Average of G
$\overline{\overline{G}}$	: Moment of G

Acronyms

2D : Two dimensional
3D : Three dimensional
BE : Boltzmann Equation
BGK : Bathnagar-Gross-Krook
BUE : BUrnett Equations
CE : Chapman-Enskog
CEV : Crew Exploration Vehicle
CFD : Computational Fluid Dynamics
CM : Command Module
DSMC : Direct Simulation Monte Carlo
FC : Fully Catalytic surface
FMF : Free Molecules Flow
EE : Euler Equations
HEO : High Earth Orbit
ISS : International Space Station
LEO : Low Earth Orbit
MD : Molecular Dynamics
ME : Maxwell Equation
MOC : Method Of Characteristics
NASA : National Aeronautics and Space Administration
NC : Non Catalytic surface
NSE : Navier-Stokes Equations
SPES : Small Planetary Entry Simulator
TSS : Tethered Satellite System
UHTC : Ultra High Temperature Ceramic
VHS : Variable Hard Sphere model
VSS : Variable Soft Sphere model

1. INTRODUCTION

The basic difference between classic aerodynamics and molecular aerodynamics is that the first one studies a flow field by the evolution of macroscopic parameters representing the state of a flow field such as velocity, temperature, density, and so on. The second one studies a flow field by the evolution of velocity, position, and internal state of each molecule of gas. Thus, molecular aerodynamics provides a more detailed, and therefore more precise, description of a fluid-dynamic system. Even though the molecular approach is of general validity, from an engineering point of view, it is aimed at studying rarefied, i.e. Free Molecules Flow (FMF), transition and low-density continuum, high velocity regimes, as per those met by a spacecraft along a high-altitude entry/re-entry path.

As is well-known, the Navier-Stokes equations (NSE) are not suitable to solve rarefied regimes because of: 1) failure of the phenomenological equations of Newton, Fourier and Fick, 2) non-equilibrium (translation, rotational, and vibrational temperatures are different), 3) anisotropy (components of translational temperature and of pressure are different along the three space directions).

Nowadays, the solution of rarefied flow fields relies on molecular methods such as Molecular Dynamics (MD) and Direct Simulation Monte Carlo (DSMC). Both MD and DSMC are computational (not numerical) methods. In fact, both do not rely on integration of differential equations. These methods consider gas as made up of molecules, whose evolution (movement, collisions with other molecules and with a body, activation/relaxation of internal degrees of freedom) is simulated by a computer. The difference between the two methods is that: MD is deterministic, DSMC is statistic. In fact, the number of simulated molecules in MD is the same as the number of real molecules, while the number of simulated molecules in DSMC is much smaller than the number of real molecules, thus the simulated molecules represent an unbiased sample of real molecules.

The Boltzmann equation (BE) should be able, in principle, to solve every flow field from FMF to low density continuum regimes. Unfortunately, this is not yet possible because BE, as shown later, is an integral-differential equation and its solution shows overwhelming theoretical and numerical difficulties; the scientific community is still searching for a solution of general validity. However, it has to be pointed out that some researchers, using simplifying assumptions and/or particular computing procedures, found the solution of particular problems. For example, Cercignani [1] found a solution of the Poiseuille flow. For this reason, BE, according to the opinion of the author, is of scarce interest from an engineering point of view, also considering that the solution of rarefied flow fields is successfully obtained by the Direct Simulation Monte Carlo (DSMC) method [2, 3, 4]. However, BE is extremely important from a theoretical point of view. The aim of this book is to show the link between BE and other equations valid at several rarefaction levels. These are quantified by the Knudsen number Kn_L ($Kn_L=\lambda/L$, is the mean free path, L is a characteristic linear dimension of the problem under study):

1) Maxwell equation (ME), $Kn_L>>1$ (FMF), 2) Burnett equations (BUE), $Kn_L\cong1$ (transitional regime), 3) Navier Stokes equations (NSE), $Kn_L<<1$ (continuum regime), 4) Euler equations (EE), $Kn_L=0$ (continuum and non-diffusive regime). The present book will show that BE has to be considered as origin, and then as “mother”, of the above mentioned equations.

The topic covered in this book is very important from an engineering point of view because the field of interest hypersonic aerodynamics essentially concerns low-density flow field, even the FMF regime. Theoretical and experimental studies of this regime have already been done extensively in 1960-1970 and were aimed at studying the aerodynamics of satellites and evaluating the aerodynamic forces, with particular regard to drag. These, although minor, can lead to significant variations in the attitude of a satellite, as well as being responsible for the orbit decay because of the very low values of atmospheric density. An estimate of these forces provides indications on the design of the propulsion systems for station keeping and for evaluating the duration of the stay in orbit for a satellite.

The joint NASA/ESA program "International Space Station" (ISS) re-launches the study of this problem, also considering that, unlike the satellites which are usually characterized by a simple shape (sphere, cylinder, flat plate etc. and/or a combination), aerodynamics of the above mentioned bodies have already been studied both theoretically and experimentally. The orbiting space station is characterized by a very complex shape, even with orientable surfaces, then aerodynamic interference effects can be important. It is advisable for students and researchers in aerospace engineering to also be informed of the aerodynamic equations alternative and, complementarily to the phenomenological formulation, use it in the courses in classic Aerodynamics and Fluid-dynamics. The book will show that the gas behavior, from a macroscopic point of view, can be completely evaluated by the knowledge of position, velocity, and internal state of the molecules by characterizing the gas from a microscopic point of view.

The mathematical processing of this topic suffers from overwhelming difficulties, thus it will be treated only with a descriptive approach and, in order to avoid heavy mathematical procedures, most formulae will be provided without proof. The present book comes out from reading, filtering, working out, and summarizing a number of books and papers, available in open literature. More specifically, the following sections will consider:

1) Characterization of a fluid-dynamic system, from a molecular point of view, by probability distribution functions (Sec.2).
2) Link among molecular (or microscopic) and thermodynamic (or macroscopic) quantities (Sec.3).
3) Boltzmann equation (Sec.4).
4) Transfer equations (Sec.5), Maxwell (Sec.6), approximation of the distribution function (Sec.7).
5) Euler (Sec.8), Navier-Stokes (Sec.9) and Burnett (Sec.10) equations.
6) Boundary conditions (Sec.11).
7) Mean free path and classification of the flow field rarefaction (Sec.12).
8) Gas-surface interaction (Sec.13).
9) Approximate theories for the computation of pressure and skin fliction coefficients (Sec.14).
10) Calculation of the aerodynamic force (Sec.15).
11) Atmospheric entry/re-entry (Sec.16)
12) Description of the DSMC method and analysis of results (Sec.17).

A meaningful part of this book will be devoted to the DSMC method. DSMC can be currently considered as the unique solution of rarefied flow fields which should otherwise be described and solved by BE. This topic is of great importance because almost any entry/re-entry path to a planet, bearing atmosphere, involves aero-assisted maneuvers like changing orbital altitude, for example transferring from High Earth Orbit (HEO) to Low Earth Orbit (LEO), changing attitude and aero-breaking. Aero-breaking is necessary for depleting kinetic energy of a capsule or of a space-plane and therefore for reducing velocity in order to avoid excessive aerodynamic and thermal loads. Using an aero-assisted procedure, instead of the propulsive one, is convenient because it reduces the amount of fuel for the rockets, which controll trajectory and attitude, and then enhances the payload of a spacecraft.

Usually, aero-breaking is carried out by a multi-pass procedure. Fig.1.1 shows the picture (out of scale) of an orbital transferring, from a planetary approach trajectory to a target orbit by a multi-pass aero-breaking. This scheme is depicted, for example, with only three orbits (or passes). The Magellan spacecraft mission to Venus developed in 730 orbits [5]. A particular case of a multi-pass aero-breaking is the “planetary aero-capture”. This is an aero-assisted maneuver where the velocity decrement, for transferring a space vehicle from the approach trajectory to the target orbit around a planet, is achieved in a single pass.

A space vehicle, during an entry pass, can experiment flow fields from FMF to continuum regimes. A flow field between continuum and FMF (or transition regime) can characterize a large portion of a pass. Thus, the solution of a flow field in this regime and the assessment of aerodynamic forces and heat flux can provide useful information for planning a spacecraft mission. For example, National Aeronautics and Space Administration (NASA) programmed sending a probe onto Titan in 2027. Titan is the largest moon of Saturn and has an atmosphere which is a mixture of Nitrogen (N_2), Methane (CH_4), and Argon (Ar). Molar fractions are about: X_{N2}=0.95, X_{CH4}=0.03, X_{AR}=0.02. The purpose of the mission is to study both the atmosphere and the surface of this moon which is similar to that of the primordial Earth and to search any clues to a possible extraterrestrial life.

Because of the complex phenomenology of the transitional regime, an unique, viable and operational mathematical model, solving the whole transitional regime, is not yet available. This difficulty involved the necessity of classifying the transition regime into sub-regimes. Hayes and Probstein [6] proposed the following classification that, from FMF to continuum flow, is: 1) first collision, 2) multiple collisions, 3) fully merged, 4) incipient merged, 5) viscosity interaction. Many attempts have been made, and are still being made, at solving this problem by approaching the solution either from continuum, namely by extending NSE to lower density flows, or from FMF, namely by extending the Boltzmann equation to higher density flows.

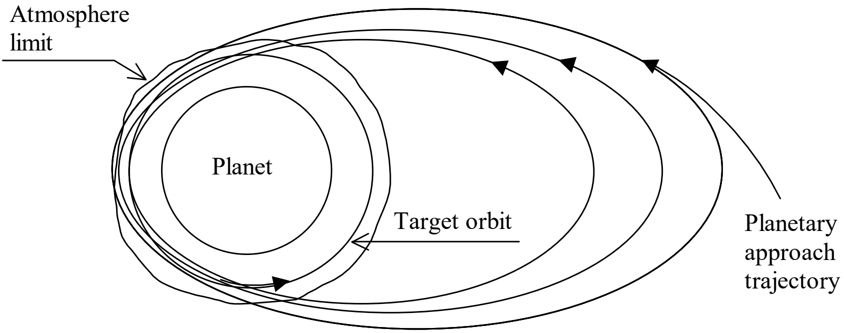

Fig.1.1 Multi-pass aero-assisted maneuvers for planetary aero-breaking.

Even though the balance and the conservation equations of fluid dynamics are valid in all flow regimes, the solution of NSE becomes lacking with increasing flow rarefaction. In fact, the numerical integration of NSE relies also on the computation of shear stress, heat flux, and diffusion of chemical species. The equations, computing these quantities, known also as phenomenological equations, consist of the gradients of macroscopic velocity, temperature, concentration of chemical species time the related transport parameter: viscosity μ (law of Newton), thermal conductivity K (law of Fourier), diffusivity D_{pq} of molecular species p and q (law of Fick). In low-density regimes, the phenomenological equations of Newton, Fourier, and Fick, computing shear stress, heat flux, and diffusion of chemical species are no longer valid. Moreover, as the density decreases, the intermolecular collisions in the gas get too few for maintaining isotropy of the pressure tensor. The conventional no-slip condition fails, and knowledge of slip velocity (u_{slip}) and temperature jump ($\Delta T=T-T_W$) is necessary for fixing the boundary conditions on the body surface. For example, the equations computing the slip velocity and the temperature jump for the solution of the flow field in a Viscous Shock Layer [7] are here reported:

$$u_{slip} = A\varepsilon^2 \left(\frac{\mu}{p} \sqrt{\frac{\gamma - 1}{\gamma} T} \left(\frac{\partial u}{\partial n} - K_s u \right) \right)_w \tag{1.1}$$

$$T - T_w = B\varepsilon^2 \left(\frac{\mu}{p} \sqrt{\frac{\gamma - 1}{\gamma} T} \frac{\partial T}{\partial n} \right)_w \tag{1.2}$$

where, besides the well-known meaning of symbols, $A = 1.2304(2 - f_t)/f_t$, $B = 2.3071(2 - f_e)/f_e$, ε is the reciprocal of the root square of the Reynolds number based on the radius of the body nose, n is the local normal to the surface, K_s is the non-dimensional surface curvature, f_t and f_e are the accommodation coefficients of tangential momentum and energy, respectively.

The Direct Simulation Monte Carlo (DSMC) method, being developed by Bird since 1963, seems to be the unique method for solving the whole transition regime. Philosophy of DSMC contrasts with classic fluid dynamics. In fact, classic fluid dynamics consider gas like a continuous medium, modeled in terms of the macroscopic, physical quantities (density, pressure, temperature, and so on). The solution of the flow field relies on the integration of differential equations. On the contrary, DSMC outlines a gas as made up of a number of discrete molecules with translational, rotational, and vibrational energies. Movement of the molecules, and collisions with other molecules and with the surface of the body under study, are governed by the equations from the kinetic theory of gases. One of the most important features of DSMC is that it does not require the equilibrium condition.

Due to the importance of this topic in the field of aerospace engineering, divulging the DSMC method to students and researchers has to be considered proper. After describing the method, (only general features are considered and all equations are reported without demonstration), four applications of DSMC are here proposed and the results discussed. The first one, related to the very simple case of a zero-dimensional flow, is aimed at describing the computer implementation of the method; the related code DSMC0S.FOR [8] is examined step by step. The second one considers a more complex phenomenology; it is related to quantification of non-equilibrium and anisotropy along the entry path in Mars' atmosphere of Pathfinder. The third example is the study of the aerodynamic behavior of the Orion capsule along a high-altitude entry path in Mars' atmosphere. Local quantities and global aerodynamic coefficients have been computed. The fourth one is the simulation of the flow field in the arc wind tunnel SPES (Small Planetary Entry Simulator) at the Department of Industrial Engineering of the University of Naples "Federico II" around specimens of Ultra High Temperature Ceramic (UHTC) materials. These DSMC simulations solved the flow field in the divergent part of the nozzle, and in the test chamber, and were aimed at getting information about the test conditions: electrical power supplied to the torch, area ratio (exit area/throat area) of the divergent part of the nozzle, and the specimen diameter. Two advanced codes for the solution of 2D/axial-symmetric flow fields (DS2V [9]) for the calculation of local quantities, and for the solution of 3D flow fields (DS3V [10]) for the calculation of global, aerodynamic coefficients, have been used.

2. PROBABILITY DENSITY, DISTRIBUTION FUNCTION AND PHASE SPACE

Gas is considered made up of a very large number of molecules. As said before, the flow field is completely described when position, velocity, and internal state of all molecules are known at each time (t). Obviously, because of the extremely large number of molecules, this approach is not feasible from an operative point of view. For example, for Earth at the sea level, the number density (n) of air molecules is about 2.5×10^{25} m^{-3}. For this reason, a statistical approach, based on the probability concept, is necessary.

The probability (dp) that a generic event X occurs is, by definition, a non-dimensional number in the closed interval [0-1]. The value of probability is suggested by an own, personal feeling and/or experience. Probability is evaluated in terms of the probability density function (p(X)). This function is such that probability, that a generic, stochastic variable X is in the interval [X¸ X+dX], is given by dp=p(X)dX. In literature, there is a number of theoretical models for p(X), each one suitable to a specific problem, such as: Gaussian, negative exponential, χ-square, uniform, and many others. Certainly, the "canonical" definition of probability is not operative from an engineering point of view. In this case, the distribution function f(X) is used in lieu of p(X), and the related probability is an engineering probability: dp=f(X)dX. For example, if the number of cases verifying an event is discrete and the distribution function is uniform (meaning that each case has the same chance to happen), probability can be computed as the ratio of the number of cases, this verifies the event and the number of all possible cases, if all cases have the same probability of happening or are unbiased. For example, if there are four white balls and six black balls in a box, the probability of pulling out a white ball is 4/10.

The state of a molecule is completely described, at each time, by a number (k) of parameters G_i, i=1,2,…,k, such as: position, velocity, energy levels of rotation, of vibration, and so on. Only mono-atomic molecules, or molecules without any interior degree of freedom which can interfere with the translational one, are here considered. Therefore, the degree of freedom of a molecule is only translational. At each time, the state of a molecule is completely defined by position $\underline{r}$ (x, y, z) and velocity $\underline{V}$ (u, v, w). Velocity is made up of macroscopic stream velocity ($\underline{V}_0$) and peculiar (or thermal) velocity ($\underline{C}$): $\underline{V} = \underline{V}_0 + \underline{C}$.

The dynamic state of a molecule can be represented in a seven dimensions space, considering at each time position and velocity. This space ($\underline{r}$, $\underline{V}$, t) is named "phase space". The state of a fluid-dynamic system, made of n molecules, is known if the 6n parameters (x, y, z, u, v, w) are known at each time (t). Since variables $\underline{r}$ and $\underline{V}$ are considered stochastically independent, an element of phase space (drdV) can be represented by two separated elements: 1) position (dr=dxdydz) at a stated velocity (Fig.2.1a), 2) velocity (dV=dudvdw) at a stated position (Fig.2.1b). The number dn of molecules, characterized by position and velocity in the ranges [$\underline{r}$, $\underline{r}$+d$\underline{r}$] and [$\underline{V}$, $\underline{V}$+d$\underline{V}$] is, according to definition of engineering probability:

$$\frac{dn(\underline{r}, \underline{r} + d\underline{r}; \underline{V}, \underline{V} + d\underline{V}; t)}{n} = f(\underline{r}, \underline{V}, t) drdV \tag{2.1}$$

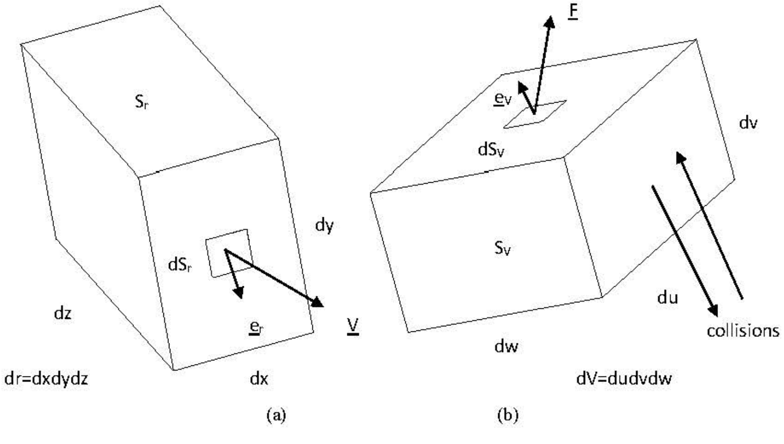

Fig.2.1 Elements of phase space: a) position (dr) at fixed velocity, b) velocity (dV) at fixed position.

The distribution function f(r, V, t) is characterized by the following properties:

1) It is normalized, i.e. its integral on both dr and dV is unity.
2) It tends to zero when r and V tend to infinity.

3) It is computed as the product of the distribution functions depending on $\underline{r}$ and that depending on $\underline{V}$: $f(\underline{r},\underline{V},t)=f(\underline{r},t)f(\underline{V},t)$. This is due to the stochastic independence of $\underline{r}$ and $\underline{V}$.

3. LINK AMONG MICROSCOPIC AND MACROSCOPIC QUANTITIES: METHOD OF MOMENTS

The distribution function f is sufficient for evaluating all fluid-dynamic quantities by means of the averages over all molecules in the phase space. If G is a generic quantity of a molecule, by definition, the average value ($\overline{G}$) is:

$$\overline{G}(t) = \frac{1}{n}\int G dn(\underline{r}, \underline{V}, t) \tag{3.1}$$

By substituting dn from Eq.2.1:

$$\overline{G}(t) = \int\int G f(\underline{r}, \underline{V}, t) dr dV \tag{3.2}$$

Integration with respect to dr and dV makes $\overline{G}(t)$ to be a constant over the phase space.

By integrating Eq.3.2 only with respect to dV, leaving $\underline{r}$ as variable and considering that dr and dV are independent of each other:

$$\overline{G}(\underline{r}, t) = dr\int G f(\underline{r}, \underline{V}, t) dV \tag{3.3}$$

Therefore, $\overline{G}(\underline{r}, t)$ is averaged only on velocity and keeps dependence on position. By dividing by dr:

$$\frac{\overline{G}(\underline{r},t)}{dr} = \overline{\overline{G}}(\underline{r},t) = \int Gf(\underline{r},\underline{V},t)dV \tag{3.4}$$

$\overline{\overline{G}}$ is called moment of G, and is characterized by the same dimensions like G, per unit volume [G/L^3]. Since its computation does not rely on integration with respect to dr, $\overline{\overline{G}}$ keeps the dependence on $\underline{r}$. In order to obtain thermodynamic quantities, one can consider a reference system moving with velocity $\underline{V}_0$ thus, the phase space will be ($\underline{r}$, $\underline{C}$, t):

3.1 Number density

G=1, the moment is the number density (n):

$$n(\underline{r},t) = \int 1 \cdot f(\underline{r},\underline{C},t)dC \tag{3.5}$$

3.2 Density

G=m (mass of a molecule), the moment is the density (ρ):

$$\rho(\underline{r},t) = \int mf(\underline{r},\underline{C},t)dC \tag{3.6}$$

3.3 Internal energy

G=1/2mC^2 (kinetic energy of a molecule), the moment is the internal energy per unit volume (e*):

$$e*(\underline{r},t) = \int \frac{1}{2} mC^2 f(\underline{r},\underline{C},t)dC \tag{3.7}$$

3.4 Stress tensor

G=-m$\underline{CC}$ (the sign "-" is because it is opposite to the momentum flux), the moment is the stress tensor ($\underset{=}{\tau}$):

$$\underline{\underline{\tau}}(\underline{r},t) = -\int m\underline{C}\underline{C}f(\underline{r},\underline{C},t)dC \tag{3.8}$$

whose components are:

$$\underline{\underline{\tau}} = -\rho\begin{bmatrix} \overline{C_x^2} & \overline{C_xC_y} & \overline{C_xC_z} \\ \overline{C_yC_x} & \overline{C_y^2} & \overline{C_yC_z} \\ \overline{C_zC_z} & \overline{C_zC_y} & \overline{C_z^2} \end{bmatrix} \tag{3.9}$$

The stress tensor is made up of a conservative part ($-p\underline{\underline{U}}$), p being the pressure and $\underline{\underline{U}}$ being the unit tensor, and a dissipative part ($\underline{\underline{\tau}}_d$) which is the difference between $\underline{\underline{\tau}}$ and -p$\underline{\underline{U}}$ ($\underline{\underline{\tau}}_d = \underline{\underline{\tau}} + p\underline{\underline{U}}$). Pressure p is, by definition, the trace of $\underline{\underline{\tau}}$ or the average of terms on the main diagonal of the matrix (3.9). It is the conservative part of the stress tensor:

$$p = -\frac{1}{3}\rho\left(\overline{C_x^2} + \overline{C_y^2} + \overline{C_z^2}\right) = -\frac{1}{3}\rho\overline{C^2} \tag{3.10}$$

then the dissipative part of $\underline{\underline{\tau}}$ is:

$$\underline{\underline{\tau}}_d = -\rho\begin{bmatrix} \overline{C_x^2} - p/\rho & \overline{C_xC_y} & \overline{C_xC_z} \\ \overline{C_yC_x} & \overline{C_y^2} - p/\rho & \overline{C_yC_z} \\ \overline{C_zC_z} & \overline{C_zC_y} & \overline{C_z^2} - p/\rho \end{bmatrix} \tag{3.11}$$

3.5 Heat flux

G=1/2mC$^2\underline{C}$ (flux of kinetic energy of a molecule), the moment is the heat flux ($\underline{\dot{q}}$):

$$\underline{\dot{q}}(\underline{r},t) = \int \frac{1}{2} mC^2\underline{C}f(\underline{r},\underline{C},t)dC \tag{3.12}$$

its components along x, y, z are:

$$\dot{q}_x = \frac{1}{2}\rho\overline{C^2 C_x}, \qquad \dot{q}_y = \frac{1}{2}\rho\overline{C^2 C_y}, \qquad \dot{q}_z = \frac{1}{2}\rho\overline{C^2 C_z} \tag{3.13}$$

4. BOLTZMANN EQUATION

The Boltzmann equation (BE [1, 2, 3, 4]), in the unknown function f, establishes a link between the distribution function f and the variables $\underline{V}$, $\underline{r}$ and t. This equation, derived by Boltzmann in 1872, is a more operative version of the Liouville equation; the Liouville equation is written in terms of probability density while BE is written in terms of distribution function.

BE relies on the following assumptions:

1)Gas is dilute. By definition, a gas is dilute if the molecular spacing δ ($\delta = n^{-1/3}$) is much greater than the molecular diameter (d): $\delta/d >> 1$. This assumption implies that the collisions are only bi-molecular and involve only weak intermolecular forces.

2)Intermolecular collisions are perfectly elastic. A collision is elastic if there is no energy exchange between translational degree of freedom (kinetic energy) and rotational and vibrational degrees of freedom (internal energy), there is no chemical reaction (dissociation, recombination and exchange), and post-collision momentum is equal to pre-collision momentum. These points imply that the molecules can be considered as rigid spheres.

3)"Molecular chaos". This assumption relies on the concept of stochastic independence; the distribution function of a generic molecule is independent of the distribution function of other molecules. This means that, chosen randomly two molecules 1 and 2 in the phase space, the distribution function, providing the probability that molecule 1 is in the position $\underline{r}_1$ with velocity $\underline{V}_1$ and molecule 2 is in the position $\underline{r}_2$ with velocity $\underline{V}_2$ is given by the product of the single distribution function:

$$f(\underline{r}_1, \underline{r}_2, \underline{V}_1, \underline{V}_2, t) = f(\underline{r}_1, \underline{V}_1, t) f(\underline{r}_2, \underline{V}_2, t) \tag{4.1}$$

Therefore, knowledge of the distribution function of a single molecule is sufficient for characterizing the distribution function of the whole system. BE provides the change of the number of molecules in the phase space. BE is made of four terms:

4.1 Change of the number of molecules in time

From Eq.2.1, the number of molecules in an element of the phase space drdV is: dn=nf($\underline{r}$,$\underline{V}$,t)drdV (whenever possible, for simplicity, the distribution function will be written hereafter just as f instead of f($\underline{r}$,$\underline{V}$,t)). The variation in time of dn is:

$$\frac{\partial n}{\partial t}=\frac{\partial f}{\partial t}n\,dr\,dV \tag{4.2}$$

4.2 Convection of molecules across S_r by effect of velocity

Velocity $\underline{V}$ is constant in the position volume dr. Since the number of molecules in the element of phase space is nfdrdV, the density of molecules, characterized by velocity $\underline{V}$ in dr is nfdV. The flux of molecules of class $\underline{V}$ (a molecule is of class $\underline{V}$ if its velocity is in the range $\underline{V}$÷$\underline{V}$+d$\underline{V}$), entering dr across S_r (Fig.2.1a), is:

$$-n\int_{S_r}\left(f\underline{V}\cdot\underline{e}_r dV\right)dS_r \tag{4.3}$$

where: S_r is the total area of the surface that defines the volume dr, $\underline{e}_r$ is the unit vector normal to dS_r (Fig.2.1a).

By the Gauss theorem, that transforms a surface integral into a volume integral and by indicating the "nabla operator" as $\partial/\partial r$, the term (4.3) reads:

$$-n\int_{dr}\left(\frac{\partial}{\partial\underline{r}}(f\underline{V})dV\right)d(dr) \tag{4.4}$$

Since f and $\underline{V}$ are constant in dr, the term (4.4) can be written as:

$$-\frac{\partial}{\partial\underline{r}}\cdot(f\underline{V})n\,dr\,dV \tag{4.5}$$

and $\underline{V}$ can put out the derivative. Therefore, the flux of molecules of class $\underline{V}$ through surface S_r finally reads: