

1. FORMULAS INVOLVED IN THE SET UP OF NORMAL SHOCK WAVE SIMULATIONS.

In this section of the course, we will perform simulations of normal shock wave using Ellipsoidal-Statistical Bhatnagar-Gross-Krook model. Before we begin with the descriptions of the steps to setup simulations, we will summarize a few relevant formulas from Gas dynamics.

1.1. Physical Characteristics of Gas. Properties of gas depend on the molecules that make up the gas. In particular, at the same temperature and pressure, argon gas will have different viscosity than, say, nitrogen. Physics, chemistry, engineering, has long developed laws that approximate behaviors of gasses under different conditions. When gas is being simulated numerically, e.g., using the kinetic equations, a number of constants is being introduced in the equations that affect properties of the solution. Also, quantities are introduced to describe the state of gas at macroscopic or microscopic level. In the following, we will briefly summarize constants and quantities that are important for simulations of rarefied gas dynamics.

m	the molecular mass, kg	This is a mass of a single molecule of the gas. Is used to convert density into number density and vice versa
$k = 1.380648813 \times 10^{-23}$	the Boltzmann constant	The Boltzmann constant is a fundamental constant of physics. It is used in a number of formulas
$R = \frac{k}{m}$	the Normal Gas constant	The normal gas constant is different for each gas and is used in a number of formulas, e.g., in the formula for the Maxwellian
d	the molecular diameter	The molecular diameter represents an idealized view of a molecule as a ball and represents a characteristic size of the that ball. It is different for each gas and is used in a number of formulas, e.g., in the estimation of the mean free path and the mean free time.
$n = \int_{R^3} f(\vec{v}) d\vec{v}$	the number density, molecules per m^3	The number density is a macroscopic quantity that gives the number of molecules per unit volume. In particular, $\rho = nm$.
$\rho = m \int_{R^3} f(\vec{v}) d\vec{v}$	the density, kg/ m^3	The density is a macroscopic quantity that gives the mass of gas per unit volume. In particular, $n = \rho/m$.

$\vec{u} = \frac{1}{n} \int_{R^3} \vec{v} f(\vec{v}) d\vec{v}$	the bulk velocity, m/s	The bulk velocity is the observable velocity of the stream of gas. It is a macroparameter. It appears in many formulas.
$T = \frac{1}{3Rn} \int_{R^3} \ \vec{v} - \vec{u}\ ^2 f(\vec{v}) d\vec{v}$	the temperature, K	The temperature is the observable temperature of the stream of gas. It is a macroparameter. It appears in many formulas.
$\tau = \frac{1}{4nd^2} \sqrt{\frac{m}{\pi kT}}$	the mean free time	Mean free time is an estimate of the time that the molecule spends between collisions on the average. It is used in estimating the length of simulations and also as a normalization parameter.
$\lambda = \frac{1}{\sqrt{2}\pi nd^2}$	the mean free path	Mean free path is an estimate of the distance that the molecule travels between collisions on the average. It is used in estimating the size of the domain in simulations and also as a normalization parameter.
$\bar{c} = \sqrt{\frac{8}{\pi} \frac{k}{m} T}$	the mean thermal velocity	Average speed of molecules as measured in the system of coordinates moving with the flow stream at the point.
$\mu = m_0(T/T_0)^\gamma$	the gas viscosity	Viscosity is a property of gas to resist motion and to dissipate energy of motion. Viscosity of gases is determined experimentally and in some instances can be derived from the microscopic properties of the gas. A popular law in Rarefied gas dynamics, aka the power viscosity law, is to express viscosity as function of temperature. $\mu = m_0(T/T_0)^\gamma$, where T_0 is some reference temperature and μ_0 is the known viscosity of the gas at the reference temperature.

2. THE BHATNAGAR-GROSS KROOK AND ELLIPSOIDAL-STATISTICAL BGK MODELS

The molecular distribution function is a solution to the Boltzmann kinetic equation

$$(1) \quad \frac{\partial}{\partial t} f(t, \vec{x}, \vec{u}) + \vec{u} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{u}) = I[f](t, \vec{x}, \vec{v}),$$

where the contribution to the change of the distribution function due to molecular collisions is modeled by the non-linear operator $Q(f)$. The complete form of the Boltzmann collision operator involves integration over five dimensional space at each point of six-dimensional phase space, thus making the solution of the Boltzmann equation computationally very challenging. A deterministic solution to the Boltzmann equation can be obtained using some approximate

models, the most widely known of which are the Bhatnagar-Gross-Krook model equation. In the BGK model, the collision operator is replaced with a simpler operator

$$I[f](t, \vec{x}, \vec{v}) = \nu(f_0(t, \vec{x}, \vec{v}) - f(t, \vec{x}, \vec{v})),$$

where $\nu(t, \vec{x})$ is the collision frequency, and $f_0(t, \vec{x})$ is the Maxwellian equilibrium distribution function

$$(2) \quad f_0 = n(t, \vec{x})(2\pi RT(t, \vec{x}))^{-3/2} \exp\left(-\frac{(\vec{u} - \vec{u}(t, \vec{x}))^2}{2RT}\right).$$

The gas density, n , bulk velocity, \vec{u} , and temperature, T , are defined as follows

$$(3) \quad \begin{aligned} n(t, \vec{x}) &= \int_{\mathbb{R}^3} f(t, \vec{x}, \vec{u}) d\vec{u}, \\ n(t, \vec{x})\vec{u}(t, \vec{x}) &= \int_{\mathbb{R}^3} \vec{u} f(t, \vec{x}, \vec{u}) d\vec{u}, \\ n(t, \vec{x})T(t, \vec{x}) &= \frac{1}{3R} \int_{\mathbb{R}^3} (\vec{u} - \vec{u})^2 f(t, \vec{x}, \vec{u}) d\vec{u}, \end{aligned}$$

where R is the normal gas constant. The collision frequency ν is determined by the expression

$$\nu = \frac{nkT}{\mu}.$$

The BGK model satisfies conservation of moments and has positive entropy generation rate.

Another popular model is the Ellipsoidal-Statistical BGK model the dimensional collision operator.

$$(4) \quad I[f](t, \vec{x}, \vec{v}) = \nu(f_{ES}(t, \vec{x}, \vec{v}) - f(t, \vec{x}, \vec{v})),$$

where

$$(5) \quad f_{ES}(t, \vec{x}, \vec{v}) = \frac{n(t, \vec{x})}{\sqrt{\det(2\pi Q)}} \exp\left(-\frac{1}{2}\vec{c}^T Q^{-1} \vec{c}\right).$$

Here $\vec{c} = \vec{v} - \vec{u}$ and

$$(6) \quad Q = (1 - \alpha)RTI + \alpha\Theta, \quad \text{where } \Theta_{pq} = \frac{1}{n(t, \vec{x})} \int_{\mathbb{R}^3} c_p c_q f(t, \vec{x}, \vec{v}) d\vec{v}.$$

Here R is the specific gas constant and I is the identity matrix. The parameter α controls the Prandtl number, \mathbf{Pr} , of the modelled gas. In particular, $\mathbf{Pr} = 1/(1 - \alpha)$. The collision frequency ν is taken to be $\nu = n(\hat{t}, \vec{x})kT(t, \vec{x})/((1 - \alpha)\mu(T))$ where k is the Boltzmann constant and $\mu(T)$ is the gas viscosity. Since the power law is often used for the viscosity dependence on the temperature, we adopt it too. As a result, the implemented collision frequency has the following dimensional form

$$\nu = \frac{n(t, \vec{x})kT}{(1 - \alpha)\mu_{\text{ref}}} \left(\frac{T_{\text{ref}}}{T}\right)^\gamma,$$

where γ is the exponent in the gas viscosity law.

3. VARIOUS CONSTANTS AND PARAMETERS

Some values that we may will use in the simulations:

gas	m , kg	R	d , m	γ
argon	6.63352e-026	2.081321e+002	3.76e-010	
nitrogen	2.325867e-026	2.96803e+002		

4. NUMERICAL EXPERIMENT. SIMULATION OF NORMAL SHOCK WAVE

The following steps are designed to help set up and run simulations of normal shock wave. In this experiment we will simulate Mach 3.0 wave. Simulation of waves with a higher Mach number is similar, but some values of parameters will change.

- Determine upstream and downstream conditions of the normal shock wave with Mach 3.0 in argon.
- Using the formulas above estimate the mean free path and mean free times for the upstream undisturbed flow.
- Use mean free path to determine the size of the domain. In most case, domain of 120 mean free paths is a good place to start. Depending on the looks of the solution you can either decrease or increase the domain later.
- Use mean free path to estimate the thickness of the shock usually 20-30 mean free paths. You will use this knowledge to set up constants in `sf02_mod.f90`.
- Set up the RKDG1D1V code to perform simulation of Mach 3.00 wave in argon. Follow the provided instructions.
 - Set up the macroparameters constants in `sf02_mod.f90` to impose the upstream and downstream conditions. Also, modify x_1 and x_2 to set up the transition zone for the initial data. We recall that the initial data is given by the following piece wise function:

$$(7) \quad f(0, x, u) = \begin{cases} f_M(u; n_U, T_u, \bar{u}_U), & x < x_1 \\ \frac{x_2 - x}{x_2 - x_1} f_M(u; n_U, T_U, \bar{u}_U) + \frac{x - x_1}{x_2 - x_1} f_M(u; n_D, T_D, \bar{u}_D), & x_1 \leq x \leq x_2 \\ f_M(u; n_D, T_D, \bar{u}_D), & x > x_2. \end{cases}$$

- Set up the macroparameters constants in `parameters.dat` to impose the upstream and downstream conditions. you can start with $k = 4$, $rk = 5$, $N = 10$, $s = 5$, $M = 10$ (these can be increased later, if necessary). Final time can be put at 150-200 mean free times (enough for a average molecule to travel through the entire domain). You may want to save solution at least 10 times during the simulation.
- Run the simulation, copy the data, the initial data files, the parameter files and the output files to your local computer and store in an organized fashion.
- To inspect the solution you can use both graphs of the solution and the graphs of macroparameters.
- To see that the solution reached steady state, plot macroparameters corresponding to consecutive in time saves. If the solution is changing, it has not reach steady state. Restart the solution from the last save.
- Determine when solution reaches steady state. Use this time as the final time for all simulations for this shock wave.
- Repeat the steps to simulate the same normal shock wave. Vary resolution in x and u .

- Specifically, perform simulations keeping the same s and M (parameters of discrete mesh in u), keep the same k , but change $N = 10, 14, 20, 28, 40, 56, 80, 113, 160$. What do you observe in terms of time demands. How much longer is the simulation time for each consecutive run? Why, in your opinion is it so?
- Specifically, perform simulations keeping the same k and N (parameters of discrete mesh in x), keep the same s , but change $M = 10, 14, 20, 28, 40, 56, 80, 113, 160$. What do you observe in terms of time demands. How much longer is the simulation time for each consecutive run? Why, in your opinion is it so?