

1. SOLUTION OF KINETIC EQUATIONS USING THE DGVLIB PACKAGE.

The DGVlib package is designed to implement nodal-DG discretization in the velocity variable in three velocity dimensions. This library can be used as a part of a larger solver. We will call such solver a driver. The driver will contain the implementation of the time and space discretizations. Currently, you are working with a driver that solves the problem of spatially homogeneous relaxation. In this case, there is no spatial discretization, but there is still tie discretization. Detail on the 3D nodal-DG discretization can be found in papers:

2014 A. Alekseenko and E. Josyula, Deterministic solution of the spatially homogeneous Boltzmann equation using discontinuous Galerkin discretizations in the velocity space, *Journal of Computational Physics*, Vol. 272, n. 1, (2014) 170–188.

2012 A. Alekseenko and E. Josyula, Deterministic solution of the Boltzmann equation using a discontinuous Galerkin velocity discretization. *Proceedings of the 28th International Symposium on Rarefied Gas Dynamics, Spain 2012*, AIP Conference Proceedings, 2012, 8 pp.

2015 A. Alekseenko and C. Euler, A Bhatnagar-Gross-Krook kinetic model with velocity-dependent collision frequency and corrected relaxation of moments. *Continuum Mechanics and Thermodynamics* DOI: 10.1007/s00161-014-0407-0

2016 A. Alekseenko, S. Gimelshein, T. Nguyen, and P. Vedula, Solution of Non-Continuum Flows Using BGK-type Model with Enforced Relaxation of Moments. *Proceedings of the 30th International Symposium on Rarefied Gas Dynamics, Canada July 2016*, AIP Conference Proceedings, 2016, 8 pp.

The library implements several models to evaluate the collision operator: The Boltzmann equation with hard spheres potential, the BGK, the ES-BGK and the Shakhov model, and also the models with enforced relaxation rates.

In the following, we will summarize a few conventions that are used in the library that will be useful to set up simulations correctly. There are three major topics to pay attention to:

- (1) DGVlib uses dimensionless formulation, so the initial data and parameters are given in dimensionless form. However, reference values are also needed in the code to make correct computations. Understanding this is important
- (2) DGVlib is a hybrid code. Specifically, different models of molecular collisions are used based on the degree of non-continuum. Understanding how this works is important.
- (3) The 0D driver determines the time to run the simulations as well as some other parameters. Parallelization can be controlled by DGVlib or by the Driver, depending on the problem and the way to parallelize (OpenMP or MPI). It is important to know the correct procedure for each way of running the code.

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 then, 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. |
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2. 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 | | |

Simulation treating argon as hard spheres gas:

| d , m | m , kg | R | μ_{ref} | T_{ref} , K | γ |
|-----------|--------------|---------------|------------------------|---------------|----------|
| 3.76e-010 | 6.63352e-026 | 2.081321e+002 | 5.337379160633744E-005 | 2000 | 0.5 |

3. DIMENSIONLESS REDUCTION IN THE VELOCITY VARIABLE

Gas dynamic constants vary greatly in scale. Caution should be exercised when these quantities are combined in a numerical method in order to avoid accumulation of the roundoff errors. However, because of the large number of integration points, accumulation of roundoff errors is difficult or even impossible to avoid completely. It is therefore desirable to build methods in such a way so as to cancel as much roundoff error as possible.

The use of dimensionless reduction when all the key quantities are of the order of unit can help avoid many (but definitely not all) obstacles caused by the roundoff errors. These reductions can be introduced for each problem and usually vary from application to application.

Let \hat{t} , \hat{x} , \hat{v} be the conventional dimensional variables. In general, all quantities bearing $\hat{\cdot}$ will be understood as conventional dimensional quantities derived in the physics consideration. In particular, $\hat{f}(\hat{t}, \hat{x}, \hat{v})$ is the molecular number density distribution function.

We assume that some time scale \mathbb{T} , reference temperature T_∞ and some length scale L were selected based on the particular application in mind. It is convenient to define $C_\infty = \sqrt{2RT_\infty}$. Also, $\mathbb{T} = L/C_\infty$ to simplify the final time dependent equations. We define:

$$(1) \quad t = \frac{\hat{t}}{\mathbb{T}}, \quad x_i = \frac{\hat{x}}{L}, \quad v = \frac{\hat{v}}{C_\infty}, \quad \text{or} \quad \hat{t} = t\mathbb{T}, \quad \hat{x} = xL, \quad \hat{v} = vC_\infty.$$

We also define the dimensionless number density

$$(2) \quad f(t, x, v) = \frac{L^3 C_\infty^3}{N} \hat{f}(t\mathbb{T}, xL, vC_\infty) = \frac{L^3 C_\infty^3}{N} \hat{f}(\hat{t}, \hat{x}, \hat{v}), \quad \text{or} \quad \hat{f}(\hat{t}, \hat{x}, \hat{v}) = \frac{N}{L^3 C_\infty^3} f(t, x, v),$$

where N is the total number of molecules in the gas volume L^3 .

With these definitions, the relationships between the macroparameters of the dimensional and dimensionless functions are as follows. We define

$$\begin{aligned}
 n(t, x) &:= \int_{R^3} f(t, x, v) dv, \\
 n(t, x) \bar{u}(t, x) &:= \int_{R^3} v f(t, x, v) dv, \\
 n(t, x) T(t, x) &:= \frac{2}{3} \int_{R^3} (v - \bar{u})^2 f(t, x, v) dv,
 \end{aligned}
 \tag{3}$$

then

$$\begin{aligned}
 n(t, x) &= \frac{L^3}{N} \hat{n}(\hat{t}, \hat{x}), \\
 \bar{u}(t, x) &= \frac{\hat{u}(\hat{t}, \hat{x})}{C_\infty}, \\
 T(t, x) &= \frac{\hat{T}(\hat{t}, \hat{x})}{T_\infty}.
 \end{aligned}
 \tag{4}$$

Next, the Maxwellian distribution with density $\hat{n}(\hat{t}, \hat{x})$, average velocity $\hat{u}_j(\hat{t}, \hat{x})$ and temperature $\hat{T}(\hat{t}, \hat{x})$ translates into the dimensionless Maxwellian distribution as follows:

$$\hat{f}_M(\hat{t}, \hat{x}, \hat{u}) = \frac{N}{L^3 C_\infty^3} f_M(t, x, u),$$

where

$$f_M(t, x, u) := n(t, x) \frac{1}{(\pi T)^{3/2}} \exp\left(-\frac{(u - \bar{u})^2}{T}\right).$$

4. FORMULAS TO COMPUTE MACROPARAMETERS OF SUMS OF MAXWELLIAN STREAMS

4.1. Derivation of the formula of macroparameters of spatially homogeneous two streams of gas. Let two spatially homogeneous streams of gas are given with the velocity distribution functions $f_1(\vec{v})$ and $f_2(\vec{v})$. Notice that the dependence on t and \vec{x} is not explicitly shown because it is important here.

Recall that the macroparameters of density, momentum and temperature are defined as

$$\begin{aligned}
 n &= \int_{R^3} f_1(\vec{v}) dv \\
 n \vec{u} &= \int_{R^3} \vec{v} f_1(\vec{v}) dv \\
 n T &= \frac{1}{3R} \int_{R^3} (\vec{v} - \vec{u})^2 f_1(\vec{v}) dv
 \end{aligned}$$

If n_1 , \vec{v}_1 , and T_1 are the macroparameters of the stream f_1 and, correspondingly, n_2 , \vec{v}_2 , and T_2 are the macroparameters of the stream f_2 , let us find the expressions of the macroparameters of the combined stream of two gases, given by $f = f_1 + f_2$.

The density and the bulk velocity of the combined stream follow immediately:

$$n = \int_{R^3} f dv = \int_{R^3} (f_1 + f_2) dv = \int_{R^3} f_1 dv + \int_{R^3} f_2 dv = n_1 + n_2;$$

$$n\vec{v} = \int_{R^3} \vec{v} f dv = \int_{R^3} \vec{v} (f_1 + f_2) dv = \int_{R^3} \vec{v} f_1 dv + \int_{R^3} \vec{v} f_2 dv = n_1 \vec{v}_1 + n_2 \vec{v}_2;$$

Therefore,

$$(7) \quad \vec{v} = \frac{n_1 \vec{v}_1 + n_2 \vec{v}_2}{n_1 + n_2};$$

Finally, for the temperature, T , we have

$$\begin{aligned} nT &= \frac{1}{3R} \int (\vec{v} - \vec{v})^2 (f_1 + f_2) dv = \frac{1}{3R} \int (\vec{v}^2 - 2\vec{v} \cdot \vec{v} + \vec{v}^2) (f_1 + f_2) dv \\ &= \frac{1}{3R} \int \vec{v}^2 (f_1 + f_2) dv - \frac{1}{3R} \int 2\vec{v} \cdot \vec{v} (f_1 + f_2) dv + \frac{1}{3R} \int \vec{v}^2 (f_1 + f_2) dv \\ &= \frac{1}{3R} \int \vec{v}^2 (f_1 + f_2) dv + \frac{1}{3R} [-2\vec{v}^2 n + \vec{v}^2 n] \\ &= \frac{1}{3R} \int \vec{v}^2 f_1 dv + \frac{1}{3R} \int \vec{v}^2 f_2 dv - \frac{1}{3R} \vec{v}^2 n \\ &= \frac{1}{3R} \int (\vec{v}^2 - 2\vec{v} \cdot \vec{v}_1 + \vec{v}_1^2) f_1 dv + \frac{1}{3R} \int 2\vec{v} \cdot \vec{v}_1 f_1 - \frac{1}{3R} \int \vec{v}_1^2 f_1 \\ &\quad + \frac{1}{3R} \int (\vec{v}^2 - 2\vec{v} \cdot \vec{v}_2 + \vec{v}_2^2) f_2 dv + \frac{1}{3R} \int 2\vec{v} \cdot \vec{v}_2 f_2 - \frac{1}{3R} \int \vec{v}_2^2 f_2 - \frac{1}{3R} \vec{v}^2 n \\ &= \frac{1}{3R} \int (\vec{v} - \vec{v}_1)^2 f_1 dv + \frac{1}{3R} [2\vec{v}_1^2 n_1 - \vec{v}_1^2 n_1] \\ &\quad + \frac{1}{3R} \int (\vec{v} - \vec{v}_2)^2 f_2 dv + \frac{1}{3R} [2\vec{v}_2^2 n_2 - \vec{v}_2^2 n_2] - \frac{1}{3R} \frac{(n_1 \vec{v}_1 + n_2 \vec{v}_2)^2}{n_1 + n_2} \\ &= T_1 n_1 + T_2 n_2 + \frac{1}{3R} (\vec{v}_1^2 n_1 + \vec{v}_2^2 n_2) - \frac{1}{3R} \frac{(n_1 \vec{v}_1 + n_2 \vec{v}_2)^2}{n_1 + n_2} \end{aligned}$$

The expression for the temperature of the mixed two streams is

$$(8) \quad T = \frac{T_1 n_1 + T_2 n_2}{n_1 + n_2} + \frac{1}{3R} \frac{(\vec{v}_1^2 n_1 + \vec{v}_2^2 n_2)}{n_1 + n_2} - \frac{1}{3R} \frac{(n_1 \vec{v}_1 + n_2 \vec{v}_2)^2}{(n_1 + n_2)^2}$$

4.2. Dimensionless reduction and the formulas for the sum of the streams of gas.

Now, let us assume that we have two streams whose dimensionless macroparameters are n_1 , n_2 , \bar{u}_1 , \bar{u}_2 , and T_1 , T_2 . The macro-parameters of the mixture of two streams are

$$\begin{aligned} n &= n_1 + n_2 \\ \bar{u} &= \frac{n_1 \bar{u}_1 + n_2 \bar{u}_2}{n} \\ (9) \quad T &= \frac{T_1 n_1 + T_2 n_2}{n} + \frac{2}{3} \frac{|u_1|^2 n_1 + |u_2|^2 n_2}{n} - \frac{2}{3} \frac{(n_1 \bar{u}_1 + n_2 \bar{u}_2)^2}{n^2} \end{aligned}$$

4.3. Moments of the dimensionless Maxwellian. These formulas are summaries of notes by Craig Euler.

Let $t, x, u = (u_1, u_2, u_3)$ be the dimensionless variables above. The following formula holds for even values of m :

$$(10) \quad \int_{R^3} u_1^m f_m(t, x, u) du = n \sum_{i=0}^{m/2} |\bar{u}|^{m-2i} \binom{m}{2i} \left(\frac{T}{2}\right)^i \prod_{j=1}^i (2j-1)$$

where $f_m =$ For odd values of m the result is zero

Finally, we state the particular cases of the formulas:

$$(11) \quad \int_{R^3} u_1^2 f_m(t, x, u) du = n|\bar{u}|^2 + n\frac{T}{2}$$

$$(12) \quad \int_{R^3} u_1^3 f_m(t, x, u) du = ??$$

$$(13) \quad \int_{R^3} u_1^4 f_m(t, x, u) du = n|\bar{u}|^4 + 3n|\bar{u}|^2 T + 3n\left(\frac{T}{2}\right)^2$$

$$(14) \quad \int_{R^3} u_1^5 f_m(t, x, u) du = ??$$

$$(15) \quad \int_{R^3} u_1^6 f_m(t, x, u) du = n|\bar{u}|^6 + \frac{15}{2}n|\bar{u}|^4 T + \frac{45}{4}n|\bar{u}|^2 T^2 + \frac{15}{8}nT^3$$

Finally, we need to add a last bunch of formulas that correspond to $\bar{u} = 0$

$$(16) \quad \int_{R^3} u_1^2 f_m(t, x, u) du = n|\bar{u}|^2 + n\frac{T}{2}$$

$$(17) \quad \int_{R^3} u_1^4 f_m(t, x, u) du = 3n\left(\frac{T}{2}\right)^2$$

$$(18) \quad \int_{R^3} u_1^6 f_m(t, x, u) du = \frac{15}{8}nT^3$$

5. SAMPLE NUMERICAL EXPERIMENT. SOLUTION OF THE PROBLEM OF SPATIALLY HOMOGENEOUS RELAXATION

The following steps are designed to help set up and run simulations of spatially homogeneous relaxation. You have been provided a sample code set up to simulate Mach 1.55 wave. Simulation of waves with a higher Mach number is similar, but some values of parameters may change.

- Determine upstream and downstream conditions of the normal shock wave with Mach 1.55 (or other Mach number) in argon.
- Using the formulas above estimate the mean free path and mean free times for the upstream undisturbed flow.
- Use mean free time to estimate the time in seconds needed to for solution to reach the steady state. In most cases the simulations close to steady state in 8-10 mean free times and the simulation can be stopped after about 20 mean free times.
- Set up the DGvlib0D3V code to perform simulation of spatially homogeneous relaxation of Mach 1.55 (or other Mach number) initial data in hard spheres argon. Follow the provided instructions.
 - Set up the macroparameters constants in `sf02_mod.f90` or `DGV_sf02.f90` to impose the upstream and downstream conditions. They are Also, modify `x1` and `x2` to set

$-x_1 = x_2$. The initial data is computed by evaluating this function as $x = 0$. We recall that the initial data is given by the following piece wise function:

$$(19) \quad f(0, x, u) = \begin{cases} f_M(u; n_U, T_u, \bar{u}_U), & x < x_1 \\ \frac{x_2-x}{x_2-x_1} f_M(u; n_U, T_U, \bar{u}_U) + \frac{x-x_1}{x_2-x_1} f_M(u; n_D, T_D, \bar{u}_D), & x_1 \leq x \leq x_2 \\ f_M(u; n_D, T_D, \bar{u}_D), & x > x_2. \end{cases}$$

- Set up the macroparameters constants in `DGVparameters.dat` and `parameters.dat`. Do not change the values of $k = 4$, $rk = 5$, $N = 10$ that were provided to you with the sample parameter files. In all simulations, you will most likely use $s = 5$. You can start with $M = 15$. The interval in x is not used in this context. The intervals in u , v , w has to stay $[-3, 3]$. 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.
- Repeat the steps to simulate the same normal shock wave. Vary resolution in the velocity variable by varying M . Use parallelization to make computations feasible.