Development of Fast Deterministic Physically Accurate Solvers for Kinetic Collision Integral for Applications of Near Space Flight and Control Devices

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A. APPENDIX A. DESCRIPTION OF MATHEMATICAL MODELS USED IN DGVLIB

This project aims at improving the existing fluid dynamics solvers by developing a software library implementing nodal discontinuous Galerkin discretization of a range of kinetic equations, including the two new approaches to evaluate the collision operator. In the first approach, modules based on the recently proposed BGK-type (Bhatnagar-Gross-Krook) model with velocity-dependent collision frequency and increased fidelity in relaxation of moments were developed. In the second approach, modules that use stochastic integration of the Boltzmann collision integral were developed. In addition, subroutines for evaluating the classical BGK model and the ellipsoidal-statistical BGK model and subroutines for evaluating full Boltzmann collision operator using formulation of [1] are included in the library. In the following, we briefly summarize the mathematical models that are employed in the library. In the description of the mathematical model we include the key formulas that the software modules use so that a future user could correctly link variables of the user's software to the variables of the library.

A.1 Dimensionless Reduction of 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. In this paper we present a reduction that was adopted from Chapter 3 in [2].

Let $\hat{t}$, $\hat{x}$, $\hat{v}$ be the conventional dimensional variables. In general, all quantities bearing $\hat{}$ 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. (usually, $\mathbb{T}$ can be selected to simplify the final equations – we will talk about it toward the end of the section).

It is convenient to define $C_\infty = \sqrt{2RT_\infty}$. We define:

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

We also define the dimensionless number density

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

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

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

Next, the Maxwellian distribution with density $\hat{n}(\hat{t},\hat{x})$, average velocity $\hat{\bar{u}}_j(\hat{t},\hat{x})$ 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

$$f_M(t,x,u) := n(t,x)\frac{1}{(\pi T)^{3/2}}\exp\Big(-\frac{(u-\bar{u})^2}{T}\Big)\,. \tag{5}$$

A.1.1 Dimensionless Reduction of Kinetic Equations

Consider a dimensional kinetic equation:

$$\frac{\partial}{\partial\hat{t}}\hat{f}(\hat{t},\hat{x},\hat{v}) + \hat{v}\cdot\nabla_{\hat{x}}\hat{f}(\hat{t},\hat{x},\hat{v}) = \hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}). \tag{6}$$

Here $\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v})$ is a dimensional molecular collision operator. We leave $\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v})$ in the most general form. In particular it can be the full Boltzmann collision operator, a classical model collision operator (e.g., in the BGK, the ES-BGK or the Shakhov form), or the velocity dependent collision frequency. In this section we will consider the dimensionless reduction of the left side of the equation (6). The dimensionless reduction of the collision operator can be added later by replacing $\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v})$ with an appropriate dimensionless expression.

By substituting $\hat{f}(\hat{t},\hat{x},\hat{v}) = \frac{N}{L^3 C_\infty^3} f(t,x,v)$ into (6) and changing derivatives $\partial/\partial\hat{t} \to \partial/\partial t$ and $\nabla_{\hat{x}} \to \nabla_x$ we obtain

$$\frac{N}{\mathbb{T}L^3C_\infty^3}\frac{\partial}{\partial t}f(t,x,v) + \frac{C_\infty N}{LL^3C_\infty^3} v\cdot\nabla_x f(t,x,v) = \hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}).$$

The latter can be re-written as

$$\frac{\partial}{\partial t}f(t,x,v) + \frac{C_\infty \mathbb{T}}{L} v\cdot\nabla_x f(t,x,v) = \frac{L^3C_\infty^3\mathbb{T}}{N}\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}).$$

If we use the standard agreement that $\mathbb{T} = L/C_\infty$, then the equation simplifies a bit more:

$$\frac{\partial}{\partial t}f(t,x,v) + v\cdot\nabla_x f(t,x,v) = \frac{L^3C_\infty^3\mathbb{T}}{N}\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}). \tag{7}$$

A.1.2 Dimensionless Reduction of the ES-BGK model

In the dimensional ES-BGK model the dimensional collision operator $\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v})$ takes the form

$$\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}) = \hat{\nu}(\hat{f}_{ES}(\hat{t},\hat{x},\hat{v}) - \hat{f}(\hat{t},\hat{x},\hat{v})), \tag{8}$$

where

$$\hat{f}_{ES}(\hat{t},\hat{x},\hat{v}) = \frac{\hat{n}(\hat{t},\hat{x})}{\sqrt{\det(2\pi\hat{Q})}}\exp\Big(-\frac{1}{2}\hat{c}^T\hat{Q}^{-1}\hat{c}\Big). \tag{9}$$

Here $\hat{c} = \hat{u} - \bar{\hat{u}}$ and

$$\hat{Q} = (1-\alpha)R\hat{T}I + \alpha\hat{\Theta}, \quad \text{where } \hat{\Theta}_{pq} = \frac{1}{\hat{n}(\hat{t})}\int_{R^3}\hat{c}_p\hat{c}_q\hat{f}(\hat{t},\hat{x},\hat{v})\,d\hat{v}\,. \tag{10}$$

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 $\hat{\nu}$ is taken to be $\hat{\nu} = \hat{n}(\hat{t},\hat{x})k\hat{T}(\hat{t},\hat{x})/((1-\alpha)\mu(\hat{T}))$ where k is the Boltzmann constant and $\mu(\hat{T})$ 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

$$\hat{\nu} = \frac{\hat{n}(\hat{t},\hat{x})k\hat{T}}{(1-\alpha)\mu_{\text{ref}}}\Big(\frac{\hat{T}_{\text{ref}}}{\hat{T}}\Big)^{\gamma},$$

where γ is the exponent in the gas viscosity law.

By substituting the relations (4) and (2) into the above formulas and using (1) we obtain the dimensionless expression for the ES-BGK model as follows:

$$\Theta_{pq} = \frac{2}{n(t)}\int_{R^3} c_p c_q f(t,x,v)\,dv \quad \text{and} \quad \Theta_{pq} = \frac{1}{RT_\infty}\hat{\Theta}_{pq}\,,$$

and

$$Q = (1-\alpha)TI + \alpha\Theta \quad \text{and} \quad Q = \frac{1}{RT_\infty}\hat{Q}\,.$$

Finally,

$$f_{ES}(t,x,u) = \frac{n(t,x)}{\sqrt{\det(\pi Q)}}\exp\Big(-c^T Q^{-1}c\Big) \quad \text{and} \quad f_{ES}(t,x,u) = \frac{L^3C_\infty^3}{N}\hat{f}_{ES}(\hat{t},\hat{x},\hat{u}).$$

The dimensionless collision frequency has the following form

$$\nu = \frac{NkT_\infty}{L^3}\frac{n(t,x)T(t,x)}{(1-\alpha)\mu(T)}, \quad \text{where} \quad \mu(T) = \mu_{\text{ref}}\Big(\frac{\hat{T}(\hat{t})}{\hat{T}_{\text{ref}}}\Big)^{\gamma} = \mu_{\text{ref}}\Big(\frac{T(t)}{T_{\text{ref}}}\Big)^{\gamma}.$$

Here $T_{\text{ref}} = \hat{T}_{\text{ref}}/T_\infty$. Summarising,

$$\hat{I}[\hat{f}](\hat{t},\hat{x},\hat{v}) = \frac{N^2kT_\infty}{L^6C_\infty^3}\frac{n(t,x)T(t,x)}{(1-\alpha)\mu(T)}(f_{ES}(t,x,v) - f(t,x,v)). \tag{11}$$

A.1.3 Formulas for Operator A in Dimensionless Variables for Hard Spheres Model

We consider the formulas for operator $A(\hat{v}_i,\hat{v}_i^1,\hat{\phi}(\hat{u}))$ in [1]:

$$A(\hat{v}_i,\hat{v}_i^1;\hat{\phi}_p^j(\hat{u})) = \frac{|\hat{g}|}{2}\int_0^{2\pi}\int_0^d (\hat{\phi}_p^j(\hat{v}_i') + \hat{\phi}_p^j(\hat{v}_1') - \hat{\phi}_p^j(\hat{v}) - \hat{\phi}_p^j(\hat{v}_1))\hat{b}\,d\hat{b}\,d\varepsilon\,. \tag{12}$$

First of all, we notice that the azimuthal angle ε is not dimensional, therefore it will not change during the dimensionless transition. Also, the transition from $\hat{v}_i$ to v_i has no impact on the local basis of e_1, e_2, and e_3. Indeed, these vectors are unit length and their direction does not change with the normalization. Let the dimensional radius of the molecules be

$\hat{d}$. We can introduce the dimensionless parameter θ, by requiring that $\hat{b} = \hat{d}\sin\theta$. We introduce $b = \hat{b}/\hat{d}$. We may think that dimensionless spheres have radius 1. Then $b = \sin\theta$ is the dimensionless collision parameter. Now we will rewrite (12) in the dimensionless variables. We will start by applying the substitution $b = \hat{b}/\hat{d}$ to (12):

$$A(\hat{v}_i, \hat{v}_i^1; \hat{\phi}_p^j(\hat{u})) = \frac{\hat{d}^2|\hat{g}|}{2}\int_0^{2\pi}\int_0^1 (\hat{\phi}_p^j(\hat{v}_i') + \hat{\phi}_p^j(\hat{v}_1') - \hat{\phi}_p^j(\hat{v}) - \hat{\phi}_p^j(\hat{v}_1))b\,db\,d\varepsilon\,.$$

Next we make a substitution $b = \sin\theta$ and introduce another dimensionless parameter $\chi = \pi - 2\theta$. We obtain:

$$\hat{A}(\hat{v}_i, \hat{v}_i^1; \hat{\phi}_p^j(\hat{u})) = \frac{\hat{d}^2|\hat{g}|}{8}\int_0^{2\pi}\int_0^{\pi} (\hat{\phi}_p^j(\hat{v}_i') + \hat{\phi}_p^j(\hat{v}_1') - \hat{\phi}_p^j(\hat{v}) - \hat{\phi}_p^j(\hat{v}_1))\sin\chi\,d\chi\,d\varepsilon\,.$$

Notice that the dimensional post-collision velocities are still calculated using the dimensionless χ according to the hard spheres model. Next we will replace them with non-dimensional velocities. We recall that

$$\hat{v}' = \frac{\hat{v}+\hat{v}_1}{2} + \frac{|\hat{g}|}{2}k,$$
$$\hat{v}_1' = \frac{\hat{v}+\hat{v}_1}{2} - \frac{|\hat{g}|}{2}k.$$

Notice, that vector k does not change because it is expressed in dimensionless variables χ and ε. Because $v = \hat{v}/C_\infty$ and $v_1 = \hat{v}_1'/C_\infty$, it is natural to introduce $v' = \hat{v}'/C_\infty$ and $v_1' = \hat{v}_1'/C_\infty$. From the above formulas it follows that

$$v' = \frac{v+v_1}{2} + \frac{|g|}{2}k,$$
$$v_1' = \frac{v+v_1}{2} - \frac{|g|}{2}k,$$

where $g := v - v_1 = \hat{g}/C_\infty$.

Next we define the dimensionless basis functions by using the following scaling:

$$\phi(v) := \hat{\phi}(C_\infty v) = \hat{\phi}(\hat{v}). \tag{13}$$

Then, of course,

$$\hat{A}(\hat{v}_i, \hat{v}_i^1; \hat{\phi}_p^j(\hat{u})) = \frac{C_\infty\hat{d}^2|g|}{8}\int_0^{2\pi}\int_0^{\pi} (\phi_p^j(v_i') + \phi_p^j(v_1') - \phi_p^j(v) - \phi_p^j(v_1))\sin\chi\,d\chi\,d\varepsilon\,.$$

We define

$$A(v_i, v_i^1; \phi_p^j(u)) := \frac{1}{C_\infty\hat{d}^2}\hat{A}(v_iC_\infty, v_i^1C_\infty; \hat{\phi}_p^j(uC_\infty)), \quad \text{or} \quad \hat{A}(\hat{v}_i, \hat{v}_i^1; \hat{\phi}_p^j(\hat{u})) = C_\infty\hat{d}^2A(v_i, v_i^1; \phi_p^j(u)). \tag{14}$$

Then the following expression is valid for $A(v_i, v_i^1; \phi_p^j(u))$:

$$A(v_i, v_i^1; \phi_p^j(u)) = \frac{|g|}{8} \int_0^{2\pi} \int_0^{\pi} (\phi_p^j(v_i') + \phi_p^j(v_1') - \phi_p^j(v) - \phi_p^j(v_1)) \sin\chi \, d\chi \, d\varepsilon \, .$$

A.1.4 Formula for $I_{\phi_p^j}$ in dimensionless variables

Next we derive the expression in the dimensionless variables for the projection of the collision operator. We begin from formula for $I_{\phi_p^j}$ in dimensional variables that can be found in [1]:

$$\hat{I}_{\hat{\phi}_p^j} = \int_{R^3} \int_{R^3} \hat{f}(\hat{t}, \hat{x}, \hat{v}) \hat{f}(\hat{t}, \hat{x}, \hat{v}_1) \hat{A}(\hat{v}, \hat{v}_1; \hat{\phi}_p^j) d\hat{v}_1 \, d\hat{v}. \tag{15}$$

Using formulas (1), (2) and (14), we obtain

$$\begin{aligned} \hat{I}_{\hat{\phi}_p^j} &= (C_\infty^6)(C_\infty \hat{d}^2) \frac{N}{L^3 C_\infty^3} \frac{N}{L^3 C_\infty^3} \int_{R^3} \int_{R^3} f(t, x, v) f(t, x, v_1) A(v, v_1; \phi_p^j) dv_1 \, dv \\ &= \frac{N^2 \hat{d}^2 C_\infty}{L^6} \int_{R^3} \int_{R^3} f(t, x, v) f(t, x, v_1) A(v, v_1; \phi_p^j) dv_1 \, dv. \end{aligned} \tag{16}$$

A.2 Nodal-DG Discretizations

Let us describe the DG velocity discretization that will be employed. We note that this description is given in the dimensionless variables. However, we note that the transition to dimensional variables can be seamless as long as the dimensionless and the dimensional velocity variables are related by $v = \hat{v}/C_\infty$ and the dimensionless basis functions and the dimensional basis functions are related by (13), namely, $\phi(\vec{v}) = \hat{\phi}(C_\infty \vec{v}) = \hat{\phi}(\hat{v})$. Also, in this section, we will denote vector variables as $\vec{u}$.

We select a rectangular parallelepiped in the (dimensionless) velocity space that is sufficiently large so that contributions of the molecular distribution function to first few moments outside of this parallelepiped are negligible. In most cases, some a-priori knowledge about the problem is available and such parallelepiped can be selected. We partition this region into rectangular parallelepipeds K_j. In this paper, only uniform partitions are considered; the advantages of using uniform partitions are explained in the next section. However, most of the approach carries over to non-uniform partitions and extensions to hierarchical and overlapping meshes are straightforward. On each element K_j, $j = 1, \ldots, M$ we introduce a finite dimensional functional basis $\phi(v)_i^j$, $i = 1, \ldots s$. Notice that in general different approximation spaces can be used on different cells K_j. Thus the number of basis functions s may be different for different velocity cells. However, the implementation of

the method presented in this paper uses the same basis functions on all elements to save on computational storage.

Let vector $\vec{v} = (u, v, w)$ and let the numbers s_u, s_v and s_w determine the degrees of the polynomial basis functions in the velocity components u, v and w, respectively. Let $K_j = [u_L^j, u_R^j] \times [v_L^j, v_R^j] \times [w_L^j, w_R^j]$. The basis functions are constructed as follows. We introduce nodes of the Gauss quadratures of orders s_u, s_v, and s_w on each of the intervals $[u_L^j, u_R^j]$, $[v_L^j, v_R^j]$, and $[w_L^j, w_R^j]$, respectively. Let these nodes be denoted $\kappa_p^{j,u}$, $p = 1, s_u$, $\kappa_q^{j,v}$, $q = 1, s_v$, and $\kappa_r^{j,w}$, $r = 1, s_w$. We define one-dimensional Lagrange basis functions as follows, see e.g., [4],

$$\phi_l^{j;u}(u) = \prod_{\substack{p=1,s^u \\ p\neq l}} \frac{\kappa_p^{j,u} - u}{\kappa_p^{j,u} - \kappa_l^{j,u}}, \quad \phi_m^{j;v}(v) = \prod_{\substack{q=1,s^v \\ q\neq m}} \frac{\kappa_q^{j,v} - v}{\kappa_q^{j,v} - \kappa_m^{j,v}}, \quad \phi_n^{j;w}(w) = \prod_{\substack{r=1,s^w \\ r\neq n}} \frac{\kappa_r^{j,w} - w}{\kappa_r^{j,w} - \kappa_n^{j,w}}. \tag{17}$$

The three-dimensional basis functions are defined as $\phi_i^j(\vec{v}) = \phi_l^{j;u}(u)\phi_m^{j;v}(v)\phi_n^{j;w}(w)$, where $i = 1, \ldots, s = s_u s_v s_w$ is the index running through all combinations of l, n, and m. (In the implementation discussed in this paper, i is computed using the following formula $i = (l-1) * s_v * s_w + (m-1) * s_w + n$.)

Orthogonality of the Nodal-DG Basis The following identities hold for basis functions $\phi_i^j(\vec{v})$:

$$\int_{K_j} \phi_p^j(\vec{v})\phi_q^j(\vec{v})\, d\vec{v} = \frac{\Delta\vec{v}^j}{8}\omega_p\delta_{pq}, \qquad \int_{K_j} \vec{v}\phi_p^j(\vec{v})\phi_q^j(\vec{v})\, d\vec{v} = \frac{\Delta\vec{v}^j}{8}\vec{v}_p^j\omega_p\delta_{pq}, \tag{18}$$

where $\Delta\vec{v}^j = (u_R^j - u_L^j)(v_R^j - v_L^j)(w_R^j - w_L^j)$, $\omega_p := \omega_l^{s_u}\omega_m^{s_v}\omega_n^{s_w}$, and $\omega_l^{s_u}$, $\omega_m^{s_v}$, and $\omega_n^{s_w}$ are the weights of the Gauss quadratures of orders s_u, s_v, and s_w, respectively and indices l, n, and m of one dimensional basis functions correspond to the three-dimensional basis function $\phi_p^j(\vec{v}) = \phi_l^{j;u}(u)\phi_m^{j;v}(v)\phi_n^{j;w}(w)$, and the vector $\vec{v}_p^j = (\kappa_l^{j,u}, \kappa_m^{j,v}, \kappa_n^{j,w})$.

We assume that on each K_j the solution to the Boltzmann equation is sought in the form

$$f(t, \vec{x}, \vec{v})|_{K_j} = \sum_{i=1,s} f_{i;j}(t, \vec{x})\phi_i^j(\vec{v}). \tag{19}$$

A.2.1 Relationship of Galerkin Coefficients to Nodal Values of the Function.

An attractive property of the constructed basis is that Galerkin coefficients commonly defined as L^2-orthogonal projections of the approximated function onto the corresponding basis functions coincide with the value of the function at the node. Indeed, to evaluate the Galerkin coefficient $f_{i;j}(t, x)$, we multiply the approximated function by a basis function

$\phi_i^j(v)$ and take the integral over the cell K_j:

$$f_{i;j}(t,x) = \frac{8}{\omega_i \Delta v^j} \int_{K_j} f(t,x,\vec{v}) \phi_i^j(v)\, dv\,.$$

By replacing integrals with Gauss quadratures on nodes $\vec{v}_p^j$, we observe that up to the truncation errors of integration,

$$f_{i;j}(t,x) = f(t,x,\vec{v}_i^j) + (\text{truncation errors}). \tag{20}$$

To derive the velocity discretization of the kinetic equation (7), we substitute representation (19) into the left side (the right side will be handled separately), multiply by the basis function $\phi_i^j(\vec{u})$ and integrate over K_j:

$$\partial_t \int_{K_j} \Big(\sum_p f_{p;j}(t,\vec{x})\phi_p^j(\vec{u})\Big)\phi_i^j(\vec{u})\, du + \int_{K_j} \vec{u}\cdot\partial_x \Big(\sum_p f_{p;j}(t,\vec{x})\phi_p^j(\vec{u})\Big)\phi_i^j(\vec{u}) = \frac{L^3 C_\infty^3 \mathbb{T}}{N} \int_{K_j} \hat{I}[\hat{f}](\hat{t},\hat{\vec{x}},\hat{\vec{u}})\phi_i^j(\vec{u})\, du.$$

Notice that instead of $\hat{I}[\hat{f}](\hat{t},\hat{\vec{x}},\hat{\vec{u}})$ one should substitute one of the dimensionless models discussed previously. The case of the full Boltzmann operator is discussed in [1] and in the above. Specifically, from (16) we conclude that:

$$\partial_t f_{i;j}(t,\vec{x}) + \vec{u}_i^j \cdot \partial_x f_{i;j}(t,\vec{x}) = \frac{N\hat{d}^2}{L^2} \frac{8}{\Delta v^j \omega_i} \int_{R^3}\int_{R^3} f(t,x,v) f(t,x,v_1) A(v,v_1;\phi_i^j) dv_1\, dv\,. \tag{21}$$

In the case of the ES-BGK model of the collision integral, the equation becomes simply:

$$\partial_t f_{i;j}(t,\vec{x}) + \vec{u}_i^j \cdot \partial_x f_{i;j}(t,\vec{x}) = \frac{NkT_\infty}{L^2 C_\infty} \frac{n(t,x)T(t,x)}{(1-\alpha)\mu(T)} (f_{ES}(t,x,v) - f(t,x,v)). \tag{22}$$

A.3 BGK Model With Velocity-Dependent Collision Frequency

In this section we briefly describe the BGK-type models with velocity dependent collision frequency that are implemented in the subroutine EvalColVelES. Two models are used in this approach. The first model will attempt to enforce exactly the relaxation rates for the selected group of moments. In this approach the number of enforced moments and the number of basis functions in the representation of the collision frequency has to be the same. A linear system of equations is solved at every time steps to determine the coefficients in the representation of the collision frequency. In the second model, the number of enforced

moments is bigger than the number of basis functions. A linear least squares problem is solved at every time step to determine the coefficients of the collision frequency. The two models are summarized below.

We note that the method is formulated in the dimensional variables, however one can use the formulas given above to derive the dimensionless form of the method. The modifications to the dimensionless case are limited to a coefficient similar to those found in (22).

A.3.1 Model with Exact Enforcement of Moments

Let $\psi_i(\vec{u})$, $i = 0, \ldots, k$ be a collection of linearly independent functions in velocity space. To allow the BGK model freedom to accommodate for specified relaxation frequencies for selected solution moments we assume that the collision frequency has the form

$$\nu(t, \vec{u}) = \sum_{i=0}^{k} c_i(t)\psi_i(\vec{u}). \tag{23}$$

In general, arbitrary linearly independent function $\psi_i(\vec{u})$ can be used in (23). However, it is expected that some choices of $\psi_i(\vec{u})$, including symmetric polynomials and trigonometric functions, will produce matrices that are near degenerate. It is best to select functions $\psi_i(\vec{u})$ so that the projection mapping between the kernels of the enforced moments and the functions $\psi_i(\vec{u})$ is invertible and is well-conditioned in a weighted L^2-norm with $f_M(t, \vec{u})$ serving as the weight. In simulations presented in the Section 3 of the Final Technical Report, the following functions $\psi_i(\vec{u})$ were used: $\psi_0(\vec{u}) = 1$, $\psi_1(\vec{u}) = u_1$, $\psi_2(\vec{u}) = u_2$, $\psi_3(\vec{u}) = u_3$, $\psi_4(\vec{u}) = u_1^2 + u_2^2 + u_3^2$, $\psi_i(\vec{u}) = P_{i-3}(u_1)$, $i = 5, \ldots, 8$, where $P_l(u_1)$ are the Legendre polynomials of degree l. As it will be seen below, functions $\psi_i(\vec{u})$ are chosen so as to match the moments that we are going to enforce. Finally, we assume that the coefficient standing with $\psi_0(\vec{u})$ in (23) has the form $c_0 + \nu_{\mathrm{BGK}} = c_0 + \alpha T(\hat{T}_0/\hat{T})^\gamma$. Thus we will seek an addition to the collision frequency of the classical BGK model that enforces relaxation speeds of selected moments. With this assumption, the new model may be considered as a generalization of the classical BGK model.

We seek the solution to the following equation

$$\partial_t f(t, \vec{u}) = \nu(t, \vec{u})(f_M(t, \vec{u}) - f(t, \vec{u}))\,. \tag{24}$$

The coefficients $c_i(t)$, $i = 1, \ldots, k$ in (23) are determined from the condition that moments $f_\varphi(t)$ of the solution relax with the prescribed relaxation frequencies ν_φ. Specifically, we multiply (24) by $\varphi(\vec{u})$ and integrate over the velocity space. Using the assumption that $\partial_t f_\varphi(t) = \nu_\varphi(f_\varphi^M - f_\varphi)$ after algebraic manipulations we obtain the system that is solved at each time step:

$$(\nu_\varphi(t) - \nu_{\mathrm{BGK}})(f_\varphi^M - f_\varphi) = \sum_{i=0}^{k} c_i(t) \int_{R^3} \psi_i(\vec{u})(f_M(t, \vec{u}) - f(t, \vec{u}))\varphi(\vec{u})\, du\,. \tag{25}$$

The relaxation frequencies are determined by evaluating the full Boltzmann collision integral using the formula:

$$\nu_\varphi(t) = -\frac{\hat{I}_\varphi}{f_\varphi(t) - f_\varphi^M(t)},$$

where $\hat{I}_\varphi$ is defined by (15). The numerical noise makes if difficult to evaluate the frequencies for higher moments when solution gets close to continuum. Therefore, in practice, the frequencies should be obtained only for solutions strongly deviating from continuum. In cases when the solution is close to continuum, models using only low order moments, or the classical BGK model should be used. Similarly, we notice that (25) becomes degenerate when solutions approach the Maxwellian distribution. Therefore, in practice, one should determine a threshold for the difference $f_M(t,\vec{u}) - f(t,\vec{u})$ and stop solving (25) when the difference drops below the threshold. In the solutions presented in this report the coefficients $c_i(t)$ are not updated whenever $\|f_M(t,\vec{u}) - f(t,\vec{u})\|_{L^1} < 0.01n$ where n is the local number density.

A.3.2 Improved Model for Enforcing Relaxation Rates of Moments

The model with exact enforcement of moments has one undesired property, namely that the kinetic models can become stiff (more stiff than the classical models) if relaxation rates are enforced for higher order moments. To reduce the stiffness one can change the way in which the relaxation rates of moments are enforced.

In the model of the previous section, the number of functions ψ_n used in (23) and the number of enforced moments f_{ϕ_n} are the same resulting in a linear system of equations (25) with a square matrix. In principle, one may desire to enforce relaxation rates for a large number of moments than the number of coefficients used in (23). In this case, the equation (25) represents an overdetermined linear system with a rectangular matrix. Let us assume that the collision operator of the kinetic equation has the form (up to a coefficient that is due to the dimensionless reduction)

$$\nu(t,\vec{x},\vec{v})(f_0(t,\vec{x},\vec{v}) - f(t,\vec{x},\vec{v})).$$

where f_0 is the desired equilibrium distribution function for a certain class of models. In particular, it can be the Maxwellian. Here ν is a velocity dependent collision frequency. We will assume that ν is expressed in terms of basis functions $\psi_k(\vec{v})$ and corresponding coefficients (or parameters) $c_k(t,\vec{x})$, (for $k = 1 \dots N_b$), as

$$\nu(t,\vec{x},\vec{v}) = \sum_{k=1}^{N_b} c_k(t)\psi_k(\vec{v}). \tag{26}$$

For convenience of later use, we define a vector of parameters, $\vec{c}$, as

$$\vec{c} \equiv (c_1, c_2, \dots, c_{N_b})^T. \tag{27}$$

For any function $\phi(\vec{v})$, the corresponding (generalized) moment can be defined as

$$f_\phi(t,\vec{x}) \equiv \int_{R^3} \phi(\vec{v}) f(t,\vec{x},\vec{v})\, dv\,. \tag{28}$$

Further, given any selection of (generalized) moments $\phi_i(\vec{v})$ for $i = 1 \ldots N_c$, we can obtain the rate of evolution (due to collisions) of any moment (or macroscopic quantity) $\langle \phi_i \rangle$ based on a weak form of the Boltzmann equation as,

$$\dot{M}^e_{\phi_i} \equiv \partial_t f_{\phi_i}|_{\text{collision}} = I_{\phi_i} \qquad \text{(see 15))} \tag{29}$$

where the right hand side of the above equation can be conveniently evaluated using certain symmetry properties of the collision operator. These properties ensure that the above right hand side term is zero (by construction) for collision invariants.

Similarly, the rate of evolution (due to collisions) obtained from our model approximations of the collision operator can be expressed as,

$$\dot{M}^a_{\phi_i} \equiv \int_{R^3} \phi_i(\vec{v})\nu(t,\vec{x},\vec{v})(f_0(t,\vec{x},\vec{v}) - f(t,\vec{x},\vec{v}))\, dv. \tag{30}$$

Based on the assumed functional form of ν, in terms of basis functions ψ_k, the rate of evolution of the generalized moment (involving ϕ_i) can be expanded as,

$$\begin{aligned} \dot{M}^a_{\phi_i}(\vec{c}) &= \int \phi_i(\vec{v}) \left(\sum_{k=1}^{N_b} c_k \psi_k(\vec{v}) \right) (f_0(t,\vec{x},\vec{v}) - f(t,\vec{x},\vec{v}))\, dv & (31)\\ &= \sum_{k=1}^{N_b} G_{ik}\ c_k = [G]\,[\vec{c}]\,, & (32) \end{aligned}$$

where

$$G_{ik} = \int \phi_i(\vec{v})\psi_k(\vec{v})(f_0(t,\vec{x},\vec{v}) - f(t,\vec{x},\vec{v}))\, dv\,. \tag{33}$$

In order to determine the unknown coefficients c_k, we define an error measure e and seek those coefficients that minimize the error, e. The error function e is chosen to be in the following form:

$$e = \sum_{i=1}^{N_c} \left[\dot{M}^e_{\phi_i} - \dot{M}^a_{\phi_i}(\vec{c}) \right]^2 = \sum_{i=1}^{N_c} \left[\dot{M}^e_{\phi_i} - [G]\,[\vec{c}] \right]^2, \tag{34}$$

where N_c denotes the number of constraints on evolution of (generalized) moments that we choose to consider. One can notice that (34) is a classical linear least squares problem

to which standard approaches could be applied. In particular, if the matrix $[G]$ is full rank then the solution to the problem is given by

$$c = [G^T G]^{-1} G^T \dot{M}^e_{\phi_i}.$$

If a matrix G is ill-conditioned or even not full rank, the problem can be regularized using the singular value decomposition.

A.4 Implementation of Korobov Integration for the Evaluation of the Collision Operator

Stochastic evaluation of the Boltzmann collision integral has been the most successful approach for obtaining solutions in multidimensional applications [7]. Stochastic methods are, indeed, the only well developed methods that beat the "curse of dimensionality" in multidimensional integration. A family of efficient quadratures is due to Korobov [6], who proposed the use of decimal parts of fractions as Monte-Carlo integration points and showed that the resulting quasi-stochastic multidimensional quadratures converge fast in the case of smooth periodic functions. Korobov integration was applied to the evaluation of the Boltzmann collision integral in [7, 5] based on discrete ordinate methods. A description of the Korobov quadratures implemented in DGVlib can be found in Chapter 3 Section 24 of [6]. In this section, we briefly summarize the approach.

Let a multidimensional function $h(x_1, \ldots, x_s)$ be periodic with period one on a s-dimensional cube $D = ([0,1])^s$. Let $h(x_1, \ldots, x_s)$ have an absolutely converging Fourier series on D with Fourier coefficients $C(m_1, \ldots, m_s)$ satisfying the inequality

$$C(m_1, \ldots, m_s) \le \frac{C}{(\bar{m}_1 \cdots \bar{m}_s)^\alpha}, \quad \text{where } \bar{m} = \max(1, |m|), \text{ for some } \alpha > 1.$$

Consider the quadrature formula

$$\int_0^1 \ldots \int_0^1 h(x_1, \ldots, x_s)\, dx_1 \ldots dx_s = \frac{1}{p} \sum_{k=1}^{p} h\Big(\Big\{\frac{a_1 k}{p}\Big\}, \ldots, \Big\{\frac{a_s k}{p}\Big\}\Big) - R_p[h], \tag{35}$$

where p is a large number, a_i, $i = 1, \ldots, s$, are some whole numbers relatively prime with p, and $\{\cdot\}$ stands for the fractional (decimal) part of the number. The following estimate holds for the truncation error $R_P[h]$:

$$|R_p[h]| \le C_1(\alpha, s) \frac{\ln^{\alpha s} p}{p^\alpha}.$$

It follows that the convergence rate α is proportional to the smoothness of the function. Specifically, a higher smoothness of the function h implies the faster convergence rate of the quadrature rule (35).

Subroutines of DGVlib implement the Korobov integration of the Galerkin projection of the Boltzmann collision integral

$$\begin{aligned}
\hat{I}_{\hat{\phi}_p^j} &= \frac{N^2\hat{d}^2C_\infty}{L^6}\int_{R^3}\int_{R^3} f(t,\vec{x},\vec{v})f(t,\vec{x},\vec{u})A(\vec{v},\vec{u};\phi_p^j)du\,dv \\
&\approx \frac{N^2\hat{d}^2C_\infty}{L^6}\int_{V}\int_{V} f(t,\vec{x},\vec{v})f(t,\vec{x},\vec{u})A(\vec{v},\vec{u};\phi_p^j)du\,dv \\
&\approx \frac{N^2\hat{d}^2C_\infty}{L^6}(\Delta V)^2\sum\frac{1}{p}\sum_{k=1}^{p} f(t,\vec{x},\vec{v}_k)f(t,\vec{x},\vec{u}_k)A(\vec{v}_k,\vec{u}_k;\phi_p^j) \\
&= \frac{N^2\hat{d}^2C_\infty}{L^6}\sum\sum_{k=1}^{p} f(t,\vec{x},\vec{v}_k)f(t,\vec{x},\vec{u}_k)\tilde{A}(\vec{v}_k,\vec{u}_k;\phi_p^j),
\end{aligned}$$

where

$$\tilde{A}(\vec{v}_k,\vec{u}_k;\phi_p^j) = \frac{(\Delta V)^2}{p}A(\vec{v}_k,\vec{u}_k;\phi_p^j)$$

and $V = [u_L,u_R]\times[v_L,v_R\times[w_L,w_R]$ is the velocity domain, and $\Delta V = (u_R-u_L)(v_R-v_L)(w_R-w_L)$ is the volume of the domain. The Korobov nodes $\vec{v}_k$, $\vec{u}_k$ are obtained by scaling, i.e.,

$$\begin{aligned}
\vec{v}_k &= \left(\frac{a_1k}{p}(u_R-u_L)+u_L, \frac{a_2k}{p}(v_R-v_L)+v_L, \frac{a_3k}{p}(w_R-w_L)+w_L,\right) \\
\vec{u}_k &= \left(\frac{a_4k}{p}(u_R-u_L)+u_L, \frac{a_5k}{p}(v_R-v_L)+v_L, \frac{a_6k}{p}(w_R-w_L)+w_L,\right)
\end{aligned}$$

The summation kernel $\tilde{A}(\vec{v}_k,\vec{u}_k;\phi_p^j)$ can be pre-computed and stored for future use.

A.4.1 Parameters of the Korobov Quadrature

It turns out that not all combinations of parameters p, $a_1,\ldots,a_6$ will produce nodes that cover the cube $[0,1]^6$ uniformly. In fact, it is a challenging mathematical problems to identify the parameters that make a good map. Some results, however, can be found in literature. In Table 1 [3], combinations of p, $a_1,\ldots,a_6$ are listed that provide a good approximation to the integral

$$I = \int_{[0,1]^6} e^{-\|\vec{x}-\vec{0.5}\|^2/T}d\vec{x},$$

where $\vec{0.5} = (.5,.5,.5,.5,.5,.5)$. The relative error of the integration using Korobov nets is given in the last column of the Table 1.

A.5 REFERENCES

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Table 1. Values of the parameters p and $a_1, \ldots, a_6$ in Korobov quadrature nets [3]

p	b or a_1	a_2	a_3	a_4	a_5	a_6	Error
256	123	25	3	113	75	9	3.9E-3
1,536	341	1,081	1,517	1,201	965	361	6.2E-4
2,048	443	1,689	707	1,905	139	137	4.6E-4
3,072	1,095	945	2,583	2,145	1,767	2,577	9.5E-4
4,096	1,271	1,617	3,111	1,441	599	3,569	2.1E-4
6,144	1,477	409	1,981	1,393	5,365	4,489	1.4E-4
8,192	67	4489	1655	3219	4389	7343	1.1E-4
12,288	5,685	729	869	785	1,093	393	1.4E-4
24,576	3771	15513	8643	4977	16779	14985	1.0E-4
32,769	4 335	16 161	32 719	16 961	27 311	2 401	1.0E-4
49,152	1,509	16,089	46,365	21,489	35,733	1,353	4.5E-4
5,536	24,565	49,273	6,861	47,409	27,365	18,673	5.2E-6
98,304	40,709	13,849	5,501	3,697	96,063	81,673	3.1E-6
131,072	33,269	54,393	20,685	41,265	128,229	50,217	1.5E-6
753,456	15,723	79,161	692,547	723,825	501,051	642,393	3.8E-7
196,608	5,209	1,777	1,5817	12,001	188,473	92,113	1.1E-5
262,144	3,851	150,137	150,067	142,641	118,811	99,881	1.6E-6
393,216	4,513	313,153	41,185	26,953	114,721	263,617	5.1E-6
24,288	67,469	444,225	434,401	138,881	245,793	394,689	1.2E-6
786,432	8,629	535,033	443,917	635,953	702,373	531,625	1.6E-6
1,048,576	9,199	735521	645327	374,337	2,479	784,225	4.8E-8
1,572,864	9,781	1,296,121	75,661	794,161	886,309	934,825	2.0E-8
2,097,152	11,027	2,057,065	459,723	549,137	855,875	549,625	8.8E-10
3,145,728	12,641	2,508,481	770,081	1,711,489	1,760,993	1,541,185	3.9E-6
4,194,304	11,587	136,841	1,263,755	2,904,313	294,915	1,267,345	5.0E-8
6,291,456	8,969	4,945,489	1,326,041	2,409,889	3,143,081	4,570,609	8.0E-10
8,388,608	13,997	2,978,025	422,773	3,585,041	7,554,429	938,873	4.2E-8
12,582,912	14,639	390,817	8,528,015	6,541,633	7,005,167	10,489,825	2.8E-12
16,777,216	15,241	14,184,273	8,076,633	1,529,761	11,534,377	3,770,609	2.0E-10
25,165,824	16,981	11,530,297	5,862,637	22,604,977	800,965	1,164,1705	3.9E-17
33,554,423	40,709	13,055,954	26,325,489	23,169,927	9,727,713	29,722,694	6.6E-16
50,331,648	19,211	16,740,985	42,163,763	20,839,729	14,105,627	47,939,113	5.1E-11
67,108,864	63,727	34,598,689	8,927,183	20,750,913	13,267,631	1,743,201	1.0E-15
100,663,296	32,119	24,997,201	61,758,887	29,889,441	26,655,959	54,969,073	1.5E-15