User's Manual for UGKS1D and UGKS2D Codes

Ruijie Wang and Kun Xu

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Contents

Chapter 1

Unified Gas-Kinetic Scheme

This chapter describes the Unified Gas-Kinetic Scheme presented in [1, 2]. This is a 1D formulation. The 2D formulation with directional splitting is presented in [3], which can be extended to develop a truly multidimensional formulation, see[4].

1.1 Model equation

The model equation is the BGK-Shakhov model. In one dimensional case,

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = \frac{f^+ - f}{\tau}, \tag{1.1}$$

where f is the distribution function, u is particle velocity, $\tau = \mu/p$ is particle collision time, μ is the dynamic viscosity, p is the pressure and f^+ is the modified equilibrium distribution function.

The modified equilibrium distribution is given by,

$$f^+ = g\left[1 + (1 - \mathrm{Pr})\mathbf{c}\cdot\mathbf{q}\left(\frac{c^2}{RT} - 5\right)/(5pRT)\right] = g + g^+, \tag{1.2}$$

where g is the Maxwellian distribution, Pr is the Prandtl number, $\mathbf{c}$ is the random velocity, $\mathbf{q}$ is heat flux, R is gas constant and T is the temperature.

The Maxwellian distribution for 1D problem is,

$$g = \rho\left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}, \tag{1.3}$$

where ρ is density, $\lambda = m/2kT$, m is molecule mass, k is Boltzmann constant, U is the macroscopic velocity, K is the number of internal degree of freedom and $\xi^2 = \xi_1^2 + \xi_2^2 ... + \xi_K^2$. For example, a monatomic gas at 1D problem has $K = 2$ to account for the motion in y, z direction, and $\xi^2 = v^2 + w^2$, where v, w are particle velocity in y, z direction.

The relation between K and the ratio of specific heat is,

$$\gamma = \frac{K+3}{K+1}. \tag{1.4}$$

The dynamic viscosity can be calculated from Sutherland's law or hard-sphere(HS)/variable hard-sphere model(VHS),

$$\mu = \mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\omega}, \tag{1.5}$$

where μ_{ref} is the reference viscosity and T_{ref} is the reference temperature, ω is the index related to HS or VHS model.

The collision term meets the requirement of conservative constraint or compatibility condition

$$\int (f^+ - f)\psi d\Xi = 0, \tag{1.6}$$

where $\psi = (1, u, 1/2(u^2 + \xi^2))^T$ is the collision invariants and $d\Xi = dud\xi$.

The macroscopic variables can be calculated via,

$$W = \begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \psi f d\Xi, \tag{1.7}$$

$$p = \frac{1}{3}\int [(u - U)^2 + \xi^2] f d\Xi, \tag{1.8}$$

$$q = \frac{1}{2}\int (u - U)[(u - U)^2 + \xi^2] f d\Xi, \tag{1.9}$$

where ρE is total energy.

An integral solution of the BGK-Shakhov model can be constructed by the method of characteristics[5],

$$f(x, t, u, \xi) = \frac{1}{\tau}\int_{t^n}^{t} f^+(x', t', u, \xi) e^{-(t-t')/\tau} dt' + e^{-(t-t^n)/\tau} f_0^n(x - u(t - t^n), t^n, u, \xi), \tag{1.10}$$

where $x' = x - u(t - t')$ is the particle trajectory and f_0^n is the initial gas distribution function at t^n.

1.2 Solution algorithm

For the numerical computation, in addition to the discretization of physical space and time, the velocity space is also discretized. That is, the distribution function is for some discrete particle velocities instead of continuous velocity space from $-\infty$ to ∞ as in [6]. Then the moments of the non-equilibrium distribution function are calculated through numerical integration(the moments of equilibrium distribution are still calculated using analytical integration). The discretization of the velocity space is determined by the choice of numerical integration method.

In the finite volume approach, if trapezoidal rule is used for the approximation of collision term, Eq. 1.1 becomes,

$$f_{i,k}^{n+1} = f_{i,k}^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} (\mathbf{f}_{i-1/2} - \mathbf{f}_{i+1/2}) dt + \frac{\Delta t}{2}\left(\frac{f_{i,k}^{+(n+1)} - f_{i,k}^{n+1}}{\tau^{n+1}} + \frac{f_{i,k}^{+(n)} - f_{i,k}^n}{\tau^n}\right), \tag{1.11}$$

where $f_{i,k}^n$ and $f_{i,k}^{n+1}$ are cell averaged distribution function of the i-th cell and k-th discrete particle velocity u_k at time t^n and t^{n+1} respectively, Δx is the cell length and Δt is the time step, $\mathbf{f}_{i-1/2}$ and $\mathbf{f}_{i+1/2}$ are the fluxes of the distribution function across the cell interface, $f_{i,k}^{+(n)}$ and $f_{i,k}^{+(n+1)}$ are modified equilibrium distribution, τ^n and τ^{n+1} are particle collision time.

Multiplying the collision invariants to Eq. 1.11 and make integration over the velocity space, the evolution of conservative flow variables becomes,

$$W_i^{n+1} = W_i^n + \frac{1}{\Delta x}(\mathbf{F}_{i-1/2} - \mathbf{F}_{i+1/2}), \tag{1.12}$$

where $\mathbf{F} = \int_{t^n}^{t^{n+1}} \int \psi \mathbf{f} d\Xi dt$.

In order to update the distribution function in Eq. 1.11, there are three unknowns to be obtained: the interface gas distribution function f, the modified equilibrium distribution $f^{+(n+1)}$ and collision time τ^{n+1} at the next time level.

The flux $\mathbf{f}$ is calculated using the integral solution Eq. 1.10 at the cell interface. Since $f^{+(n+1)}$ and τ^{n+1} have one-to-one correspondence to the macroscopic variables, they are obtained by using the updated conservative variables in Eq. 1.12.

In order to remove the dependence of distribution functions on the internal degree of freedom ξ, the reduced distribution function [7, 8] is used in real computation, which is defined as,

$$h = \int_{-\infty}^{\infty} f d\xi, \quad b = \int_{-\infty}^{\infty} \xi^2 f d\xi, \tag{1.13}$$

and the reduced modified equilibrium distributions are,

$$h^+ = H + H^+, \quad b^+ = B + B^+,$$

where the corresponding reduced Maxwellian distribution g becomes,

$$H = \int_{-\infty}^{\infty} g d\xi = \rho \left(\frac{\lambda}{\pi}\right)^{1/2} e^{-\lambda(u-U)^2}, \quad B = \int_{-\infty}^{\infty} \xi^2 g d\xi = \frac{K}{2\lambda} H, \tag{1.14}$$

and the corresponding terms related to g^+ becomes,

$$\begin{aligned} H^+ &= \int_{-\infty}^{\infty} g^+ d\xi = \frac{4(1-\Pr)\lambda^2}{5\rho}(u-U)q(2\lambda(u-U)^2 + K - 5)H, \\ B^+ &= \int_{-\infty}^{\infty} \xi^2 g^+ d\xi = \frac{4(1-\Pr)\lambda^2}{5\rho}(u-U)q(2\lambda(u-U)^2 + K - 3)B, \end{aligned} \tag{1.15}$$

Then the update of f using Eq. 1.11 becomes two similar equations for the update of h and b, respectively.

The overview flow chart of the solution algorithm in one iteration is shown in Figure. 1.1.

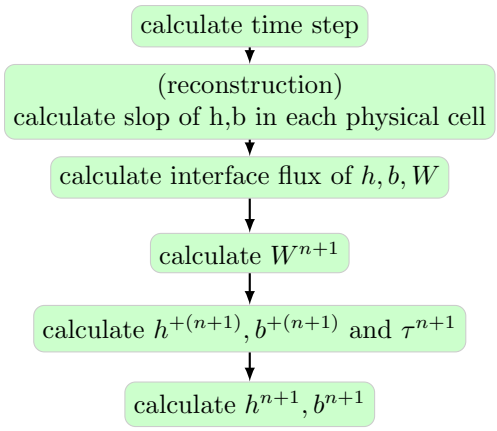


Figure 1.1: solution algorithm in one iteration

1.3 Nondimensionalization

In the program, the following nondimensionalization is used,

$$\begin{aligned} \hat{t} = \frac{t}{t_\infty},\ \hat{u}_x = \frac{u_x}{C_\infty},\ \hat{x} = \frac{x}{L_\infty},\ \hat{\rho} = \frac{\rho}{\rho_\infty},\ \hat{T} = \frac{T}{T_\infty}, \hat{p} = \frac{p}{\rho_\infty C_\infty^2}, \\ \hat{q} = \frac{q}{\rho_\infty C_\infty^3},\ \hat{h} = \frac{h}{\rho_\infty / C_\infty},\ \hat{b} = \frac{b}{\rho_\infty C_\infty},\ \hat{E} = \frac{E}{C_\infty^2}, \hat{\mu} = \frac{\mu}{\rho_\infty C_\infty L_\infty}, \end{aligned}$$

The free stream variables are related through,

$$C_\infty = \sqrt{2RT_\infty},\ t_\infty = \frac{L_\infty}{C_\infty},\ \lambda_\infty = 1/C_\infty^2.$$

In the following, all variables are nondimensionalized, but we will drop the "ˆ" for simplicity. After nondimensionalization and using the reduced distribution function, the expressions for macroscopic variables become,

$$\begin{aligned}
\rho &= \int h\mathrm{du} = \sum \alpha_k h_k, \\
\rho U &= \int hu\mathrm{du} = \sum \alpha_k h_k u_k, \\
\rho E &= \frac{1}{2}\left(\int hu^2\mathrm{du} + \int b\mathrm{du}\right) = \frac{1}{2}\left(\sum \alpha_k h_k u_k^2 + \sum \alpha_k b_k\right),
\end{aligned} \tag{1.16}$$

$$(K+1)p = \int (u-U)^2 h\mathrm{du} + \int b\mathrm{du} = \sum \alpha_k (u_k - U)^2 h_k + \sum \alpha_k b_k, \tag{1.17}$$

$$\begin{aligned}
q &= \frac{1}{2}\left[\int (u-U)(u-U)^2 h\mathrm{du} + \int (u-U) b\mathrm{du}\right] \\
&= \frac{1}{2}\left[\sum \alpha_k (u_k - U)(u_k - U)^2 h_k + \sum \alpha_k (u_k - U) b_k\right],
\end{aligned} \tag{1.18}$$

where α_k is the weight of the numerical integration at the k-th particle velocity. The summation is over all the discrete particle velocity.

The equation of state is,

$$p = \frac{1}{2}\rho T, \quad \lambda = \frac{1}{T}. \tag{1.19}$$

1.4 Time step and reconstruction

The time step is determined by the CFL condition

$$\Delta t = \mathrm{CFL}\frac{\Delta x}{|U| + c}, \tag{1.20}$$

where CFL is the CFL number, c is the speed of sound. The macroscopic velocity $|U| + c$ can also be replaced by $\max(|u|)$.

In the program, the van Leer limiter is used for the reconstruction. For example, the slope of h at the i-th cell and k-th particle velocity is,

$$\sigma_{i,k}^h = (\mathrm{sign}(s_1) + \mathrm{sign}(s_2))\frac{|s_1||s_2|}{|s_1| + |s_2|}, \tag{1.21}$$

where $s_1 = (h_{i,k} - h_{i-1,k})/(x_i - x_{i-1}), s_2 = (h_{i+1,k} - h_{i,k})/(x_{i+1} - x_i)$.

The slope of b is calculated in the same way.

1.5 The algorithm

Take the interface $x_{i+1/2} = 0$ at $t^n = 0$ as example.

1.5.1 The calculation of interface fluxes

Here the original distribution function is used for illustration. From Eq. 1.10, the integral solution at the cell interface is,

$$f(0,t,u_k,\xi)=\frac{1}{\tau}\int_0^t f^+(x',t',u_k,\xi)e^{-(t-t')/\tau}dt'+e^{-t/\tau}f_0(-u_kt,0,u_k,\xi). \tag{1.22}$$

The initial distribution function around the interface f_0 is,

$$f_0(x,0,u_k,\xi)=\begin{cases}f^L_{i+1/2,k}+\sigma_{i,k}x, & x\leqslant 0,\\ f^R_{i+1/2,k}+\sigma_{i+1,k}x, & x>0,\end{cases} \tag{1.23}$$

where $f^L_{i+1/2,k}, f^R_{i+1/2,k}$ are the reconstructed initial distribution functions at the left and right side of the interface.

The Maxwellian distribution around the interface in f^+ is approximated by Taylor expansion,

$$g(x,t,u,\xi)=g_0[1+(1-H[x])a^Lx+H[x]a^Rx+At], \tag{1.24}$$

where g_0 is the Maxwellian distribution at $x=0,t=0$ and $H[x]$ is the Heaviside function

$$H[x]=\begin{cases}0, & x<0,\\ 1, & x\geqslant 0.\end{cases}$$

a^L, a^R and A have the same form [6],

$$a=a_1+a_2u+a_3\frac{1}{2}(u^2+\xi^2),$$

where a_1, a_2, a_3 are local constants.

Inserting Eq. 1.23 and Eq. 1.24 into Eq. 1.22, one obtains,

$$\begin{aligned}f(0,t,u_k,\xi)=&(1-e^{-t/\tau})(g_0+g^+)\\ &+(\tau(-1+e^{-t/\tau})+te^{-t/\tau})(a^LH[u_k]+a^R(1-H[u_k]))u_kg_0\\ &+\tau(t/\tau-1+e^{-t/\tau})Ag_0\\ &+e^{-t/\tau}((f^L_{i+1/2,k}-u_kt\sigma_{i,k})H[u_k]+(f^R_{i+1/2,k}-u_kt\sigma_{i+1,k})(1-H[u_k]))\\ =&\tilde{g}_{i+1/2,k}+\tilde{f}_{i+1/2,k},\end{aligned} \tag{1.25}$$

where $\tilde{g}_{i+1/2,k}$ is the first three terms related to equilibrium distribution, $\tilde{f}_{i+1/2,k}$ is the last term related to the initial non-equilibrium distribution.

Here g_0 or W_0 in Eq. 1.24 can be obtained by applying the compatibility condition at $x=0,t=0$,

$$\int(f^+-f)|_{x=0,t=0}\psi d\Xi=0,$$

which gives,

$$W_0=\int g_0\psi d\Xi=\int f_0(0,0,u_k,\xi)\psi d\Xi. \tag{1.26}$$

Then, a^L, a^R, A are obtained from the slope of conservative variables,

$$\left(\frac{\partial W}{\partial x}\right)^L=\int a^Lg_0\psi d\Xi,\quad \left(\frac{\partial W}{\partial x}\right)^R=\int a^Rg_0\psi d\Xi, \tag{1.27}$$

$$\frac{\partial W}{\partial t}=\int Ag_0\psi d\Xi. \tag{1.28}$$

The time derivative of W can be calculated via the compatibility condition,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int (f^+ - f)\psi d\Xi\Big|_{x=0,t=0} = 0,$$

which gives,

$$\frac{\partial W}{\partial t} = -\int \left(a^L H[u] + a^R(1-H[u])\right) u g_0 \psi d\Xi. \tag{1.29}$$

1.5.2 The numerical procedure

The flow chart of the numerical procedure is shown in Figure. 1.2

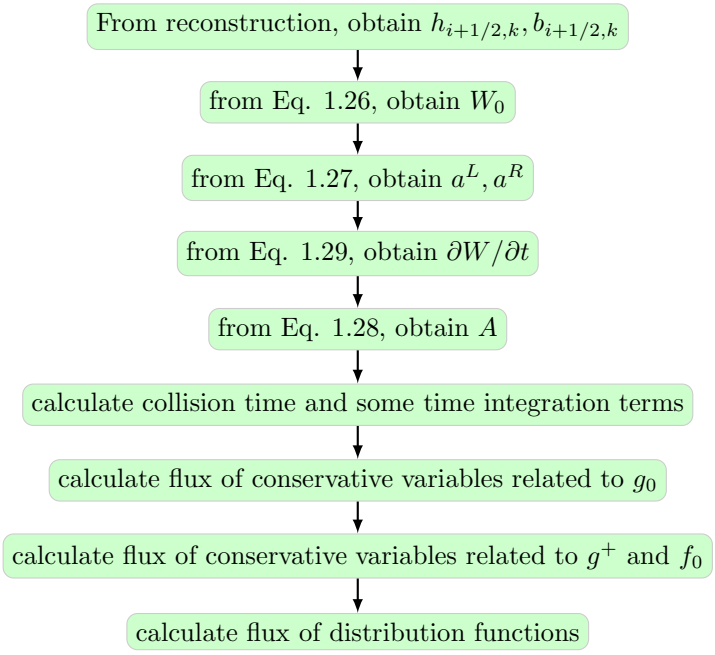


Figure 1.2: interface flux calculation

Reconstruct initial distribution

Take h as example. Since we take value from $h^L_{i+1/2,k}$ only if $u_k \geqslant 0$ and take value from $h^R_{i+1/2,k}$ only if $u_k < 0$ (see Eq. 1.25), there is no need to store the left and right values separately.

We define the variable,

$$h_{i+1/2,k} = \begin{cases} h_{i,k} + (x_{i+1/2} - x_i)\sigma^h_{i,k}, & u_k \geqslant 0, \\ h_{i+1,k} - (x_{i+1} - x_{i+1/2})\sigma^h_{i+1,k}, & u_k < 0, \end{cases}$$

and similarly,

$$\sigma^h_{i+1/2,k} = \begin{cases} \sigma^h_{i,k}, & u_k \geqslant 0, \\ \sigma^h_{i+1,k}, & u_k < 0. \end{cases}$$

In the program, they are written as,

$$\sigma^h_{i+1/2,k} = \sigma^h_{i,k} H[u_k] + \sigma^h_{i+1,k}(1 - H[u_k]),$$

and,

$$h_{i+1/2,k} = (h_{i,k} + (x_{i+1/2} - x_i)\sigma^h_{i,k})H[u_k] + (h_{i+1,k} - (x_{i+1} - x_{i+1/2})\sigma^h_{i+1,k})(1 - H[u_k]).$$

Calculate W_0

W_0 is calculated from Eq. 1.16, with $h_k = h_{i+1/2,k}, b_k = b_{i+1/2,k}$.

Then the primary variables is obtained from the relation (the expression for λ below only holds for equilibrium state),

$$\rho_0 = \rho_0, \quad U_0 = \frac{\rho_0 U_0}{\rho_0}, \quad \lambda_0 = \frac{(K+1)\rho_0}{4\left(\rho_0 E_0 - \frac{1}{2}\rho U_0^2\right)}.$$

The heat flux is calculated by Eq. 1.18, with $h_k = h_{i+1/2,k}, b_k = b_{i+1/2,k}, U = U_0$.

Calculate a^L, a^R

The macroscopic slope is approximated by,

$$\left(\frac{\partial W}{\partial x}\right)^L \approx \frac{W_0 - W_i}{x_{i+1/2} - x_i}, \quad \left(\frac{\partial W}{\partial x}\right)^R \approx \frac{W_{i+1} - W_0}{x_{i+1} - x_{i+1/2}},$$

and the three components of a^L, a^R are calculated from,

$$\begin{aligned} a_3 &= \frac{4\lambda_0^2}{(K+1)\rho_0}\left[2\frac{\partial \rho E}{\partial x} + \left(U_0^2 - \frac{K+1}{2\lambda_0}\right)\frac{\partial \rho}{\partial x} - 2U_0\frac{\partial \rho U}{\partial x}\right], \\ a_2 &= \frac{2\lambda_0}{\rho_0}\left(\frac{\partial \rho U}{\partial x} - U_0\frac{\partial \rho}{\partial x}\right) - U_0 a_3, \\ a_1 &= \frac{1}{\rho_0}\frac{\partial \rho}{\partial x} - U_0 a_2 - \frac{1}{2}\left(U_0^2 + \frac{K+1}{2\lambda_0}\right)a_3. \end{aligned} \tag{1.30}$$

Calculate $\partial W/\partial t$ and A

From Eq. 1.29, the time derivative of W is calculated from,

$$\frac{\partial W}{\partial t} = -\rho_0\left(< a^L u\psi >_{>0} + < a^R u\psi >_{<0}\right),$$

where $< ... >$ is the moments of Maxwellian distribution function. The detail definition and calculation can be found in [6] and also Appendix A: Moments of Maxwellian distribution function.

A is calculated in the same way as a^L, a^R using Eq. 1.30.

Calculate collision time and some time integration terms

From Eq. 1.5 and Eq. 1.19, the collision time is,

$$\tau = \frac{2\lambda_0^{1-\omega}}{\rho_0}\mu_\infty.$$

Some time integrals used in the evaluation of flux are listed below,

$$
\begin{aligned}
Mt_4 &= \int_{t^n}^{t^{n+1}} e^{-t/\tau} dt = \tau(1 - e^{-\Delta t/\tau}), \\
Mt_5 &= \int_{t^n}^{t^{n+1}} te^{-t/\tau} dt = -\tau \Delta t e^{-\Delta t/\tau} + \tau Mt_4, \\
Mt_1 &= \int_{t^n}^{t^{n+1}} (1 - e^{-t/\tau}) dt = \Delta t - Mt_4, \\
Mt_2 &= \int_{t^n}^{t^{n+1}} (\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}) dt = -\tau Mt_1 + Mt_5, \\
Mt_3 &= \int_{t^n}^{t^{n+1}} \tau(t/\tau - 1 + e^{-t/\tau}) dt = \frac{1}{2}\Delta t^2 - \tau Mt_1.
\end{aligned}
$$

Calculate the flux of conservative variables related to g_0

Theoretically, $\int_{t^n}^{t^{n+1}} \int \tilde{g}_{i+1/2} u\psi d\Xi dt$ can be calculated analytically. But the integration related to g^+ is too complex, and will be calculated with numerical integration. Only the terms related to g_0 will be integrated analytically here.

$$
\mathbf{F}_{g_0} = Mt_1 \rho_0 < u\psi > + Mt_2 \rho_0 \left(< a^L u^2 \psi >_{>0} + < a^R u^2 \psi >_{<0} \right) + Mt_3 \rho_0 < Au\psi >
$$

Calculate the flux of conservative variables related to g^+ and f_0

First evaluate H_k, B_k corresponding to g_0 by Eq. 1.14,

$$
H_k = \rho_0 \left(\frac{\lambda_0}{\pi} \right)^{1/2} e^{-\lambda_0 (u_k - U_0)^2}, \quad B_k = \frac{K}{2\lambda_0} H_k,
$$

and then evaluate H_k^+, B_k^+ corresponding to g^+ by Eq. 1.15,

$$
\begin{aligned}
H_k^+ &= \frac{4(1 - \Pr)\lambda_0^2}{5\rho_0} (u_k - U_0) q (2\lambda_0 (u_k - U_0)^2 + K - 5) H_k, \\
B_k^+ &= \frac{4(1 - \Pr)\lambda_0^2}{5\rho_0} (u_k - U_0) q (2\lambda_0 (u_k - U_0)^2 + K - 3) B_k.
\end{aligned}
$$

The flux of conservative variables related to g^+ is,

$$
\mathbf{F}_{g^+} = Mt_1 \begin{pmatrix} \sum \alpha_k u_k H_k^+ \\ \sum \alpha_k u_k^2 H_k^+ \\ \frac{1}{2} \left(\sum \alpha_k u_k^3 H_k^+ + \sum \alpha_k u_k B_k^+ \right) \end{pmatrix}.
$$

The flux of conservative variables related to f_0 is,

$$
\mathbf{F}_{f_0} = Mt_4 \begin{pmatrix} \sum \alpha_k u_k h_{i+1/2,k} \\ \sum \alpha_k u_k^2 h_{i+1/2,k} \\ \frac{1}{2} \left(\sum \alpha_k u_k^3 h_{i+1/2,k} + \sum \alpha_k u_k b_{i+1/2,k} \right) \end{pmatrix} - Mt_5 \begin{pmatrix} \sum \alpha_k u_k^2 \sigma_{i+1/2,k}^h \\ \sum \alpha_k u_k^3 \sigma_{i+1/2,k}^h \\ \frac{1}{2} \left(\sum \alpha_k u_k^4 \sigma_{i+1/2,k}^h + \sum \alpha_k u_k^2 \sigma_{i+1/2,k}^b \right) \end{pmatrix}.
$$

The flux of conservative variables is,

$$
\mathbf{F}_{i+1/2} = \int_{t^n}^{t^{n+1}} \int f_{i+1/2} u\psi d\Xi dt = \mathbf{F}_{g_0} + \mathbf{F}_{g^+} + \mathbf{F}_{f_0}.
$$

Calculate the flux of distribution functions

The flux of reduced distribution function h is calculated by,

$$\begin{aligned}\int_{t^n}^{t^{n+1}} \mathbf{f}^h_{i+1/2,k} dt &= \int_{t^n}^{t^{n+1}} \int f_{i+1/2,k} u_k d\xi dt \\ &= Mt_1 u_k (H_k + H_k^+) \\ &+ Mt_2 u_k^2 \left(a_1^L H_k + a_2^L u_k H_k + \frac{1}{2} a_3^L (u_k^2 H_k + B_k) \right) H[u_k] \\ &+ Mt_2 u_k^2 \left(a_1^R H_k + a_2^R u_k H_k + \frac{1}{2} a_3^R (u_k^2 H_k + B_k) \right) (1 - H[u_k]) \\ &+ Mt_3 u_k \left(A_1 H_k + A_2 u_k H_k + \frac{1}{2} A_3 (u_k^2 H_k + B_k) \right) \\ &+ Mt_4 u_k h_{i+1/2,k} - Mt_5 u_k^2 \sigma^h_{i+1/2,k}.\end{aligned}$$

The flux of reduced distribution function b is calculated by,

$$\begin{aligned}\int_{t^n}^{t^{n+1}} \mathbf{f}^h_{i+1/2,k} dt &= \int_{t^n}^{t^{n+1}} \int f_{i+1/2,k} u_k d\xi dt \\ &= Mt_1 u_k (B_k + B_k^+) \\ &+ Mt_2 u_k^2 \left(a_1^L B_k + a_2^L u_k B_k + \frac{1}{2} a_3^L (u_k^2 B_k + < \xi^4 > H_k) \right) H[u_k] \\ &+ Mt_2 u_k^2 \left(a_1^R B_k + a_2^R u_k B_k + \frac{1}{2} a_3^R (u_k^2 B_k + < \xi^4 > H_k) \right) (1 - H[u_k]) \\ &+ Mt_3 u_k \left(A_1 B_k + A_2 u_k B_k + \frac{1}{2} A_3 (u_k^2 B_k + < \xi^4 > H_k) \right) \\ &+ Mt_4 u_k b_{i+1/2,k} - Mt_5 u_k^2 \sigma^b_{i+1/2,k}.\end{aligned}$$

1.6 Update cell averaged value

The procedure is shown in Figure. 1.3

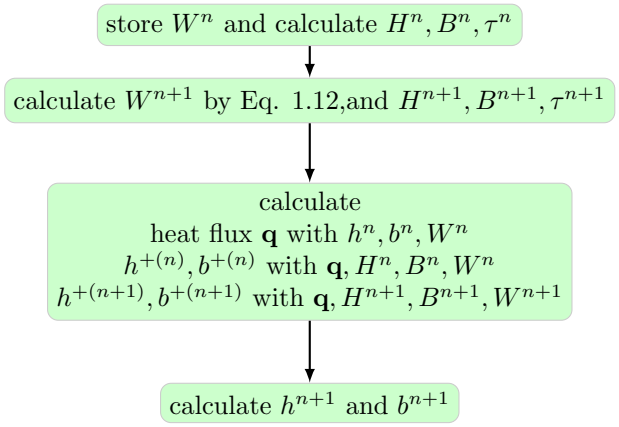


Figure 1.3: update cell averaged value

The equation for updating h^{n+1} and b^{n+1} can be obtained from Eq. 1.11,

$$h_{i,k}^{n+1} = \left(1 + \frac{\Delta t}{2\tau^{n+1}}\right)^{-1} \left[h_{i,k}^{n} + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} (\mathbf{f}_{i-1/2}^{h} - \mathbf{f}_{i+1/2}^{h})dt + \frac{\Delta t}{2}\left(\frac{h_{i,k}^{+(n+1)}}{\tau^{n+1}} + \frac{h_{i,k}^{+(n)} - h_{i,k}^{n}}{\tau^{n}}\right)\right],$$

$$b_{i,k}^{n+1} = \left(1 + \frac{\Delta t}{2\tau^{n+1}}\right)^{-1} \left[b_{i,k}^{n} + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} (\mathbf{f}_{i-1/2}^{b} - \mathbf{f}_{i+1/2}^{b})dt + \frac{\Delta t}{2}\left(\frac{b_{i,k}^{+(n+1)}}{\tau^{n+1}} + \frac{b_{i,k}^{+(n)} - b_{i,k}^{n}}{\tau^{n}}\right)\right].$$

1.7 Boundary condition

Only isothermal wall boundary condition with complete accommodation is discussed. Assuming left wall ($x = 1/2$). The boundary condition described here is quiet simple, the incoming distribution function is directly obtained through interpolation. This kind of boundary treatment is sufficient for Knudsen number case $\mathrm{Kn} = 0.075, 1.0, 10.0$. For flow in continuum regime, one need to use the same method as the inner region to calculate the incoming distribution function and flux.

First, obtain h_k^{in}, b_k^{in} by one-sided interpolation from the interior region. For example,

$$h_k^{in} = h_{1,k} - \sigma_{1,k}^{h}\frac{\Delta x}{2}.$$

Second, calculate the density at the wall with the condition that no particle penetrating the wall,

$$\int_{t^n}^{t^{n+1}}\int_{u>0} u g_w d\Xi dt + \int_{t^n}^{t^{n+1}}\int_{u<0} u f^{in} d\Xi dt = 0,$$

which gives,

$$\rho_w = -\frac{\sum \alpha_k u_k h_k^{in}}{\left(\frac{\lambda_w}{\pi}\right)^{1/2}\sum \alpha_k u_k e^{-\lambda_w(u_k - U_w)^2}},$$

where $g_w, \rho_w, \lambda_w, U_w$ are the variables at the wall.

The corresponding reduced Maxwellian distribution at the wall H_k^w, B_k^w is also obtained.

Thirdly, the distribution function at the boundary interface is expressed by (same holds for b_k),

$$h_k = H_k^w H[u_k] + h_k^{in}(1 - H[u_k]).$$

Finally, the flux across the wall is calculated by,

$$\mathbf{F}_{1/2} = \Delta t \begin{pmatrix} \sum \alpha_k u_k h_k \\ \sum \alpha_k u_k^2 h_k \\ \sum \alpha_k \frac{1}{2}\left(u_k^3 h_k + u_k b_k\right) \end{pmatrix},$$

and,

$$\int_{t^n}^{t^{n+1}} \mathbf{f}_{1/2,k}^{h} dt = \Delta t u_k h_k,$$

$$\int_{t^n}^{t^{n+1}} \mathbf{F}_{1/2,k}^{b} dt = \Delta t u_k b_k.$$

Chapter 2

UGKS Codes

2.1 Usage

2.1.1 Compiling

A makefile is provided to compile the program under Linux. If you are using any IDE (e.g. Visual Studio), use the compiling function provided by the IDE.

The makefile can be used to compile the two codes, UGKS1D and UGKS2D, and also this manual. There are several requirements for the makefile to work.

- Fortran Compiler: either **ifort** or **gfortran** , supporting Fortran 2003
- Bash shell
- Latex: only for compilation of the manual. It requires **hyperref** , **parskip** , **amsmath** , **amssymb** , **fullpage** , **appendix** , **graphicx** , **subfigure** , **xcolor** , **listings** or **minted** packages, and also **bibtex** , **dvips** and **ps2pdf** .

By default, the make command will compile both UGKS1D and UGKS2D with openmp and ifort. This behavior can be changed by specifying the target and passing parameters.

1. Compile both UGKS1D and UGKS2D with openmp and ifort

   ```
   make
   ```

2. Only compile UGKS1D

   ```
   make 1D
   ```

3. Only compile UGKS2D

   ```
   make 2D
   ```

4. Compile both UGKS1D and UGKS2D, but **WITHOUT** openmp, and **WITH** gfortran

   ```
   make OMP=no FC=gfortran
   ```

5. Compile the manual

   ```
   make manual
   ```

6. Clean the compilation

   ```
   make clean
   ```

The executables will be put into the bin directory, and the compiled manual.pdf will in the doc directory.

2.1.2 Running

Just type the program name to run it under the bin directory, no input file or data is required.

The code will generate two files,

- *.hst : record the convergence history every 10 iterations.
- *.dat : record the final result of the program.

Both files are in tecplot format and will be put into current working directory.

2.1.3 Other information

The comments in the program are written in doxygen format, and can be used to generate documentation of the code. But the doxygen configuration file is not included, and the documentation generation is not tested.

This program uses GIT for version control, and the source repository is published on GitHub. To obtain the code via git, use the following command,

```
git clone git://github.com/lainme/UGKS.git
```

2.2 UGKS1D Code

Once the flow condition before the normal shock is known (upstream), the flow variables after the shock (downstream) can be calculated by normal shock relation,

$$\begin{aligned} M_2 &= \sqrt{\frac{M_1^2(\gamma-1)+2}{2\gamma M_1^2-(\gamma-1)}}, \\ \frac{\rho_2}{\rho_1} &= \frac{(\gamma+1)M_1^2}{(\gamma-1)M_1^2+2}, \\ \frac{T_2}{T_1} &= \frac{(1+\frac{\gamma-1}{2}M_1^2)(\frac{2\gamma}{\gamma-1}M_1^2-1)}{M_1^2(\frac{2\gamma}{\gamma-1}+\frac{\gamma-1}{2})}, \end{aligned} \tag{2.1}$$

where M_1, ρ_1, T_1 are upstream Mach number, density and temperature. M_2, ρ_2, T_2 are downstream Mach number, density and temperature.

For shock structure calculation, the upstream and downstream conditions are specified at the two boundaries (via ghost cell). And the flux across the interfaces are calculated through the same method described in section 1.5.

In the UGKS1D code, the reference state is,

$$L_\infty = l_{mfp,1}, \quad T_\infty = T_1, \quad \rho_\infty = \rho_1,$$

where $l_{mfp,1}$ is the upstream mean free path.

There are several important options in the code,

- **method_output**: the method to output the solution. If set to **ORIGINAL** , the original nondimensionalized values will be written to the result file. If set to **NORMALIZE** , the density will be normalized by $\rho = (\rho - \rho_1)/(\rho_2 - \rho_1)$ and the temperature is also normalized by the same way
- **mu_ref**: the reference viscosity coefficient μ_∞, which can be specified directly or calculated through the provided function **get_mu** . This function calculate the viscosity coefficient through,

$$\mu_\infty = \frac{5(\alpha+1)(\alpha+2)\sqrt{\pi}}{4\alpha(5-2\omega)(7-2\omega)}\mathrm{Kn}_\infty,$$

where α, ω are coefficients related to molecule model.

The default settings in the code is for Argon shock structure calculation at Ma = 8.0, see [2].

- Argon gas with Prandlt number Pr = 2.0/3.0 and variable hard-sphere model $\omega = 0.72$
- Mach number 8.0
- Newton-Cotes integration with 100 velocity points ranges from -15 to 15.
- Computation domain is 50 times of the upstream mean free path
- Cell size is half of the upstream mean free path
- Output solution at $t = 250$

Figure. 2.1 shows the comparison of the simulated density with the experimental measurements [9] and also temperature profile .

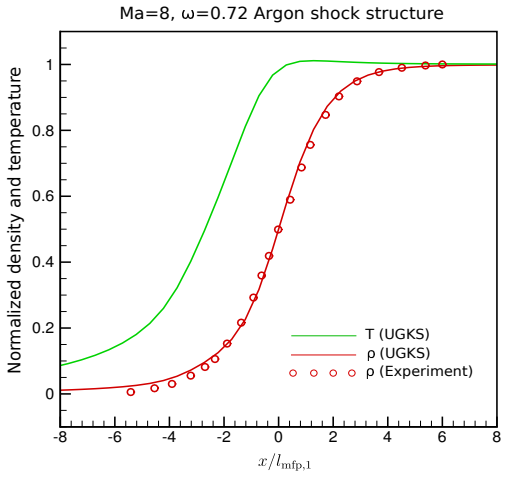


Figure 2.1: Argon shock structure at Ma = 8.0.

2.3 UGKS2D Code

2.3.1 Differences with 1D

For 2D problem, many expressions need to be slightly changed. For example,

$$g = \rho \left(\frac{\lambda}{\pi}\right)^{\frac{K+2}{2}} e^{-\lambda((u-U)^2+(v-V)^2+\xi^2)},$$

where v is particle velocity in y direction, V is macroscopic velocity in y direction.

The relation between K and γ becomes,

$$\gamma = \frac{K+4}{K+2}.$$

The reduced Maxwellian distribution becomes (B is not changed),

$$H = \int_{-\infty}^{\infty} g d\xi = \rho \left(\frac{\lambda}{\pi}\right) e^{-\lambda((u-U)^2+(v-V)^2)}.$$

The collision invariants are $\psi = (1, u, v, 1/2(u^2+v^2+\xi^2))^T$. And the expressions for macroscopic variables are correspondingly changed. For example, the nondimensionalized pressure is calculated via,

$$\frac{K+2}{2}p = \int ((u-U)^2 + (v-V)^2)hdu + \int bdu.$$

When calculating the flux, the slopes related to Maxwellian become,

$$a = a_1 + a_2 u + a_3 v + a_4 \frac{1}{2}(u^2 + v^2 + \xi^2),$$

and the components are calculated via,

$$\begin{aligned}
a_4 &= \frac{4\lambda_0^2}{(K+2)\rho_0}\left[2\frac{\partial \rho E}{\partial x} + \left(U_0^2 + V_0^2 - \frac{K+2}{2\lambda_0}\right)\frac{\partial \rho}{\partial x} - 2U_0\frac{\partial \rho U}{\partial x} - 2V_0\frac{\partial \rho V}{\partial x}\right], \\
a_3 &= \frac{2\lambda_0}{\rho_0}\left(\frac{\partial \rho V}{\partial x} - V_0\frac{\partial \rho}{\partial x}\right) - V_0 a_4, \\
a_2 &= \frac{2\lambda_0}{\rho_0}\left(\frac{\partial \rho U}{\partial x} - U_0\frac{\partial \rho}{\partial x}\right) - U_0 a_4, \\
a_1 &= \frac{1}{\rho_0}\frac{\partial \rho}{\partial x} - U_0 a_2 - V_0 a_3 - \frac{1}{2}\left(U_0^2 + V_0^2 + \frac{k+2}{2\lambda_0}\right)a_4.
\end{aligned}$$

2.3.2 Lid-driven cavity problem

The test case included in UGKS2D code is Lid-driven cavity problem[3]. The argon gas is enclosed by four walls to form a rectangular shape. The upper wall is moving in tangential direction with velocity U_W, other walls are stationary. All walls are kept at a constant temperature T_W, and full accommodation is assumed. The gas is initially at rest with the same temperature as the wall. Figure. 2.2 shows the schematic of the problem.

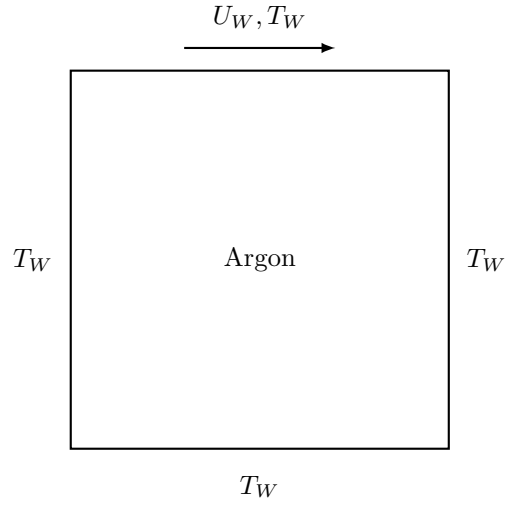


Figure 2.2: Schematic of Lid-driven cavity problem

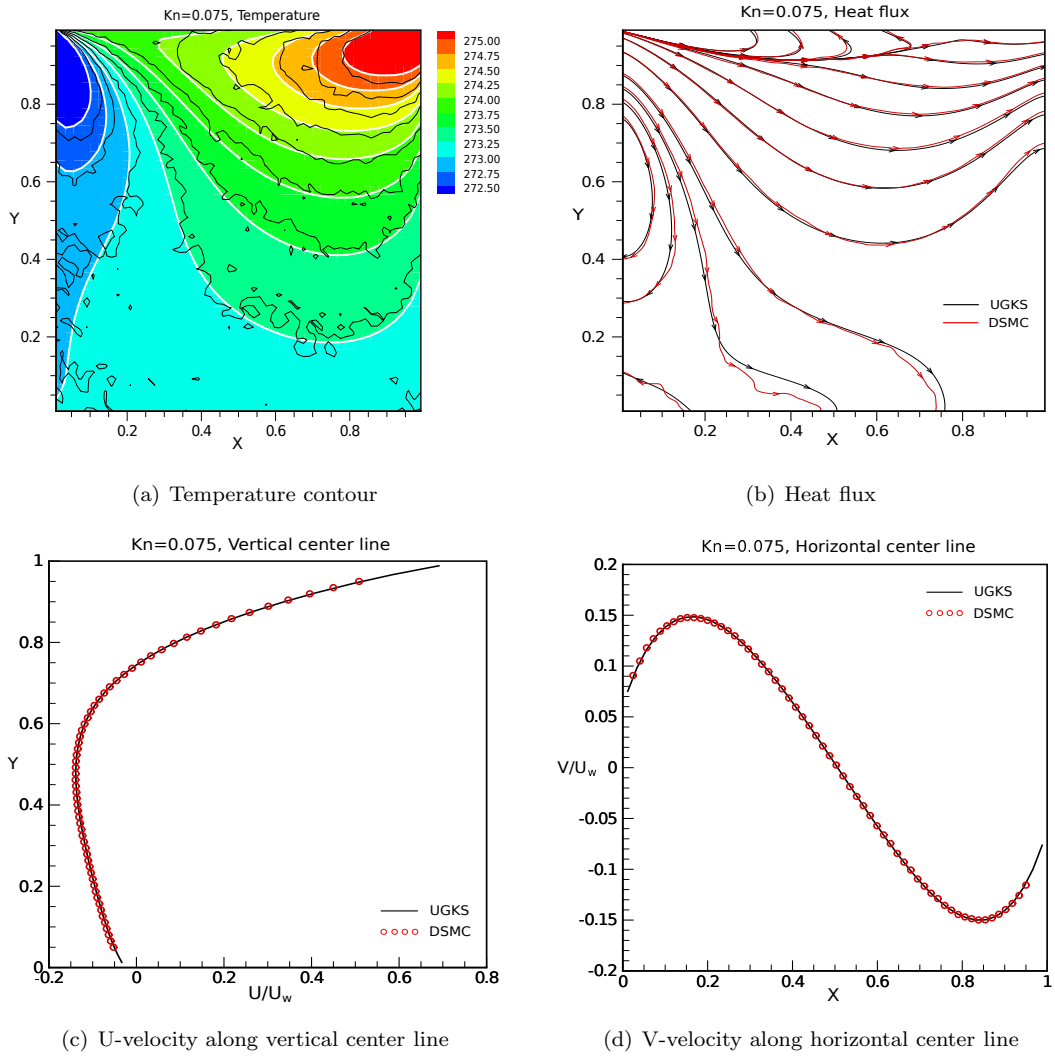
In the code, the default test case is for $T_W = 273K, U_W = 50m/s, \mathrm{Kn} = l_{mfp}/L = 0.075$, where l_{mfp} is mean free path and L is the domain length.

Choose the initial condition as reference state, the settings are

- Second order interpolation
- VHS model for collision time and HS model for reference state

- Prandtl number Pr = 2.0/3.0, Knudsen number $\mathrm{Kn}_\infty = 0.075$ (at reference state)
- $T_W = 1, U_W = 0.15$
- $L = 1$ with 45x45 grids
- Gaussian quadrature with 28x28 velocity points

Figure. 2.3 shows the result for the above setup, and compared with the DSMC solution[10].



(a) Temperature contour

(b) Heat flux

(c) U-velocity along vertical center line

(d) V-velocity along horizontal center line

Figure 2.3: Cavity flow at Kn = 0.075. In the temperature contour, the black lines are from DSMC, the white lines and background contour are from UGKS

2.3.3 Other information

The Gaussian quadrature used in the code is from Table IIa of [11], which is better than Gaussian-Hermite quadrature in high Knudsen number case. But for the cavity problem with Kn >= 1, Newton-Cotes formula of 61x61 velocity grids with velocity range $u, v = -4 - 4$ can avoid oscillating in the solution, which happens using Gaussian quadrature and second order interpolation. For example, the setting for Newton-Cotes integration

```
subroutine init()
!variable declarations...
```

```
real(kind=RKD) :: umin,vmin !declare smallest discrete velocity

umin = -4.0
vmin = -4.0
!largest discrete velocity. Global variables
umax = 4.0
vmax = 4.0
!number of velocity points. Global variables
unum = 61
vnum = 61

call init_velocity_newton(unum,umin,umax,vnum,vmin,vmax) !set the velocity space
!other commands...
end subroutine init
```

On Intel® Core™ Quad Processor Q9450 (12M Cache, 2.66 GHz, 1333 MHz FSB) with openmp enabled, the computation time of the above setup is about 16 minutes (with openmp). With 65x65 physical space, the computation time is about 35 minutes.

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Appendix A: Moments of Maxwellian distribution function

In the program, the moments of Maxwellian distribution function is frequently used, and they are usually obtained from subroutines.

The moments of Maxwellian distribution function is defined as,

$$\rho < ... >= \int (...) g d\Xi,$$

and have the property that,

$$< u^n \xi^m >=< u^n >< \xi^m >,$$

where m, n are integers.

Moments of ξ^m

$$< \xi^2 >= \left(\frac{K}{2\lambda}\right), \quad < \xi^4 >= \left(\frac{3K}{4\lambda^2} + \frac{K(K-1)}{4\lambda^2}\right).$$

Moments of u^n

The integration limits of $< u^n >$ is from $-\infty$ to ∞,

$$\begin{aligned} < u^0 > &= 1, \\ < u^1 > &= U, \\ < u^{n+2} > &= U < u^{n+1} > + \frac{n+1}{2\lambda} < u^n > . \end{aligned}$$

The integration limits of $< u^n >_{>0}$ is from 0 to ∞,

$$\begin{aligned} < u^0 >_{>0} &= \frac{1}{2}\mathrm{erfc}(-\sqrt{\lambda}U), \\ < u^1 >_{>0} &= U < u^0 >_{>0} + \frac{1}{2}\frac{e^{-\lambda U^2}}{\sqrt{\pi\lambda}}, \\ < u^{n+2} >_{>0} &= U < u^{n+1} >_{>0} + \frac{n+1}{2\lambda} < u^n >_{>0} . \end{aligned}$$

The integration limits of $< u^n >_{<0}$ is from $-\infty$ to 0,

$$\begin{aligned} < u^0 >_{<0} &= \frac{1}{2}\mathrm{erfc}(\sqrt{\lambda}U), \\ < u^1 >_{<0} &= U < u^0 >_{<0} - \frac{1}{2}\frac{e^{-\lambda U^2}}{\sqrt{\pi\lambda}}, \\ < u^{n+2} >_{<0} &= U < u^{n+1} >_{<0} + \frac{n+1}{2\lambda} < u^n >_{<0} . \end{aligned}$$

Moments of $< u^n \xi^m \psi >$

There are three components for 1D problem,

$$< u^n \xi^m \psi >= \begin{pmatrix} < u^n >< \xi^m > \\ < u^{n+1} >< \xi^m > \\ \frac{1}{2}\left(< u^{n+2} >< \xi^m > + < u^n >< \xi^{m+2} >\right) \end{pmatrix}.$$

Moments of $< a u^n \psi >$

There are three components for 1D problem,

$$< a u^n \psi >= a_1 < u^n \psi > + a_2 < u^{n+1} \psi > + \frac{1}{2} a_3 \left(< u^{n+2} \psi > + < u^n \xi^2 \psi >\right).$$

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