User Manual for UGKS1D and UGKS2D Code

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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], and can be extended to a truly multi-dimensional 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

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

where g is the Maxwellian distribution, Pr is the Prandtl number, $\mathbf{c}$ is the random velocity, 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 capability 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 E 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 ∞. Then the moments of the non-equilibrium distribution function are calculated through numerical integration(the moments of equilibrium distribution are still calculated from analytical integration). The discretization of the velocity space is determined by the chosen numerical integration method.

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

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

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 $t = t^n$ and $t = t^{n+1}$ 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 flux of the distribution function across the cell interface integrated over the whole time step, $f_{i,k}^{+(n)}$ 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 variables becomes

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

where $\mathbf{W} = \int \psi \mathbf{F} d\Xi$

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

The flux $\mathbf{F}$ is calculated by 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 can be obtained by updating the conservative variables first using Eq. 1.12.

In order to remove the dependence of distribution functions on the internal degree of freedom ξ, the reduced distribution function [6] 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 distribution

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

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 reduced g^+ becomes

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

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

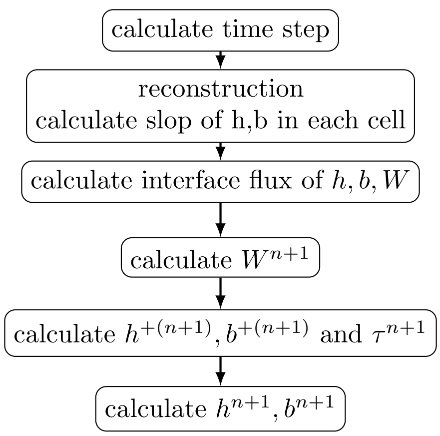

Figure 1.1: solution algorithm in one iteration

1.3 Nondimensionalization

In the program, the following nondimensionalization is used,

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

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

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

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

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

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

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

Other expressions are not changed.

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 can also be replace by $\max(U, u)$

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 Calculation of interface flux

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

1.5.1 The algorithm

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,

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

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 two terms related to the initial non-equilibrium distribution

g_0 or W_0 can be obtained by applying the capability condition at $x=0, t=0$

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

which gives

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

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

$$\frac{1}{\rho_0}\left(\frac{\partial W}{\partial x}\right)^L = \int a^Lg_0\psi d\Xi, \quad \frac{1}{\rho_0}\left(\frac{\partial W}{\partial x}\right)^R = \int a^Rg_0\psi d\Xi \tag{1.27}$$

$$\frac{1}{\rho_0}\frac{\partial W}{\partial t} = \int Ag_0\psi d\Xi \tag{1.28}$$

The time derivative of W can be calculated via the capability condition

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

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

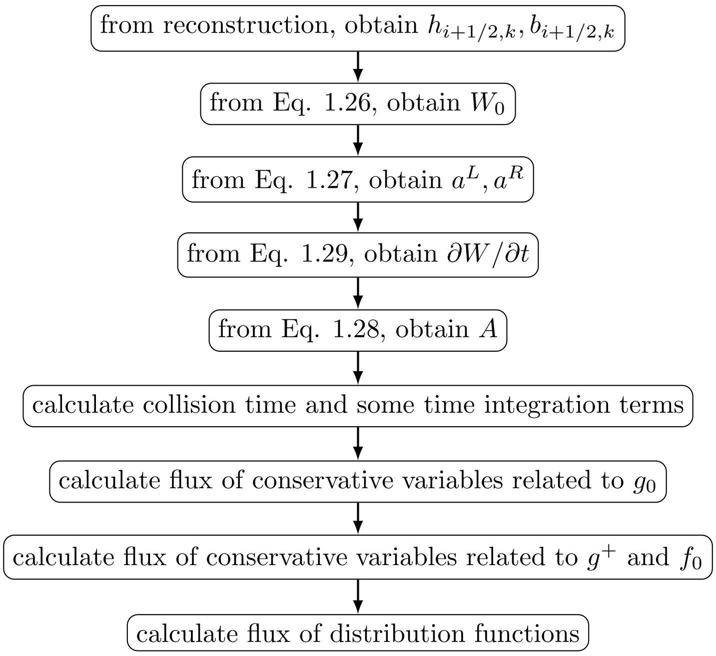

Figure 1.2: interface flux calculation

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.

Instead, 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

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

and

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

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 only holds for equilibrium state)

$$\rho_0 = \rho_0, \quad U_0 = \frac{\rho_0 U_0}{\rho_0}, \quad \lambda_0 = \frac{(K+1)\rho_0}{4\left(\rho_0 E_0 - \frac{1}{2}\rho(U_0^2 + V_0^2)\right)}$$

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 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

$$\tau = \frac{2\lambda_0^{1-\omega}}{\rho_0}\mu_{ref}\lambda_{ref}^{\omega}$$

where $\lambda_{ref} = 1/T_{ref}$

Some time integrals used in the evaluation of flux is 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.

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

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

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

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

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

The flux of conservative variables related to f_0 is,

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

The flux of conservative variables is

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

Calculate the flux of distribution functions

The flux of reduced distribution function h is calculated by

$$
\begin{aligned}
\mathbf{F}^h_{i+1/2,k} &= \int_{t^n}^{t^{n+1}} \int f_{i+1/2,k} u_k d\xi dt \\
&= M t_1 u_k (H_k + H_k^+) \\
&+ M t_2 u_k^2 \left(a_1^L H_k + a_2^L u_k H_k + \frac{1}{2} a_3^L (u_k^2 H_k + B_k) \right) H[u_k] \\
&+ M t_2 u_k^2 \left(a_1^R H_k + a_2^R u_k H_k + \frac{1}{2} a_3^R (u_k^2 H_k + B_k) \right) (1 - H[u_k]) \\
&+ M t_3 u_k \left(A_1 H_k + A_2 u_k H_k + \frac{1}{2} A_3 (u_k^2 H_k + B_k) \right) \\
&+ M t_4 u_k h_{i+1/2,k} - M t_5 u_k^2 \sigma^h_{i+1/2,k}
\end{aligned}
$$

The flux of reduced distribution function b is calculated by

$$
\begin{aligned}
\mathbf{F}^h_{i+1/2,k} &= \int_{t^n}^{t^{n+1}} \int f_{i+1/2,k} u_k d\xi dt \\
&= M t_1 u_k (B_k + B_k^+) \\
&+ M t_2 u_k^2 \left(a_1^L B_k + a_2^L u_k B_k + \frac{1}{2} a_3^L (u_k^2 B_k + < \xi^4 > H_k) \right) H[u_k] \\
&+ M t_2 u_k^2 \left(a_1^R B_k + a_2^R u_k B_k + \frac{1}{2} a_3^R (u_k^2 B_k + < \xi^4 > H_k) \right) (1 - H[u_k]) \\
&+ M t_3 u_k \left(A_1 B_k + A_2 u_k B_k + \frac{1}{2} A_3 (u_k^2 B_k + < \xi^4 > H_k) \right) \\
&+ M t_4 u_k b_{i+1/2,k} - M t_5 u_k^2 \sigma^b_{i+1/2,k}
\end{aligned}
$$

1.6 Update cell averaged value

The procedure is shown in Figure. 1.3

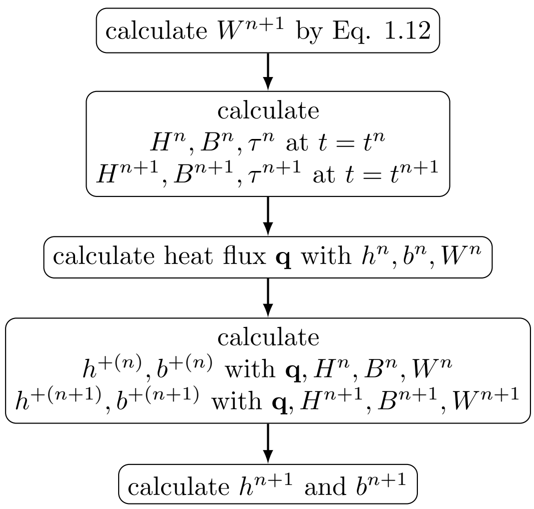

Figure 1.3: update cell averaged value

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

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

1.7 Boundary condition

Only isothermal wall boundary condition with complete accommodation is discussed. Assuming left wall($x = 1/2$)

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.

Finally, the flux across the wall is calculated by

$$\mathbf{W}_{1/2} = H[u_k] \begin{pmatrix} \sum \alpha_k u_k H_k^w \\ \sum \alpha_k u_k^2 H_k^w \\ \sum \alpha_k \frac{1}{2} \left(u_k^3 H_k^w + u_k B_k^w \right) \end{pmatrix} + (1 - H[u_k]) \begin{pmatrix} \sum \alpha_k u_k h_k^{in} \\ \sum \alpha_k u_k^2 h_k^{in} \\ \sum \alpha_k \frac{1}{2} \left(u_k^3 h_k^{in} + u_k b_k^{in} \right) \end{pmatrix}$$

and

$$\mathbf{F}_{1/2,k}^{h} = (u_k H_k^w) H[u_k] + (u_k h_k^{in})(1 - H[u_k])$$
$$\mathbf{F}_{1/2,k}^{b} = (u_k B_k^w) H[u_k] + (u_k b_k^{in})(1 - H[u_k])$$

Chapter 2

UGKS1D Code

This chapter describes the structure and the included shock structure test case at Ma=8.0 in the UGKS1D code.

Chapter 3

UGKS2D Code

This chapter describes the structure and the included lid-driven cavity test case in the UGKS2D code.

3.1 test

test

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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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