

User Manual for UGKS1D and UGKS2D Code

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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 dimension case,

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = \frac{f^+ - f}{\tau} \quad (1.1)$$

where f is the distribution function, u is partical velocity, τ is particle collision time and f^+ is the modified equilibrium distribution function.

The collision time is given by $\tau = \mu/p$, where μ is the dynamic viscosity and p is the pressure

The modified equilibrium distribution is

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

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

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

where ρ is density, $\lambda = m/2kT$, m is molecule mass, k is Boltzmann constant, K is the number of internal degree of freedom and $\xi^2 = \xi_1^2 + \xi_2^2 \dots + \xi_K^2$. 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 collision invariants are $\psi = (1, u, 1/2(u^2 + \xi^2))^T$, and the macroscopic variables can be calculated via

$$w = \begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \psi f d\Xi \quad (1.4)$$

$$p = \frac{1}{3} \int [(u - U)^2 + \xi^2] f d\Xi \quad (1.5)$$

$$q = \frac{1}{2} \int (u - U)[(u - U)^2 + \xi^2] f d\xi \quad (1.6)$$

where U is the macroscopic velocity, E is total energy and $d\xi = du d\xi$

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

$$f(x, t, u, \xi) = \frac{1}{\tau} \int_{t^n}^t f^+(x', t', u, \xi) e^{-(t-t')/\tau} dt' + e^{-(t-t^n)/\tau} f_0^n(x - u(t - t^n), t^n, u, \xi) \quad (1.7)$$

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 distribution function are calculated through numerical 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,

$$f_{i,k}^{n+1} = f_{i,k}^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} (\mathbf{F}_{i-1/2} - \mathbf{F}_{i+1/2}) dt + \frac{\Delta t}{2} \left(\frac{f_{i,k}^{+(n+1)} - f_{i,k}^{n+1}}{\tau^{n+1}} + \frac{f_{i,k}^{+(n)} - f_{i,k}^n}{\tau^n} \right) \quad (1.8)$$

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, $f_{i,k}^{+(n)}$ 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. 1.8 and make integration over the velocity space, the evolution of conservative variables becomes

$$w_i^{n+1} = w_i^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int \psi (\mathbf{F}_{i-1/2} - \mathbf{F}_{i+1/2}) d\xi dt \quad (1.9)$$

In order to update the distribution function in Eq. 1.8, 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. 1.7 at the cell interface. Since $f^{+(n+1)}$ and τ^{n+1} have one-to-one correspondance to the macroscopic variables, they can be obtained by updating the conservative variables first using Eq. 1.9.

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

$$h = \int_{-\infty}^{\infty} f d\xi, \quad b = \int_{-\infty}^{\infty} \xi^2 f d\xi \quad (1.10)$$

and the reduced modified equilibrium distribution

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

where the corresponding reduced Maxwellian distribution g becomes

$$H = \int_{-\infty}^{\infty} g d\xi = \rho \left(\frac{\lambda}{\pi} \right)^{1/2} e^{-\lambda(u-U)^2}, \quad B = \int_{-\infty}^{\infty} \xi^2 g d\xi = \frac{k}{2\lambda} H \quad (1.11)$$

and the corresponding reduced g^+ becomes

$$\begin{aligned} H^+ &= \int_{-\infty}^{\infty} g^+ d\xi = \frac{4(1-\text{Pr})\lambda^2}{5\rho} (u-U)q(2\lambda(u-U)^2 + k-5)H \\ B^+ &= \int_{-\infty}^{\infty} \xi^2 g^+ d\xi = \frac{4(1-\text{Pr})\lambda^2}{5\rho} (u-U)q(2\lambda(u-U)^2 + k-3)B \end{aligned} \quad (1.12)$$

Then the update of f using Eq. 1.8 becomes two similar equations for the update of h and b , respectively

The overview flow chart of the solution algorithm in one iteration is as follows

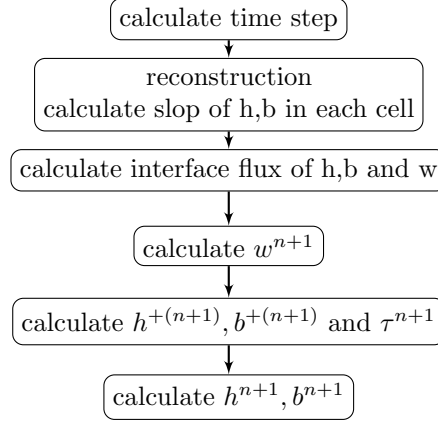


Figure 1.1: solution algorithm in one iteration

1.3 Nondimensionalization

In the program, the following nondimensionalization is used,

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

The free stream variables are related through

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

In the following, all variables are nondimensioned, but we will drop the $\hat{\cdot}$ for simplicity. After nondimensionalization and using the reduced distribution function, the expressions for macroscopic variables become

$$\begin{aligned} \rho &= \int h du = \sum \alpha_k h_k \\ \rho U &= \int h u du = \sum \alpha_k h_k u_k \end{aligned} \quad (1.13)$$

$$\rho E = \frac{1}{2} \left(\int h u^2 du + \int b du \right) = \frac{1}{2} \left(\sum \alpha_k h_k u_k^2 + \sum \alpha_k b_k \right)$$

$$\frac{k+1}{2} p = \int (u-U)^2 h du + \int b du = \sum \alpha_k (u_k - U)^2 h_k + \sum \alpha_k b_k \quad (1.14)$$

$$\begin{aligned}
q &= \frac{1}{2} \left[\int (u - U)(u - U)^2 h du + \int (u - U) b du \right] \\
&= \frac{1}{2} \left[\sum \alpha_k (u_k - U)(u_k - U)^2 h_k + \sum \alpha_k (u_k - U) b_k \right]
\end{aligned} \tag{1.15}$$

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

$$p = \frac{1}{2} \rho T, \quad \lambda = \frac{1}{T} \tag{1.16}$$

Other expressions are not changed.

1.4 Time step and reconstruction

The time step is determined by the CFL condition

$$\Delta t = \text{CFL} \frac{\Delta x}{|U| + c} \tag{1.17}$$

where CFL is the CFL number, c is the speed of sound. The macroscopic velocity U can also be replaced 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

$$\sigma_{i,k}^h = (\text{sign}(s_1) + \text{sign}(s_2)) \frac{|s_1||s_2|}{|s_1| + |s_2|} \tag{1.18}$$

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. 1.7, the integral solution at the cell interface is

$$f(0, t, u_k, \xi) = \frac{1}{\tau} \int_0^t f^+(x', t', u_k, \xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_0(-u_k t, 0, u_k, \xi) \tag{1.19}$$

The initial distribution function f_0 is

$$f_0(-u_k t, 0, u_k, \xi) = \begin{cases} f_{i+1/2,k}^L - \sigma_{i,k} u_k t, & u_k \geq 0 \\ f_{i+1/2,k}^R - \sigma_{i+1,k} u_k t, & u_k < 0 \end{cases} \tag{1.20}$$

where $f_{i+1/2,k}^L, f_{i+1/2,k}^R$ are obtained through the reconstruction

The Maxwellian distribution in f^+ is approximated by

$$g(x, t, u, \xi) = g_0 [1 + (1 - H[x]) a^L x + H[x] a^R x + At] \tag{1.21}$$

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

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

1.5.2 The numerical procedure

1.6 Update cell averaged value

1.7 Boundary condition

Chapter 2

Usage

This chapter describes how to compile the source code and documentation. Currently, it's only tested under Linux.

2.1 Compile under *nix

2.2 Compile under windows

Chapter 3

UGKS1D Code

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

Chapter 4

UGKS2D Code

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

4.1 test

test

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