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 truely multi-dimensional formulation, see[4].

1.1 Model equation

The model equation is the BGK-Shakhov model. In one dimensioanl 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 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

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

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, 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 collision invariants are $\psi = (1, u, 1/2(u^2 + \xi^2))^T$, and the macroscopic variables can be calculated via

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

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

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

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

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

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

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 algrithm

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

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

where f_i^n and f_i^{n+1} are cell averaged distribution function of the i-th cell 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 interface, $f^{+(n)}$ and $f^{+(n+1)}$ are modified equilibrium distribution, τ^n and τ^{n+1} are particle collision time.

Multiplying the collision invarients to Eq. 1.8 and make integration over the velocity space, the evolution of conservative variables becomes

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

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

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

And the corresponding reduced Maxwellian distribution g becomes

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

The corresponding reduced g^+ becomes

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

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

1.3 Nondimensionalization

1.4 Time step and reconstruction

1.5 Calculation of interface flux

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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