Assignment - Part II

Ph.D. Course 2012:
Nodal DG-FEM for solving partial differential equations

This the second part of the mandatory part of the course and completion of it is required to pass the course with full credit.

This part should, in combination with the results for Assignment part I, form a report which must be submitted electronically no later than

Friday, August 31, 2012

Mathematical model

We shall consider the BGK approximation of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = -\frac{1}{\tau}\left(f - f^{eq}(\rho, \mathbf{u})\right), \quad (x, y) \in \Omega \tag{1}$$

which describes statistical behavior of fluid motion at the microscopic level under the assumption that the fluid is a gas statistically described in terms of a particle distribution function $f(t, \boldsymbol{\xi}, \mathbf{x})$. $\boldsymbol{\xi} = (\xi_x, \xi_y)$ is the microscopic velocity, $\mathbf{x} = (x, y)$ is the spatial Cartesian coordinates and τ the relaxation time.

Flow properties

The solution for a fluid in uniform state is given by the local equilibrium distribution function in 2D

$$f^{eq} = \frac{\rho}{2\pi RT} \exp\left(-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2RT}\right) \tag{2}$$

where R is the gas constant and T is the temperature. This function is dependent on the macroscopic flow properties characterized by density ρ and flow velocity $\mathbf{u} = (u, v)$ expressed in terms of horizontal and vertical components.

The macroscopic flow properties can be derived from the particle distribution. For example density and momentum as

$$\rho = \int_{-\infty}^{\infty} f d\boldsymbol{\xi}, \quad \rho u = \int_{-\infty}^{\infty} \xi_x f d\boldsymbol{\xi}, \quad \rho v = \int_{-\infty}^{\infty} \xi_y f d\boldsymbol{\xi} \tag{3}$$

In the following, we will follow the suggested procedure described by Tölke, Kraftczyk, Schulz & Rank (2000) for deriving a set of governing equations that can be used to solve Boltzman equation approximately by a Galerkin formulation.

By assuming absolute equilibrium and setting $\mathbf{u} = 0$, the particle distribution function can be approximated $\hat{f} \sim f$ by introducing a Hermite expansion of the form

$$\hat{f} = \frac{1}{2\pi RT} \exp\left(-\frac{\tilde{\xi}_x^2 + \tilde{\xi}_y^2}{2}\right) \sum_{k=1}^{\infty} a_k(t, \mathbf{x}) \varphi(\tilde{\xi}_x, \tilde{\xi}_y) \tag{4}$$

where scaled velocity components have been introduced $\tilde{\boldsymbol{\xi}} = (\tilde{\xi}_x, \tilde{\xi}_y) = (\xi_x, \xi_y)/\sqrt{RT}$ and with the first six trial functions defined in terms of orthogonal Hermite polynomials as

$$\begin{aligned}
\varphi_1(x,y) &= H_1(x)H_1(y), \quad & \varphi_2(x,y) &= H_2(x)H_1(y) \\
\varphi_3(x,y) &= H_1(x)H_2(y), \quad & \varphi_4(x,y) &= H_2(x)H_2(y) \\
\varphi_5(x,y) &= H_3(x)H_1(y), \quad & \varphi_6(x,y) &= H_1(x)H_3(y)
\end{aligned}$$

Approximations to the macroscopic flow properties can be expressed in terms of the Hermite coefficients. For example

$$\begin{aligned}
\rho &= \int_{-\infty}^{\infty} \hat{f} d\boldsymbol{\xi} = a_1 \\
\rho u &= \int_{-\infty}^{\infty} \xi_x \hat{f} d\boldsymbol{\xi} = a_2\sqrt{RT} \\
\rho v &= \int_{-\infty}^{\infty} \xi_y \hat{f} d\boldsymbol{\xi} = a_3\sqrt{RT} \\
\sigma_{11} &= \int_{-\infty}^{\infty} (\xi_x - u)^2 \hat{f} d\boldsymbol{\xi} + RT\rho = -RT\left(\sqrt{2}a_5 - \frac{a_2^2}{a_1}\right) \\
\sigma_{22} &= \int_{-\infty}^{\infty} (\xi_y - v)^2 \hat{f} d\boldsymbol{\xi} + RT\rho = -RT\left(\sqrt{2}a_6 - \frac{a_3^2}{a_1}\right) \\
\sigma_{12} &= \int_{-\infty}^{\infty} (\xi_x - u)(\xi_y - v) \hat{f} d\boldsymbol{\xi} = -RT\left(a_4 - \frac{a_2 a_3}{a_1}\right)
\end{aligned}$$

which enables direct conversion between series coefficients and macroscopic properties.

The kinematic viscosity $\nu = RT\tau$ can be used to define the Reynolds Number $Re = UL/\nu$ and $RT = 1$ can be assumed, such that L is a characteristic length. Assume $L = 1$ in the tests defined below.

Governing equations

A set of governing equation can be obtained by a Galerkin procedure where residual equation arising when a truncated Hermite expansion with only

6 terms retained is substituted for f in the Boltzman equation and the resulting residual equations R_h are required to be orthogonal with respect to the test functions

$$\int_{-\infty}^{\infty} \varphi_k R_h d\boldsymbol{\xi} = 0, \quad k = 1, ..., 6 \tag{5}$$

This procedure generates a set of governing equations that can be expressed as a coupled set of partial differential equations

$$\frac{\partial a_1}{\partial t} + \sqrt{RT}\left(\frac{\partial a_2}{\partial x} + \frac{\partial a_3}{\partial y}\right) = 0 \tag{6}$$

$$\frac{\partial a_2}{\partial t} + \sqrt{RT}\left(\frac{\partial a_1}{\partial x} + \sqrt{2}\frac{\partial a_5}{\partial x} + \frac{\partial a_4}{\partial y}\right) = 0 \tag{7}$$

$$\frac{\partial a_3}{\partial t} + \sqrt{RT}\left(\frac{\partial a_4}{\partial x} + \frac{\partial a_1}{\partial y} + \sqrt{2}\frac{\partial a_6}{\partial y}\right) = 0 \tag{8}$$

$$\frac{\partial a_4}{\partial t} + \sqrt{RT}\left(\frac{\partial a_3}{\partial x} + \frac{\partial a_2}{\partial y}\right) = \frac{1}{\tau}\left(a_4 - \frac{a_2 a_3}{a_1}\right) \tag{9}$$

$$\frac{\partial a_5}{\partial t} + \sqrt{2RT}\left(\frac{\partial a_2}{\partial x}\right) = -\frac{1}{\tau}\left(a_5 - \frac{a_2^2}{\sqrt{2}a_1}\right) \tag{10}$$

$$\frac{\partial a_6}{\partial t} + \sqrt{2RT}\left(\frac{\partial a_3}{\partial y}\right) = -\frac{1}{\tau}\left(a_6 - \frac{a_3^2}{\sqrt{2}a_1}\right) \tag{11}$$

By closely examining this system it should be clear that it is linear in all spatial differential operations. The system can be expressed in the general compact form as a conservation law

$$\frac{\partial \mathbf{a}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{c} \tag{12}$$

where the gradient operator is two-dimensional $\nabla = (\partial/\partial x, \partial/\partial y)$, the vector function $\mathbf{F} = (\mathbf{A}, \mathbf{B})\mathbf{a}$ where $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{6\times 6}$, $\mathbf{a}, \mathbf{c} \in \mathbb{R}^6$ and the source vector $\mathbf{c} = \mathbf{c}(\mathbf{a})$ defined in terms of nonlinear contributions from Hermite coefficients appearing on the right hand side of the equations. This forms the basis for numerical discretization in the time-space domain.

Numerical discretization

1. Formulate a two-dimensional DG-FEM formulation to be used as a basis for solving the Boltzman equation approximately.
2. Give expressions for $\mathbf{A}, \mathbf{B}$ and $\mathbf{c}$.
3. Describe how the Lax-Friedrich flux would look like.
4. Detail how you choose the numerical fluxes. Describe how the Lax-Friedrich flux would look like and derive a proper upwinding scheme for the DGFEM formulation.

5. Implement a discrete two-dimensional DG-FEM solver based on the formulated nodal DG-FEM scheme.

6. Discuss how you decide on the time-step.

7. To test the implemented solver you can setup the test case for steady Poiseuille flow described. Tölke, Kraftczyk, Schulz & Rank (2000) presented numerical experiments for Poiseuille flow which should be reproduced as a first test case using your solver. Confirm that the solver is stable and make sure the solution is converged.

8. Plot a couple of snap-shots of the computed solution

Now that we have implemented and tested the code, you should be ready to use it for more complex problems.

CASE 1: Rectangular Driven cavity

Consider a driven cavity defined on $(x, y) \in \Omega([0, 1]^2)$ with a lid at $y = 1$ (north boundary) suddenly driven at a velocity $U = 1$ for time $t \geq 0$.

Assume no-slip boundary conditions at west, east and south boundaries

$$u = v = 0$$

At the north boundary a lid is driven with velocity $U = 1$ in the horizontal direction. For computational purposes it may be necessary to smooth the velocity profile smoothly from 0 to 1 near the corners of the cavity.

As initial conditions you can take all variables to zero except for the density, $\rho = 1$. Since these initial conditions lead to a discontinuity at the upper boundary, you should consider how to start up the problem without causing too many problems, e.g., one could ramp up the lid-speed in time, you could use a heavy filter initially and then remove it or some other approach to avoid problems.

Results of numerical experiments can be used for comparison with computed results are presented in Ghia et al. (1984). See Table I for the u-velocity and Table II for the v-velocity profiles found for the steady state solution for different Reynolds numbers. Consider Reynolds numbers Re corresponding to 100 and 400. See if you can reproduce the velocity profiles for the vertical and horizontal cuts through the geometric center of the cavity as a test of code.

1. Generate different grids to enable a convergence study and test that the computed solution(s) converge toward a grid-independent solution.

2. Run the code for different values of the Re and discuss your observations.

3. Plot a couple of snap-shots of the computed solution - you can plot velocities, vorticities, streamlines or something else. The references have plots you can compare with.

CASE 2: Triangular Driven cavity

Consider a driven cavity defined on isosceles triangular domain. Consult the reference by Erturk & Gokcol (2007) and the example presented in Fig 6 in that reference.

Reproduce the results for Reynolds numbers 12.5, 25, and 100.

1. Generate different grids to enable a convergence study and test that the computed solution(s) converge toward a grid-independent solution.
2. Run the code for different values of the Re and discuss your observations.
3. Plot a couple of snap-shots of the computed solution - you can plot velocities, vorticities, streamlines or something else. The references have plots you can compare with.

CASE 3: Driven cavity with internal structure (OPTIONAL)

If time permits, decide on your own experiment with the solver. For example, try to produce a snapshot of a driven cavity flow with an internal structure positioned inside the cavity, e.g. a square or circular wall.

Enjoy !