Числен анализ на газови микротечения (Numerical analysis of gas microflows)

Кирил Щерев
Направление „Математическо моделиране и числени симулации”
Общоинститутски семинар
20.06.2018г., София
Outline

- Applications of rarefied gas dynamics
- Consider a flow past square problem to illustrate issues in methods and codes
- Considerations about convective terms approximation
- Some recent Direct Simulation Monte Carlo (DSMC) results
Applications of rarefied gas dynamics
Типични микроустройства (MEMS) и приложения на нанотехнологии съответстващи на число на Кнудсен, при стандартни атмосферни условия, и свързания с това режим (континуален, с приплъзване, преходен и свободно молекулен режим), M. Gad-el-Hak 2006.
Rarefied Gas Dynamics at upper layers of atmosphere

Rarefied Gas Dynamics at upper layers of atmosphere

Consider a flow past square problem to illustrate issues in methods and codes
Flow past square in a microchannel
The transition (neutral) curve

The transition (neutral) curve obtained for unconfined flow past a square and flow past square confined in a microchannel for $B = 20, 10, 5$ and $3$ and subsonic regimes.
The transition (neutral) curve for narrow channel $B=3$
At lower Knudsen, $Kn=0.0001$, $M=2.43$ (higher Reynolds numbers) TVD scheme obtains unphysical oscillations.

Horizontal velocity along the center line, narrow channel ($B=3$), $M=2.43$, $Kn=0.0001$.
At lower Knudsen, $Kn=0.0001$, $M=2.43$ (higher Reynolds numbers) upwind first order scheme obtains physical realistic results but needs a lot of resources to obtain correct result.

Horizontal velocity along the center line, narrow channel ($B=3$), $M=2.43$, $Kn=0.0001$.

Continuum model
Where is the problem?

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} &= 0 \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho uu)}{\partial x} + \frac{\partial (\rho vu)}{\partial y} &= \rho g_x - A \frac{\partial p}{\partial x} + B \left[ \frac{\partial}{\partial x} \left( \Gamma \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial u}{\partial y} \right) \right] + B \left[ \frac{\partial}{\partial x} \left( \Gamma \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial v}{\partial y} \right) - \frac{2}{3} \frac{\partial}{\partial x} \left( \Gamma \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] \\
\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho uv)}{\partial x} + \frac{\partial (\rho vv)}{\partial y} &= \rho g_y - A \frac{\partial p}{\partial y} + B \left[ \frac{\partial}{\partial x} \left( \Gamma \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma \frac{\partial v}{\partial y} \right) \right] + B \left[ \frac{\partial}{\partial y} \left( \Gamma \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial x} \left( \Gamma \frac{\partial u}{\partial x} \right) - \frac{2}{3} \frac{\partial}{\partial y} \left( \Gamma \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] \\
\frac{\partial (\rho T)}{\partial t} + \frac{\partial (\rho uT)}{\partial x} + \frac{\partial (\rho vT)}{\partial y} &= C^{T1} \left[ \frac{\partial}{\partial x} \left( \Gamma^2 \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma^2 \frac{\partial T}{\partial y} \right) \right] + C^{T2} \Gamma \Phi + C^{T3} \frac{Dp}{Dt}
\end{align*}
\]

\[p = \rho T\]

where:

\[\Phi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2 - \frac{2}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2\]

Газът е описан използвайки континуален модел изграден на базата на уравненията на Навие-Стокс-Фурие за свиваем, вискозен газ от твърди сфери с дифузионни коефициенти, определени в първо приближение по теорията на Чепмен-Енског за малки числа на Кнудсен, виж. Стефанов, Русинов и Черчиняни 2002.
Considerations about convective terms approximation
Typical advection flow example is oil in water

Oil follows river’s streamlines without mixing with neighbor streamline.

When velocity is zero, the oil stays still and doesn’t mix with water - no diffusion.

Kiril Shterev
The steady convection-diffusion equation for a general property $\phi$

$$
\rho \frac{\partial (u\phi)}{\partial x} + \rho \frac{\partial (v\phi)}{\partial y} = \Gamma \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right),
$$

where $u$ and $v$ are velocities along x- and y-axis, $\Gamma$ is diffusion coefficient.
Diffusion and convective terms

\[ \rho \frac{\partial (u\phi)}{\partial x} + \rho \frac{\partial (v\phi)}{\partial y} = \Gamma \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) \]

Schematic propagation information area for diffusion dominated problem (a) and convection dominated problem (b).

The information about \( \phi \) is not available outside the cone.
Transport of fluid particle through a streamtube

\[ \rho \frac{\partial (u\phi)}{\partial x} + \rho \frac{\partial (v\phi)}{\partial y} \]

A fluid particle propagation through a streamtube.
Information propagation in mesh

Propagation information cone of convection dominated problem at mesh nodes.
Information propagation that reaches nodes \((i,j)\)

Reverse propagation information cone in node \((i,j)\) keeps nodes that information reach it.
Shape function

Shape function that corresponds to convective terms.

\[ f^{\text{shape}}(x, y) = c_0 + c_1 x + c_2 y \]
Numerical equation

Advection equation (pure convection) can be derived from convection-diffusion equation when $\Gamma = 0$:

$$\rho \frac{\partial (u\phi)}{\partial x} + \rho \frac{\partial (v\phi)}{\partial y} = 0$$

Integration over control volume (consider $\rho = \text{const}$):

$$\int_{CV} \rho \frac{\partial (u\phi)}{\partial x} + \rho \frac{\partial (v\phi)}{\partial y} dV \approx \rho u^{\text{average}} \int_{CV} \frac{\partial (f_{\text{shape}}(x, y))}{\partial x} dV + \rho v^{\text{average}} \int_{CV} \frac{\partial (f_{\text{shape}}(x, y))}{\partial y} dV$$

$$= \rho u^{\text{average}} c_1 V + \rho v^{\text{average}} c_2 V$$

After simplification numerical equation becomes:

$$\phi_0 = (a_1 \phi_1 + a_1 \phi_2) / a_0,$$

where

$$a_0 = a_1 + a_2$$

$$a_1 = u^{\text{average}} (y_0 - y_2) - v^{\text{average}} (x_0 - x_2), \quad a_2 = v^{\text{average}} (x_0 - x_1) - u^{\text{average}} (y_0 - y_1)$$

Second order TVD schemes for 2D fluid flow need around 120 floating point operations per equation.
Advection of a step profile: (a) physical domain, (b) $\phi$ profile at $y = 0.8$. 
## Performance comparisons

<table>
<thead>
<tr>
<th>Approximation scheme</th>
<th>$\alpha$</th>
<th>Iterations</th>
<th>max residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upwind</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R1</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R2</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R3</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R4</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R5</td>
<td>1.0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Min-Mod</td>
<td>0.95</td>
<td>36</td>
<td>$8.1 \times 10^{-9}$</td>
</tr>
<tr>
<td>QUICK(TVD)</td>
<td>0.95</td>
<td>49</td>
<td>$6.2 \times 10^{-9}$</td>
</tr>
<tr>
<td>SUPERBEE</td>
<td>0.95</td>
<td>151</td>
<td>$9.4 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

Relaxation coefficient, number of iterations and obtained maximum residual of considered schemes for advection of a step profile and convergence criteria $\varepsilon = 10^{-8}$
Smith and Hutton problem
Smith and Hutton problem numerical solutions
Smith and Hutton problem, \( \alpha = 1000, \Gamma = 0 \), contour plots of schemes for mesh 40x20 nodes.
### Performance comparisons

<table>
<thead>
<tr>
<th>Approximation scheme</th>
<th>$\alpha$</th>
<th>Iterations</th>
<th>max residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upwind</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R1</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R2</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R3</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R4</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>UpwindM R5</td>
<td>1.0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Min-Mod</td>
<td>0.95</td>
<td>81</td>
<td>$5.5 \times 10^{-9}$</td>
</tr>
<tr>
<td>QUICK(TVD)</td>
<td>0.85</td>
<td>62</td>
<td>$9.0 \times 10^{-9}$</td>
</tr>
<tr>
<td>SUPERBEE</td>
<td>0.1</td>
<td>50000</td>
<td>$10^{-3}$</td>
</tr>
</tbody>
</table>

Relaxation coefficient, number of iterations and obtained maximum residual of considered schemes for Smith and Hutton problem for mesh 40x20 nodes and convergence criteria $\varepsilon = 10^{-8}$. 
Proposed approach looks very promising because:

- Naturally approximates first derivatives in partial differential equations that are big issue!
- All independent variables can be defined in the same nodes
- Easy application on unstructured meshes
- Easy application on adaptive mesh refinement
- It can be applied as meshfree method
- This approach can be applied to Finite Volume Method SIMPLE-TS for calculation of Navier-Stokes-Fourier equations

Direct Simulation Monte Carlo DSMC

New DSMC code is under active development, testing, and validation.

A lots of background work has been done:

- The code is written from scratch in C++ on the basis of Prof. Stefanov’s FORTRAN code
- Adaptive time step
- Spatial adaptive mesh. It is implemented Transient Adaptive Subcells (TAS) approach. This reduce computational resources significantly. Some problems need 20 times less number of particles to reach the same spatial accuracy as code without TAS.
- Import 2D geometry from CAD systems
Supersonic flow past NACA0012 airfoil, $M=2$, $Kn=0.031$
Direct Simulation Monte Carlo DSMC

What’s next:

- Parallel organization based MPI standard for CPU calculations
- C++ code can and will be ported to GPU
- Present 2D code can be easily extended for 3D problems where 3D geometry will be import from CAD systems
Thank you!