

- main ingredients: [LM (M3AS 00, JCP 00)]
 - plane flow: 2D BGK Model
 - conservative and entropic velocity discretization
 - space discretization: finite volume, curvilinear grids
 - time discretization: backward Euler (transient solutions), linearized implicit scheme (steady flows)

- ▶▶▶▶ new features (2007) : [Aoki-Degond-LM (JCP 07)]
 - ▶▶▶ reduced distribution technique: $v \in \mathbb{R}^2$ instead of \mathbb{R}^3
 - ▶▶▶ implicit boundary conditions (faster convergence to steady state)
- ▶▶▶▶ various boundary conditions can be used on any arbitrary part of the boundaries of domain (diffuse reflection, symmetry axis, periodic condition, out/in-flow condition, temperature gradient on solid wall, evaporation/condensation)
- ▶▶▶▶ parallel implementation (Open-MP)
- ▶▶▶▶ tested on 16 processors of the Altix 3700 (SGI)

▣▣▣▣ F is independent of $z \Rightarrow$ the transport operator does not contain explicitly the velocity v_z .

▣▣▣▣ define the reduced distribution function

$$f(t, x, y, v_x, v_y) = \int_{\mathbb{R}} F dv_z, \text{ and integrate BGK w.r.t } v_z$$

$$\partial_t F + v \cdot \nabla_x F = \nu(\mathcal{M}[\rho, u, T] - F)$$

$$\Downarrow \int_{\mathbb{R}} \cdot dv_z$$

$$\partial_t f + v \cdot \nabla_x f = \nu(M[\rho, u, T] - f),$$

where $M[\rho, u, T]$ is the reduced Maxwellian defined by

$$M[\rho, u, T] = \int_{\mathbb{R}} \mathcal{M}[\rho, u, T] dv_z = \frac{\rho}{2\pi RT} \exp\left(-\frac{(v_x - u_x)^2 + (v_y - u_y)^2}{2RT}\right),$$

but T cannot be defined through f only:

$$\begin{aligned} E &= \frac{1}{2}\rho|u|^2 + \frac{3}{2}\rho RT \\ &= \int_{\mathbb{R}^3} \frac{1}{2}|v|^2 F(t, x, v) dv \\ &= \int_{\mathbb{R}^3} \frac{1}{2}|v_x^2 + v_y^2 + v_z^2| F(t, x, v) dv \\ &= \int_{\mathbb{R}^2} \frac{1}{2}|v_x^2 + v_y^2| f(t, x, v) dv_x dv_y + \int_{\mathbb{R}^2} g(t, x, v) dv_x dv_y \end{aligned}$$

where $g(t, x, y, v_x, v_y) = \int_{\mathbb{R}} \frac{1}{2}v_z^2 F dv_z$.

- ▶▶▶ as for f , an equation for g is derived
- ▶▶▶ finally, we get the coupled system of kinetic equations:

$$\partial_t f + v \cdot \nabla_x f = \nu(M[\rho, u, T] - f),$$

$$\partial_t g + v \cdot \nabla_x g = \nu\left(\frac{RT}{2}M[\rho, u, T] - g\right),$$

and the macroscopic quantities are obtained through f and g by

$$\rho = \int_{\mathbb{R}^2} f \, dv^2, \quad \rho u = \int_{\mathbb{R}^2} v f \, dv^2,$$
$$\frac{1}{2}\rho|u|^2 + \frac{3}{2}\rho RT = \int_{\mathbb{R}^2} \left(\frac{1}{2}|v|^2 f + g\right) \, dv^2.$$

► for given ρ, u, T , the Maxwellian $M[\rho, u, T]$ satisfies

$$\text{conservation: } \int_{\mathbb{R}^2} \begin{pmatrix} \frac{1}{v} \\ \frac{1}{2}|v|^2 \end{pmatrix} M[\rho, u, T] dv = \begin{pmatrix} \rho \\ \rho u \\ \frac{1}{2}\rho|u|^2 + \rho RT \end{pmatrix}$$

$$\text{entropy: } \int_{\mathbb{R}^2} M[\rho, u, T] \log M dv = \min \left\{ \int_{\mathbb{R}^2} f \log f dv \right\}$$

► \mathbb{R}^2 is truncated to $[v_{\min}, v_{\max}]^2$ and discretized by $(v_k)_{k=1}^N$

► $\int_{\mathbb{R}^2} f dv$ is replaced by $\sum_{k=1}^N f_k \Delta v$

► we can define $(M_k)_{k=1}^N$ that satisfies discrete conservation and entropy properties (\Rightarrow existence and convergence results)

equation for f : finite volumes, upwind scheme, curvilinear grid

$$\partial_t f + v \cdot \nabla_x f = \nu(M[\rho, u, T] - f),$$

↓

$$\begin{aligned} \partial_t f_{\mathbf{k},i,j} + \frac{1}{\Delta x} (\phi_{i+\frac{1}{2},j}(f_{\mathbf{k}}) - \phi_{i-\frac{1}{2},j}(f_{\mathbf{k}})) + \frac{1}{\Delta y} (\phi_{i,j+\frac{1}{2}}(f_{\mathbf{k}}) - \phi_{i,j-\frac{1}{2}}(f_{\mathbf{k}})) \\ = \nu_{i,j} (M_{\mathbf{k}}[\rho_{i,j}, u_{i,j}, T_{i,j}] - f_{\mathbf{k},i,j}), \end{aligned}$$

where the numerical fluxes are defined by

$$\begin{aligned} \phi_{i+\frac{1}{2},j}(f_{\mathbf{k}}) &= \frac{1}{2} \left(v_{x,k}(f_{\mathbf{k},i+1,j} + f_{\mathbf{k},i,j}) - |v_{x,k}|(\Delta f_{\mathbf{k},i+\frac{1}{2},j} - \Phi_{\mathbf{k},i+\frac{1}{2},j}) \right) \\ \phi_{i,j+\frac{1}{2}}(f_{\mathbf{k}}) &= \frac{1}{2} \left(v_{y,k}(f_{\mathbf{k},i,j+1} + f_{\mathbf{k},i,j}) - |v_{y,k}|(\Delta f_{\mathbf{k},i,j+\frac{1}{2}} - \Phi_{\mathbf{k},i,j+\frac{1}{2}}) \right) \end{aligned}$$

transient solutions: first order backward euler

$$\begin{aligned} \frac{1}{\Delta t} (f_{k,i,j}^{n+1} - f_{k,i,j}^n) &+ \frac{1}{\Delta x} (\phi_{i+\frac{1}{2},j}(f_k^n) - \phi_{i-\frac{1}{2},j}(f_k^n)) \\ &+ \frac{1}{\Delta y} (\phi_{i,j+\frac{1}{2}}(f_k^n) - \phi_{i,j-\frac{1}{2}}(f_k^n)) \\ &= \nu_{i,j}^n (M_k[\rho_{i,j}^n, u_{i,j}^n, T_{i,j}^n] - f_{k,i,j}^n) \end{aligned}$$

stability if

$$\Delta t \leq \frac{1}{\max_{i,j}(\nu_{i,j}^n)} \quad \text{and} \quad \frac{\Delta t}{\Delta x} \leq \frac{1}{\max_k |v_k|}$$

restrictive condition for: rapid or dense flows, and steady state

steady solutions: forward euler (implicit)

$$\begin{aligned} \frac{1}{\Delta t} (f_{k,i,j}^{n+1} - f_{k,i,j}^n) &+ \frac{1}{\Delta x} (\phi_{i+\frac{1}{2},j}(f_k^{n+1}) - \phi_{i-\frac{1}{2},j}(f_k^{n+1})) \\ &+ \frac{1}{\Delta y} (\phi_{i,j+\frac{1}{2}}(f_k^{n+1}) - \phi_{i,j-\frac{1}{2}}(f_k^{n+1})) \\ &= \nu_{i,j}^n (M_k[\boldsymbol{\mu}_{i,j}^{n+1}] - f_{k,i,j}^{n+1}) \end{aligned}$$

then linearization:

$$M_k[\boldsymbol{\mu}_{i,j}^{n+1}] \approx M_k[\boldsymbol{\mu}_{i,j}^n] + \partial_{\boldsymbol{\mu}} M_k[\boldsymbol{\mu}_{i,j}^{n+1}] (\boldsymbol{\mu}_{i,j}^{n+1} - \boldsymbol{\mu}_{i,j}^n)$$

where $\boldsymbol{\mu} = (\rho, \rho u, \frac{1}{2}\rho|u|^2 + \frac{3}{2}\rho RT)$

δ -matrix form of the scheme: set $U^n = (\{f_{k,i,j}^n\}_{k,i,j}, \{g_{k,i,j}^n\}_{k,i,j})$

Then the scheme is

$$\left(\frac{I}{\Delta t} + T + B + R^n \right) \delta U^n = RHS^n,$$

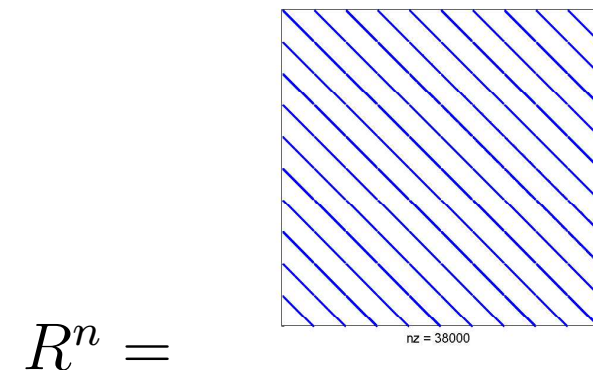
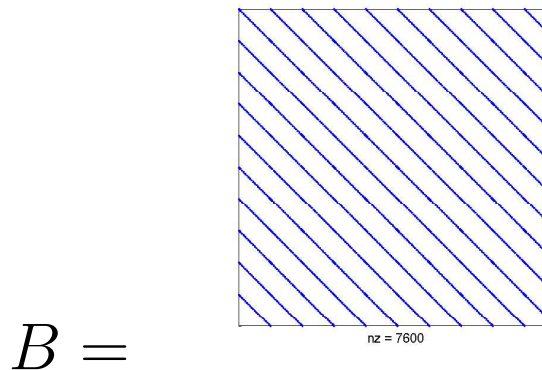
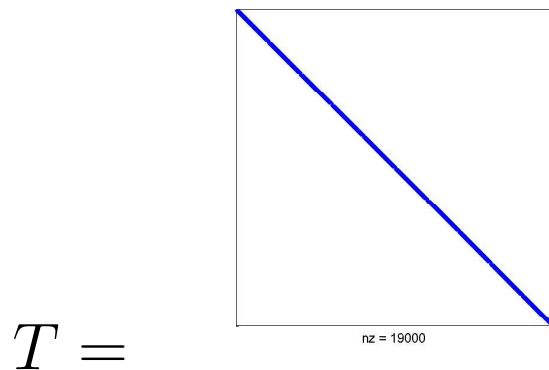
where

- $\delta U^n = U^{n+1} - U^n$,
- I is the unit matrix,
- T contains the transport coefficients, (b. c. in in B)
- B contains the boundary condition coefficients,
- R^n is the Jacobian matrix of the collision operator,
- RHS^n is the residual (transport and collision operators applied to U^n).

$$\left(\frac{I}{\Delta t} + T + B + R^n \right) \delta U^n = RHS^n,$$

➡ very large linear system

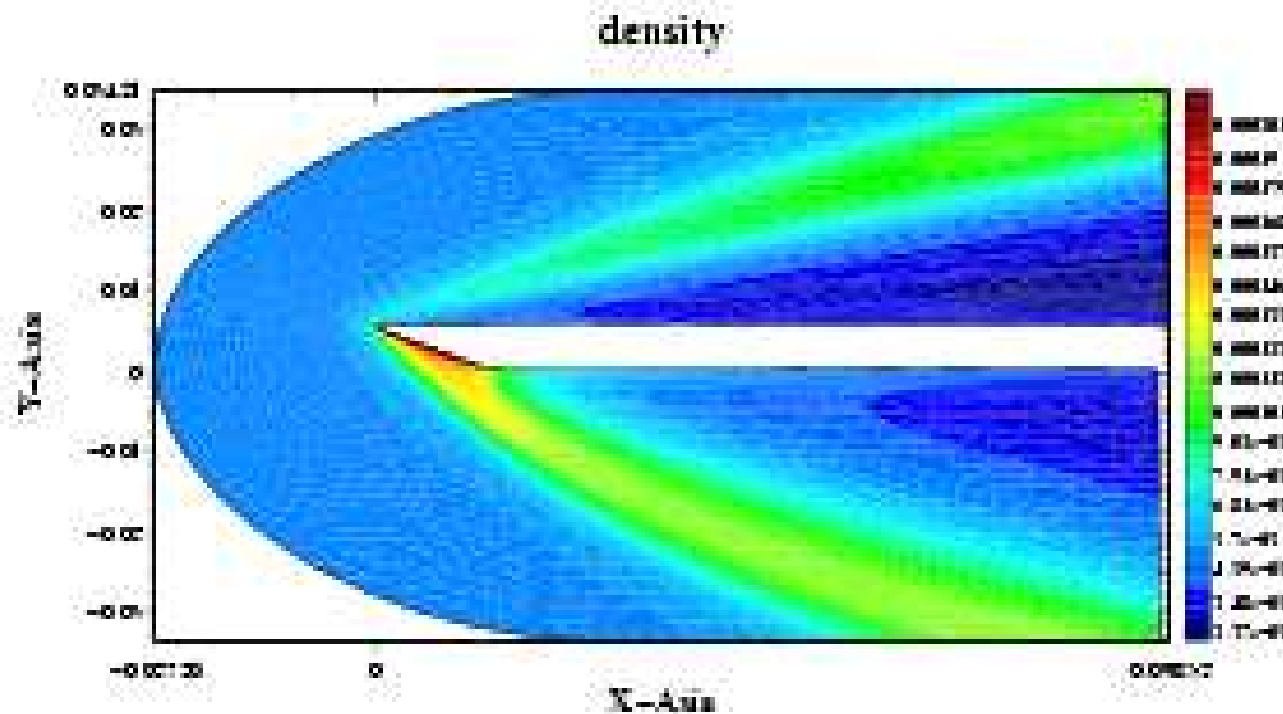
➡ sparse matrices



➡ an adapted iterative solver is used

Hypersonic external flow:

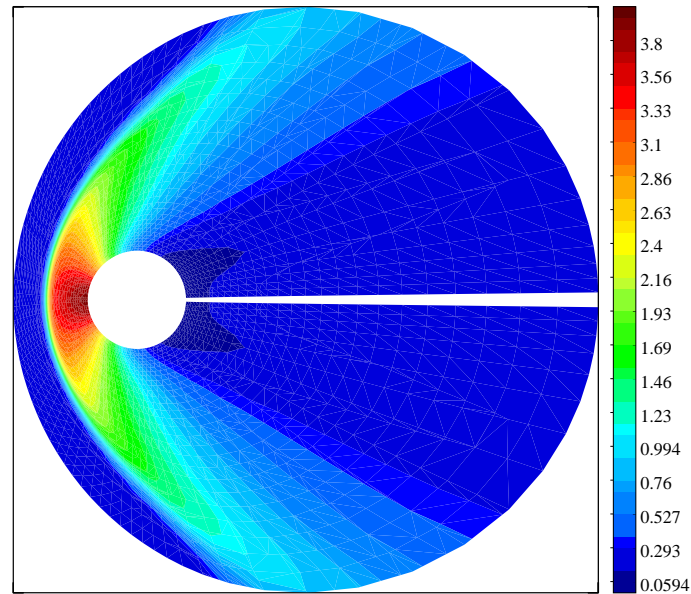
Mach = 18.3, Kn = 0.014



Supersonic external flow:

Mach 4, $Kn = 0.0358$

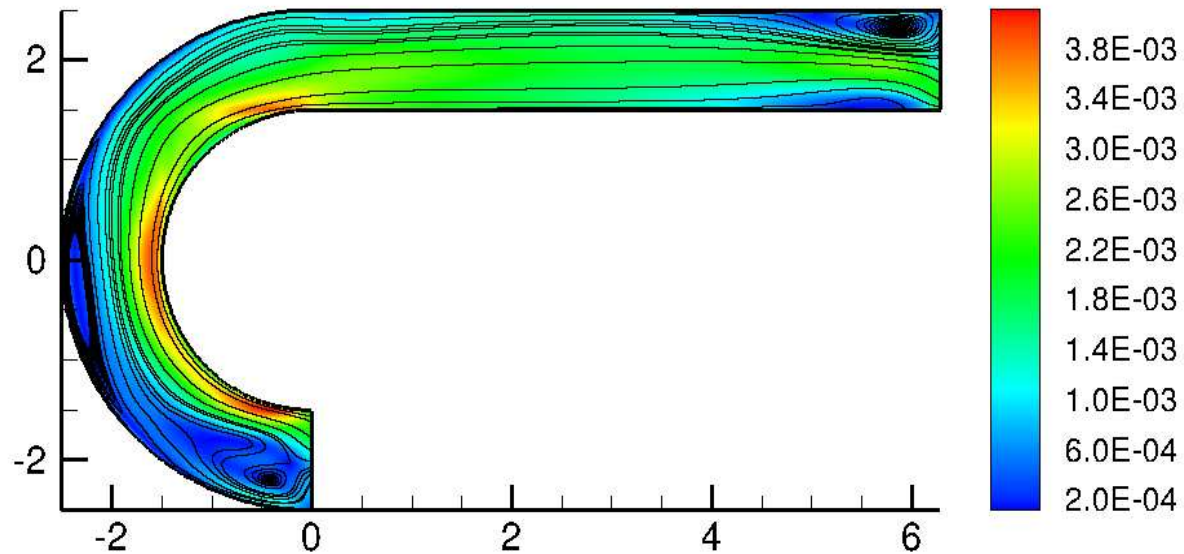
pressure around a cylinder



Internal slow flow:

Mach 0.001, Kn=0.5

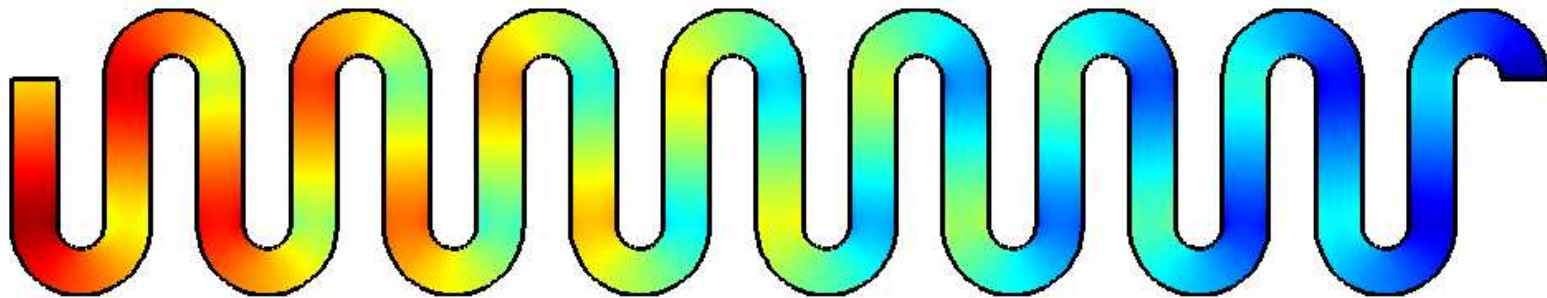
Velocity magnitude and streamlines in half of a ring-shaped channel



Internal slow flow:

Mach 0.001, Kn=0.5

pressure in a micro-pump



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- 3D code
 - unstructured 2D code
 - include polyatomic effects