Numerical simulations of rarefied gases in curved channels: thermal creep, circulating flow, and pumping effect.

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Introduction

- study new systems of micro-pumps by using properties of rarefied gases
- simplified mathematical and physical models
- numerical simulations
Thermal creep flow and pumping effect

Rarefied gas: \[ Kn = \frac{\text{mean free path}}{\text{characteristic length}} = \frac{\lambda}{D} \approx 1 \]

- the density of the gas is small enough
- or the width of the channel is small enough
Thermal creep flow and pumping effect

apply a temperature gradient on the wall

\[ T_{low} \rightarrow T_{High} \]
Thermal creep flow and pumping effect

- on the walls: particles coming from the right have more energy than particles coming from the left

\[ T_{low} \rightarrow T_{High} \]

- the gas gives a net momentum from right to left to the walls
The walls are fixed: by reaction, the gas moves from the left to the right.

This is the thermal creep flow.
Thermal creep flow and pumping effect

- the thermal creep flow disappears if $\frac{\lambda}{D} \rightarrow 0$ (fluid regime)
- known as “thermal transpiration” since Reynolds (1888), Maxwell (1889), Knudsen (1910)
- Sone (1966): analytical demonstration of the thermal creep flow by asymptotic theory
Thermal creep flow and pumping effect

- natural application:
  create flow and pumping effect **without** moving mechanical part

- physical conditions: rarefied regime

\[ Kn = \frac{\text{mean free path}}{\text{characteristic length}} \]

is not too small

- weak pressure gas

- or small devices: Micro-Electro-Mechanical-Systems (MEMS)
  (e.g.: air at atmospheric pressure \(\Rightarrow\) width \(\approx 0.1\mu m\))
Pumping effect

- thermal creep flow ⇒ a flow is generated, and a pressure difference is obtained \((p_R > p_L)\)

- problem:
  - very weak effect: velocity \(u\) is small
  - \(u\) depends on the temperature gradient
  - a very large temperature gradient is technologically impossible
Pumping effect

- idea: maintain the two tanks at the same temperature
- increase and decrease the wall temperature
- two opposed thermal creep flows
- no pressure difference
Pumping effect

- how to get a net flow with two opposed temperature gradients?
- idea: use a ditch (Aoki, Sone et al, 1996)

- the opposite flow is confined to the ditch
- there is a global mass flow
- a pumping effect is possible
- similar idea by Knudsen (1910)
Pumping effect

- more efficiency of the pump with a cascade system: Knuden compressor

- experiments and numerical simulations (Aoki, Sone et al.),
- mathematical modeling (Aoki, Degond)
A new Knudsen compressor: the project

new (simpler) idea: channel with varying curvature
(Aoki-Degond-LM-Takata-Yoshida)

project: numerical simulations and mathematical modeling
A new Knudsen compressor: simulations

- steady 2D kinetic simulations: standard method is DSMC → very expensive (slow flow)

- instead: deterministic kinetic simulations

- for large number of units: asymptotic model (small width approximation)
Kinetic theory

- monoatomic gas: distribution function of molecular velocities $F(t, x, v)$
- defined such as $F(t, x, v)dx dv = \text{mass of molecules that at time } t \text{ have position } x \pm dx \text{ and velocity } v \pm dv$
- macroscopic quantities: moments of $F$ w.r.t $v$

  mass density $\rho = \int_{\mathbb{R}^3} F(t, x, v) \, dv$,

  momentum $\rho u = \int_{\mathbb{R}^3} v F(t, x, v) \, dv$,

  total energy $E = \int_{\mathbb{R}^3} \frac{1}{2} |v|^2 F(t, x, v) \, dv$. 
temperature $T$ defined by $E = \frac{1}{2} \rho |u|^2 + \frac{3}{2} \rho RT$

equilibrium state: Maxwellian distribution, depends only on $v, \rho, u, T$

$$\mathcal{M}[\rho, u, T](v) = \frac{\rho}{(2\pi RT)^{\frac{3}{2}}} \exp \left( -\frac{|v - u|^2}{2RT} \right)$$
Kinetic theory

- evolution of $F$ described by a kinetic equation

$$\partial_t F + u \cdot \nabla_x F = Q(F)$$

- $Q(F)$ is the Boltzmann collision operator, but often the simpler BGK model is used:

$$Q(F) = \nu (\mathcal{M} [\rho, u, T] - F)$$

effect of collisions = relaxation of $F$ towards the Maxwellian equilibrium
Deterministic numerical method

- main ingredients: [LM (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)
Deterministic numerical method

- new features: [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)

- parallel implementation (Open-MP)

- typical simulation for 1 unit: $400 \times 100$ space cells, $40 \times 40$ discrete velocities
Numerical method: reduced distribution technique

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

- define the reduced distribution function

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

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

\[
\Downarrow \int_{\mathbb{R}} . \, dv_z
\]

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

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

\[
M[\rho, u, T] = \int_{\mathbb{R}} M[\rho, u, T] \, dv_z = \frac{\rho}{2\pi RT} \exp \left( -\frac{(v_x - u_x)^2 + (v_y - u_y)^2}{2RT} \right),
\]
but $T$ cannot be defined through $f$ only:

\[
E = \frac{1}{2} \rho |u|^2 + \frac{3}{2} \rho RT
\]

\[
= \int_{\mathbb{R}^3} \frac{1}{2} |v|^2 F(t, x, v) \, dv
\]

\[
= \int_{\mathbb{R}^3} \frac{1}{2} |v_x^2 + v_y^2 + v_z^2| F(t, x, v) \, dv
\]

\[
= \int_{\mathbb{R}^2} \frac{1}{2} |v_x^2 + v_y^2| f(t, x, v) \, dv_x dv_y + \int_{\mathbb{R}^2} g(t, x, v) \, dv_x dv_y
\]

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

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

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

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

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 $\rho, u, T$, the Maxwellian $M[\rho, u, T]$ satisfies

conservation: $\int_{\mathbb{R}^2} \left( \frac{1}{2} |v|^2 \right) M[\rho, u, T] \, dv = \left( \frac{1}{2} \rho |u|^2 + \rho RT \right)$

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

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

$$\downarrow$$

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

where the numerical fluxes are defined by

$$\phi_{i+\frac{1}{2},j}(f_k) = \frac{1}{2} \left( v_{x,k} (f_{k,i+1,j} + f_{k,i,j}) - |v_{x,k}|(\Delta f_{k,i+\frac{1}{2},j} - \Phi_{k,i+\frac{1}{2},j}) \right)$$

$$\phi_{i,j+\frac{1}{2}}(f_k) = \frac{1}{2} \left( v_{y,k} (f_{k,i,j+1} + f_{k,i,j}) - |v_{y,k}|(\Delta f_{k,i,j+\frac{1}{2}} - \Phi_{k,i,j+\frac{1}{2}}) \right)$$
Numerical method: time discretization

transient solutions: first order backward euler

\[
\frac{1}{\Delta t} (f_{k+1}^{n+1} - f_k^{n}) + \frac{1}{\Delta x} (\phi_{i+\frac{1}{2},j}^n (f_k^n) - \phi_{i-\frac{1}{2},j}^n (f_k^n)) + \frac{1}{\Delta y} (\phi_{i,j+\frac{1}{2}}^n (f_k^n) - \phi_{i,j-\frac{1}{2}}^n (f_k^n))
\]

\[
= \nu_{i,j}^n (M_k [\rho_{i,j}^n, u_{i,j}^n, T_{i,j}^n] - f_k^{n})
\]

stability if

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

restrictive condition for: rapid or dense flows, and steady state
Numerical method: time discretization

steady solutions: forward euler (implicit)

\[
\frac{1}{\Delta t} (f_{k,i,j}^{n+1} - f_{k,i,j}^n) + \frac{1}{\Delta x} (\phi_{i+1/2,j} (f_{k}^{n+1}) - \phi_{i-1/2,j} (f_{k}^{n+1})) \\
+ \frac{1}{\Delta y} (\phi_{i,j+1/2} (f_{k}^{n+1}) - \phi_{i,j-1/2} (f_{k}^{n+1})) \\
= \nu^n_{i,j} (M_k [\mu_{i,j}^{n+1}] - f_{k,i,j}^{n+1})
\]

then linearization:

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

where \( \mu = (\rho, \rho u, \frac{1}{2} \rho |u|^2 + \frac{3}{2} \rho RT) \)
\textbf{Numerical method: time discretization}

\(\delta\)-matrix form of the scheme: set \(U^n = (\{f^n_{k,i,j}\}_{k,i,j}, \{g^n_{k,i,j}\}_{k,i,j})\)

Then the scheme is

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

where

\[ \bullet \quad \delta U^n = U^{n+1} - U^n, \]
\[ \bullet \quad I \text{ is the unit matrix}, \]
\[ \bullet \quad T \text{ contains the transport coefficients, (b. c. in in } B) \]
\[ \bullet \quad R^n \text{ is the Jacobian matrix of the collision operator}, \]
\[ \bullet \quad RHS^n \text{ is the residual (transport and collision operators applied to } U^n). \]
Numerical method: linear system

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

- very large linear system
- sparse matrices

\[
T = \begin{array}{c}
\text{nz = 19000}
\end{array} \quad B = \begin{array}{c}
\text{nz = 7600}
\end{array} \quad R^n = \begin{array}{c}
\text{nz = 36000}
\end{array}
\]

- an adapted iterative solver is used
Numerical simulations

Basic unit of our devices: a hook shaped channel.
Three sizes: thick ($D/R = 1$), medium (0.5), thin (0.2)
Three Knudsen numbers: $Kn = 1, 0.5, 0.1$
Numerical simulations: Circulating flow
Numerical simulations: Circulating flow
Numerical simulations: *Circulating flow*

![Numerical simulations](image-url)
Numerical simulations: *Circulating flow*

Mass flow rate in the ring-shaped channel as a function of the Knudsen number.

Each curve corresponds to one of the three different size of channel.
Numerical simulations: Circulating flow

time evolution of the density and velocity fields + mass flow rate:
Closed cascade device to generate a pumping effect.
Pressure field in the closed cascade device: 2, 4, 8 and 16 units.
Non-dimensionalized average pressure (left) and density (right) profiles for the pumping device with several numbers $N$ of units. Thick case with $Kn = 0.5$. 
Pressure (left) and density gain (right) for the pumping device with several numbers $N$ of units. Thick case with $Kn = 0.5$. 
Numerical simulations: Micro-Pump

comparison BGK/DSMC
Asymptotic model

- problem: simulation impossible for a large number of units
- idea: develop a simplified mathematical model (asymptotic analysis)
- result: fluid model (no particles), one space dimension only
- diffusion model, induced by the boundaries
- very fast simulations, arbitrary number of units
Asymptotic model

[Aoki-Degond-LM-Takata-Yoshida (MMS 07)]

BGK equation:

\[ \partial_t f + v \cdot \nabla_x f = Q(f), \]

Local coordinates:

\[ \partial_t f + (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_{v_s} f \]

\[ - \kappa (1 - \kappa r)^{-1} v_s^2 \partial_{v_r} f = A c \rho(M[\rho, u, 2RT] - f). \]
Asymptotic model

[Aoki-Degond-LM-Takata-Yoshida (MMS 07)]

BGK equation:

\[ \partial_t f + v \cdot \nabla_x f = Q(f), \]

Local coordinates:

\[
\partial_t f + (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_{v_s} f
\]

\[
- \kappa (1 - \kappa r)^{-1} v_s^2 \partial_{v_r} f = A_c \rho (M[\rho, u, 2RT] - f).
\]

re-scaling: \( \epsilon = \frac{D}{L_s} \ll 1, \quad t' = \epsilon^2 t \quad \text{and} \quad s' = \epsilon s \)
Asymptotic model

[Aoki-Degond-LM-Takata-Yoshida (MMS 07)]

BGK equation:

\[ \partial_t f + v \cdot \nabla_x f = Q(f), \]

Local coordinates:

\[ \epsilon^2 \partial_t f + \epsilon (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_{v_s} f \]

\[ - \kappa (1 - \kappa r)^{-1} v_s^2 \partial_{v_r} f = \frac{1}{K_0} \rho \left( M[\rho, u, T] - f \right) \]

re-scaling: \( \epsilon = \frac{D}{L_s} \ll 1, \quad t' = \epsilon^2 t \) and \( s' = \epsilon s \)
Asymptotic model

conservation of the averaged density:

$$\partial_t \varrho + \partial_s j = 0,$$

where

$$\varrho(s, t) = \int_{-1/2}^{1/2} \int_{\mathbb{R}^3} f(1-\kappa r) \, dv \, dr \quad \text{and} \quad j(s, t) = \frac{1}{\epsilon} \int_{-1/2}^{1/2} \int_{\mathbb{R}^3} v_s f \, dv \, dr$$

limit $\epsilon \to 0 : 1$D macroscopic model (variable $s$ only)
Asymptotic model

**Theorem** (formal)

(i) \( \varrho \to \rho_0 \), solution of

\[
\partial_t \rho_0 + \partial_s j_1 = 0,
\]

\[
j_1 = \sqrt{T_w} M_P \partial_s \rho_0 + \frac{\rho_0}{\sqrt{T_w}} (M_P + M_T) \partial_s T_w,
\]

(\text{where } M_P \text{ and } M_T \text{ are non-linear functions of } \rho_0)

(ii) \( M_P \leq 0 \)

(iii) \( \varrho - \rho_0 = O(\epsilon^2) \) and \( j - j_1 = O(\epsilon^2) \)
Asymptotic model

\[ \epsilon^2 \partial_t f + \epsilon (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_{v_s} f \]

\[ - \kappa (1 - \kappa r)^{-1} v_s^2 \partial_{v_r} f = \frac{1}{K_0} \rho \left( M[\rho, u, T] - f \right) \]

Hilbert expansion: \( f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \ldots \)

\[ f_0 = \rho_0 (s, t) M[1, 0, T_w(s)] \]

\[ \downarrow \]

\( \rho_0 \) to be determined, and \( j_0 = \frac{1}{\epsilon} \int_{-1/2}^{1/2} \int_{\mathbb{R}^3} v_s f_0 \ d\mathbf{v} \ dr = 0 \)
Asymptotic model

\[ \epsilon^2 \partial_t f + \epsilon (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_v f \]

\[ - \kappa (1 - \kappa r)^{-1} v_s^2 \partial_v f = \frac{1}{K_0} \rho(M[\rho, u, T] - f) \]

Hilbert expansion: \( f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \ldots \)

\[ L f_1 = -(1 - \kappa r)^{-1} v_s \partial_s f_0 \quad \text{(1D linear kinetic eq.)} \]

\[ \downarrow \]

\[ \rho_1 = 0 \quad \text{and} \]

\[ j_1(s, t) = \int_{-1/2}^{1/2} \int_{\mathbb{R}^3} v_s f_1 \, dvdr = \sqrt{T_w} M_P \partial_s \rho_0 + \frac{\rho_0}{\sqrt{T_w}} (M_P + M_T) \partial_s T_w \]
Numerical computations:

- \( M_P \) and \( M_T \):
  - depend only on \( s \) through \( K \) and \( \kappa \)
  - are averaged fluxes given by solutions of auxiliary linear kinetic problems, 1D in \( r \), local in \( s \)
  - these problems are numerically solved for many values of \( K \) and \( \varepsilon \)
  - construction of a database for \( M_P \) and \( M_T \)
Asymptotic model

Numerical computations:

- discontinuity of the curvature is taken into account (boundary layer corrector)
- the diffusion model is numerically solved
- comparison with a fully kinetic simulations (2D BGK)
- simulation of a 100 unit pump
Asymptotic model

Comparison with 2D BGK: circulating flow
Comparison with 2D BGK: circulating flow
Asymptotic model

Comparison with 2D BGK: micro-pump

100 unit pump: pressure gain = factor 6
Perspectives

g► test different geometries

► optimization of the shape of the channel

► simulation of a 3D Knudsen pump (pipe):
  ➤ Derive a diffusion model
  ➤ Compute the transport coefficients

► experimental studies