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

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3. A new Knudsen compressor
4. Kinetic theory
5. Deterministic numerical method
6. Numerical simulations
7. Asymptotic model
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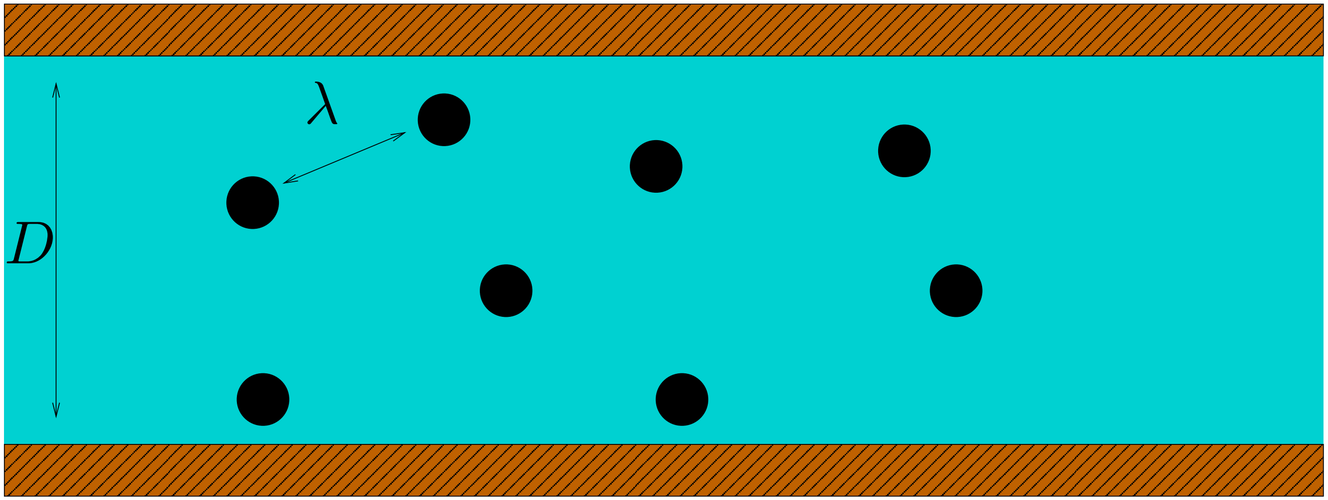
Introduction

- 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: $\mathrm{Kn} = \frac{\text{mean free path}}{\text{characteristic length}} = \frac{\lambda}{D} \approx 1$

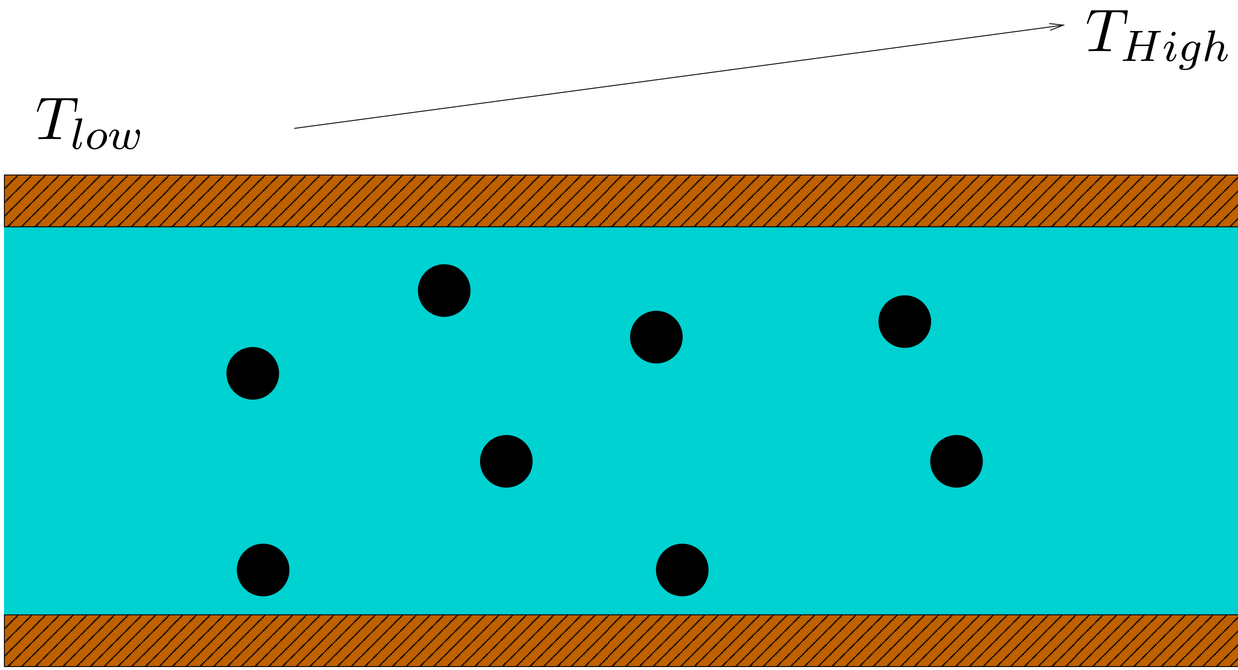


➠ the density of the gas is small enough

➠ or the width of the channel is small enough

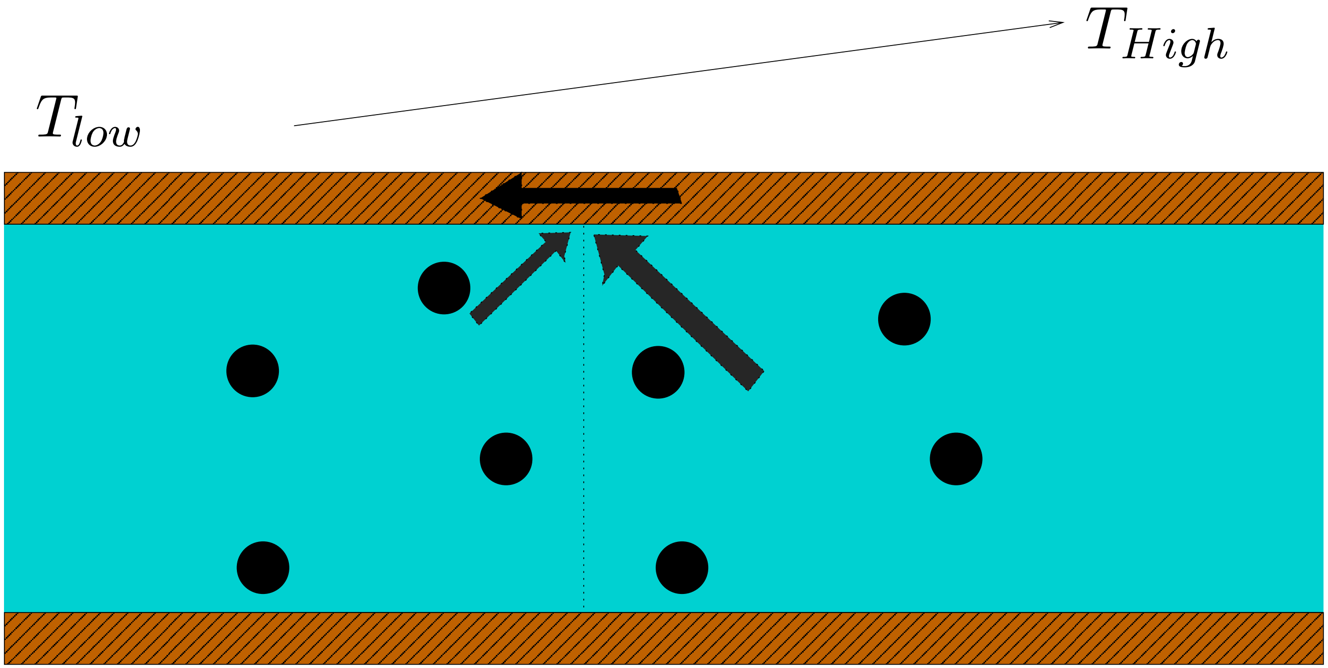
Thermal creep flow and pumping effect

- apply a temperature gradient on the wall



Thermal creep flow and pumping effect

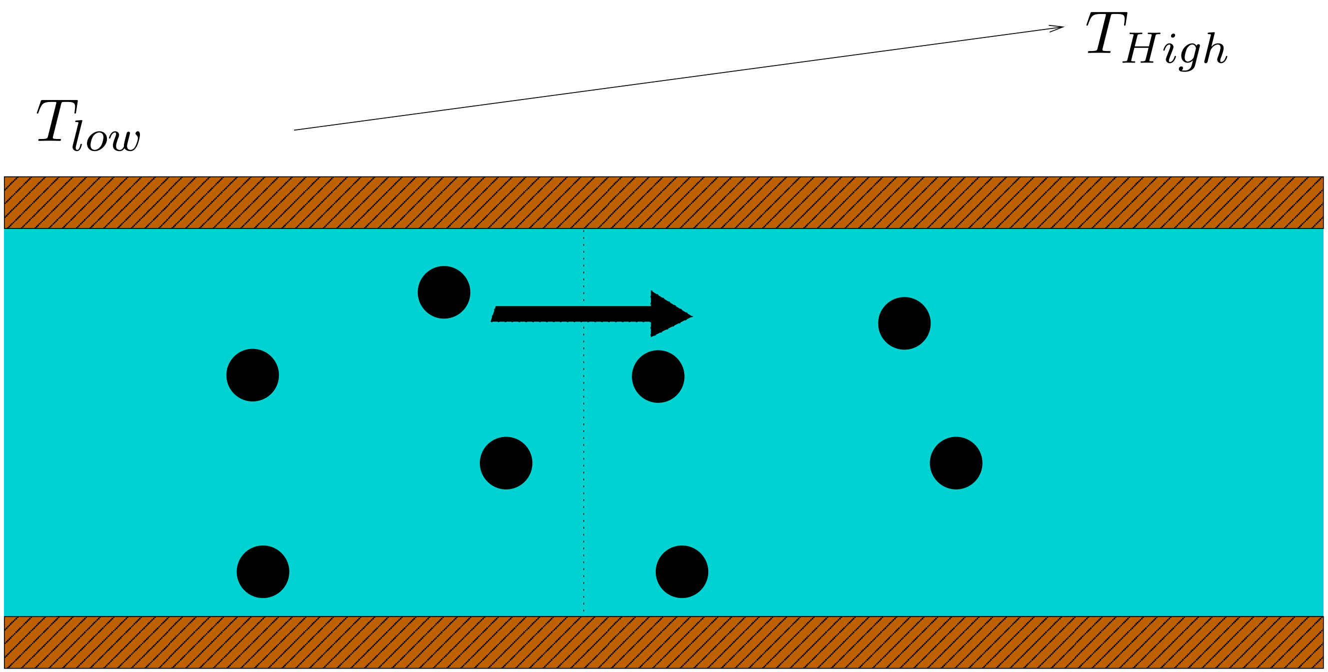
- on the walls: particles coming from the right have more energy than particles coming from the left



- the gas gives a net momentum from right to left to the walls

Thermal creep flow and pumping effect

- 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 $\frac{\lambda}{D} \longrightarrow 0$ (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

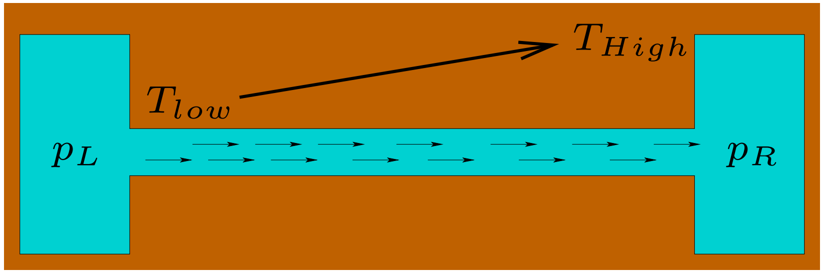
- natural application:
  create flow and pumping effect <u>without</u> moving mechanical part

- physical conditions: rarefied regime

$$\text{Kn} = \frac{\text{mean free path}}{\text{characteristic length}} \quad \text{is not too small}$$

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

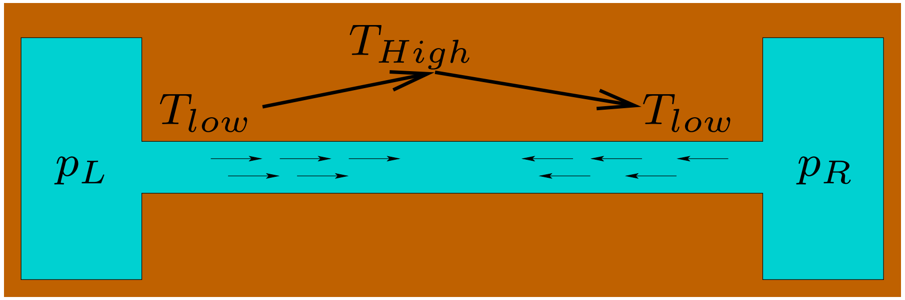
Pumping effect



- thermal creep flow $\Rightarrow$ 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

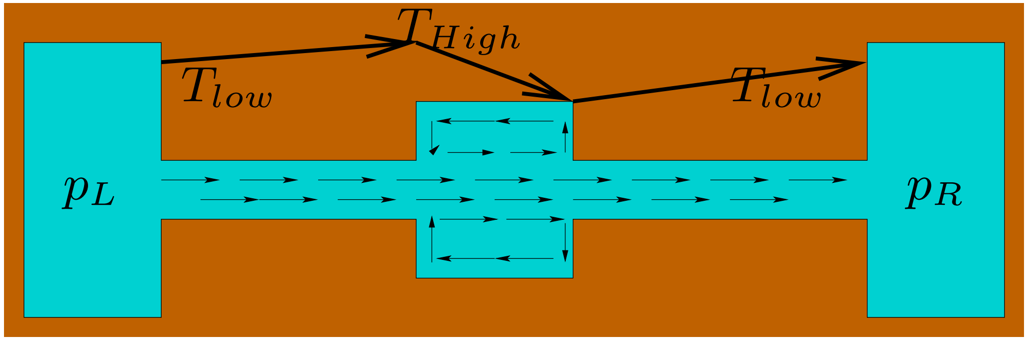
- idea: maintain the two tanks at the same temperature
- increase and decrease the wall temperature



- two opposed thermal creep flows
- no pressure difference

Pumping effect

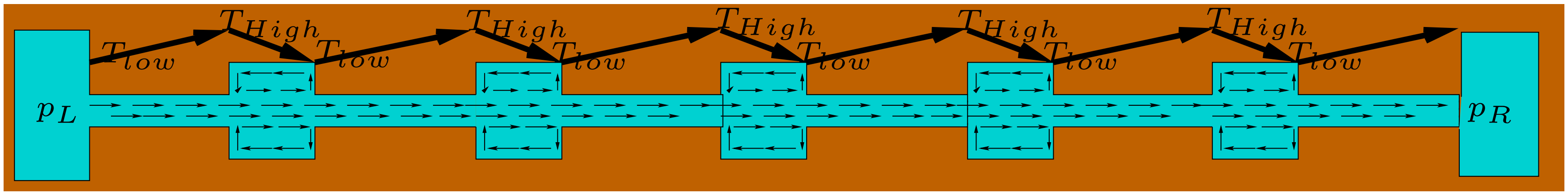
- how to get a net flow with two opposed temperature gradients ?
- idea: use a ditch (Aoki, Sone et al, 1996)



  - the opposit 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

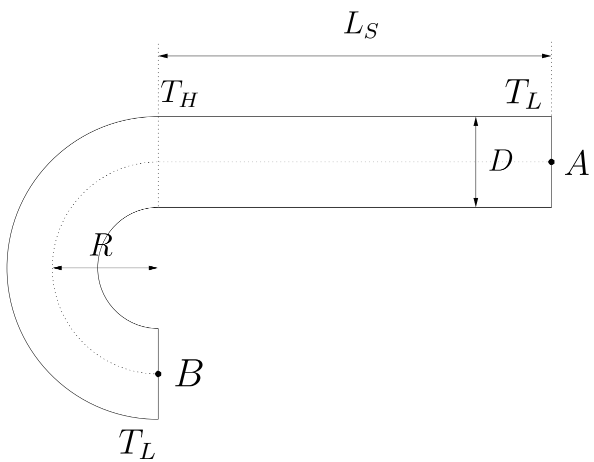


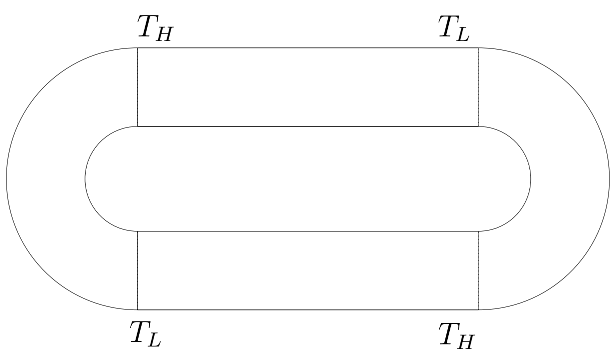
- experiments and numerical simulations (Aoki, Sone et al.),
- mathematical modeling (Aoki, Degond)

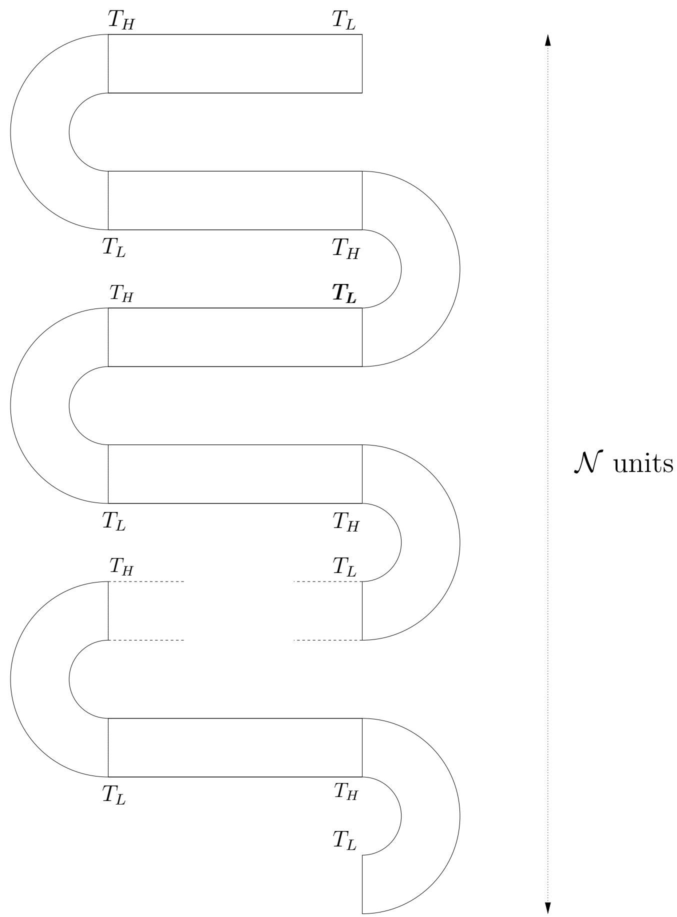
A new Knudsen compressor: the project

- 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 $\rightarrow$ very expensive (slow flow)

- instead: deterministic kinetic simulations

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

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

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

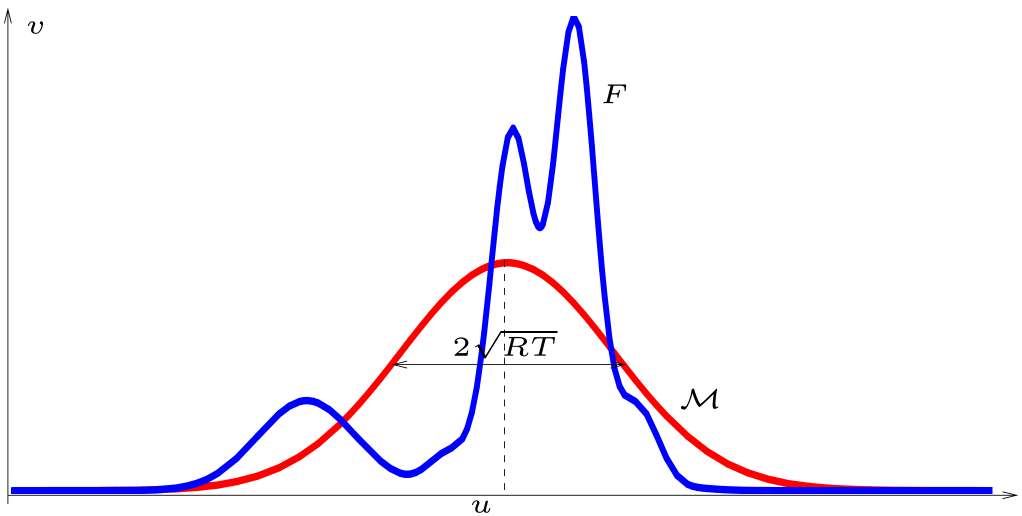
$$\text{momentum } \rho u = \int_{\mathbb{R}^3} vF(t, x, v)\, dv,$$

$$\text{total energy } E = \int_{\mathbb{R}^3} \tfrac{1}{2}|v|^2 F(t, x, v)\, dv.$$

Kinetic theory

- temperature T defined by $E = \frac{1}{2}\rho|u|^2 + \frac{3}{2}\rho RT$
- equilibrium state: Maxwellian distribution, depends only on v, ρ, 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

$$\underbrace{\partial_t F + v \cdot \nabla_x F}_{\text{transport}} = \underbrace{Q(F)}_{\text{collisions}}$$

- $Q(F)$ 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: 400×100 space cells, 40×40 discrete velocities

- F is independent of $z \Rightarrow$ the transport operator does not contain explicitely the velocity v_z.
- define the reduced distribution function $f(t,x,y,v_x,v_y) = \int_{\mathbb{R}} F\, dv_z$, and integrate BGK w.r.t v_z

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

$$\Downarrow \qquad \int_{\mathbb{R}} .\, dv_z$$

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

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

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

Numerical method: *reduced distribution technique*

but T cannot be defined through f only:

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

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

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

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

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

and the macroscopic quantities are obtained through f and g by

$$\rho = \int_{\mathbb{R}^2} f \, dv^2, \qquad \rho u = \int_{\mathbb{R}^2} v f \, dv^2,$$

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

Numerical method: *velocity discretization*

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

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

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 $(v_k)_{k=1}^N$

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

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

Numerical method: *space discretization*

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

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

$$\downarrow$$

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

where the numerical fluxes are defined by

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

$$\phi_{i,j+\frac{1}{2}}(f_{\mathrm{k}}) = \frac{1}{2}\Big(v_{y,k}(f_{\mathrm{k},i,j+1} + f_{\mathrm{k},i,j}) - |v_{y,k}|(\Delta f_{\mathrm{k},i,j+\frac{1}{2}} - \Phi_{\mathrm{k},i,j+\frac{1}{2}})\Big)$$

Numerical method: *time discretization*

transient solutions: first order backward euler

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

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)

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

then linearization:

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

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

Numerical method: *time discretization*

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

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

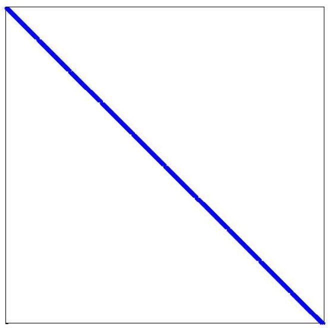
where

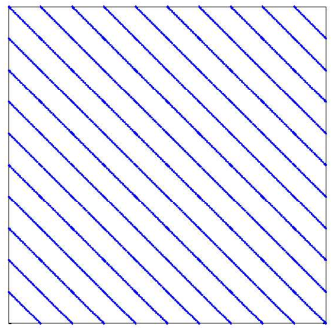
- $\delta U^n = U^{n+1} - U^n$,
- I is the unit matrix,
- T contains the transport coeffi cients, (b. c. in in B)
- R^n is the Jacobian matrix of the collision operator,
- RHS^n is the residual (transport and collision operators applied to U^n).

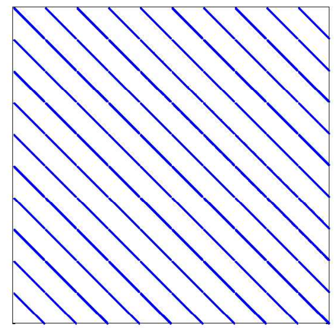
Numerical method: *linear system*

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

- very large linear system
- sparse matrices

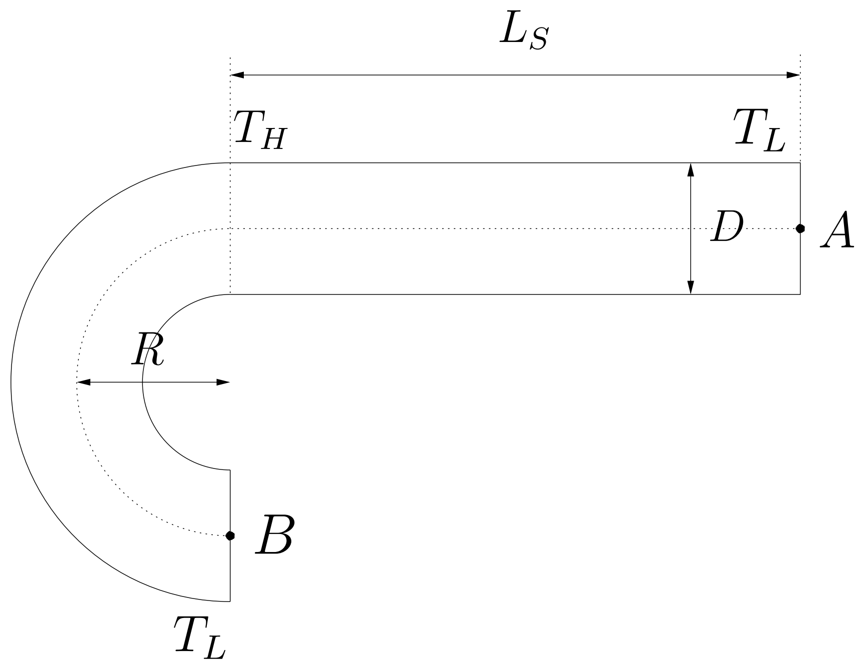
$T =$ 

$B =$ 

$R^n =$ 

- an adapted iterative solver is used

Numerical simulations

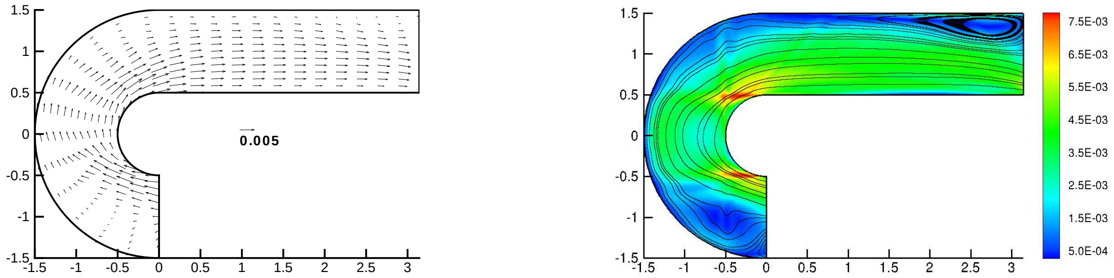


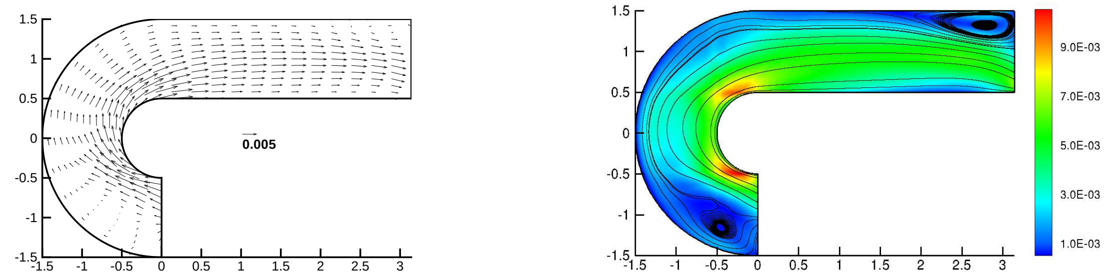
Basic unit of our devices : a hook shaped channel.

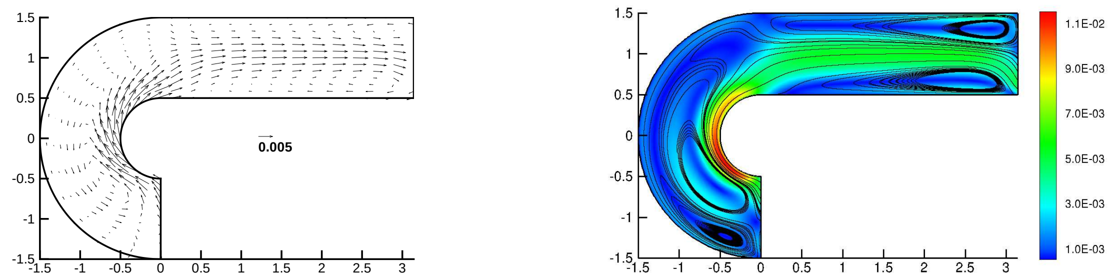
Three sizes: thick ($D/R = 1$), medium (0.5), thin (0.2)

Three Knudsen numbers: Kn $= 1, 0.5, 0.1$

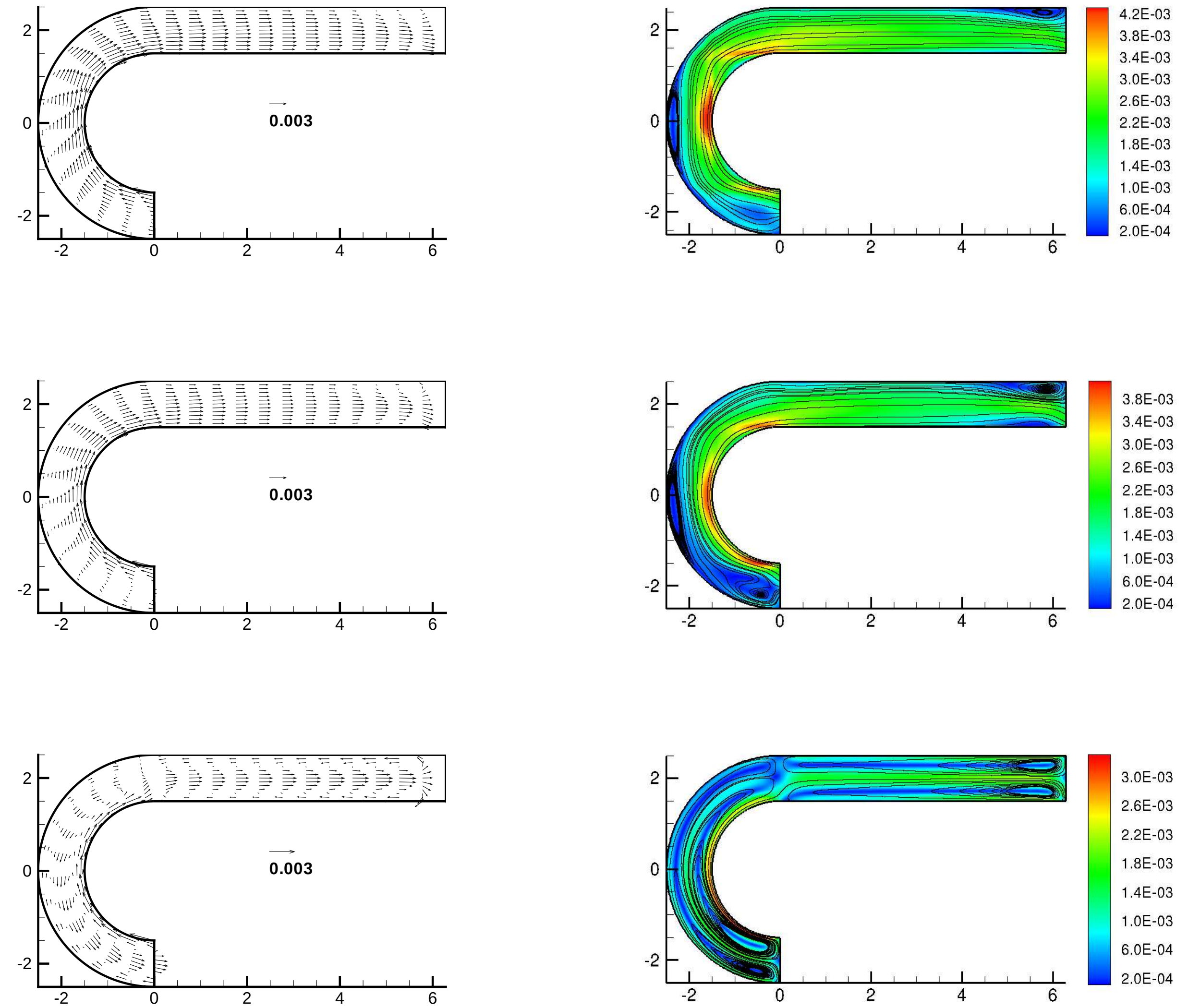
Numerical simulations: *Circulating flow*



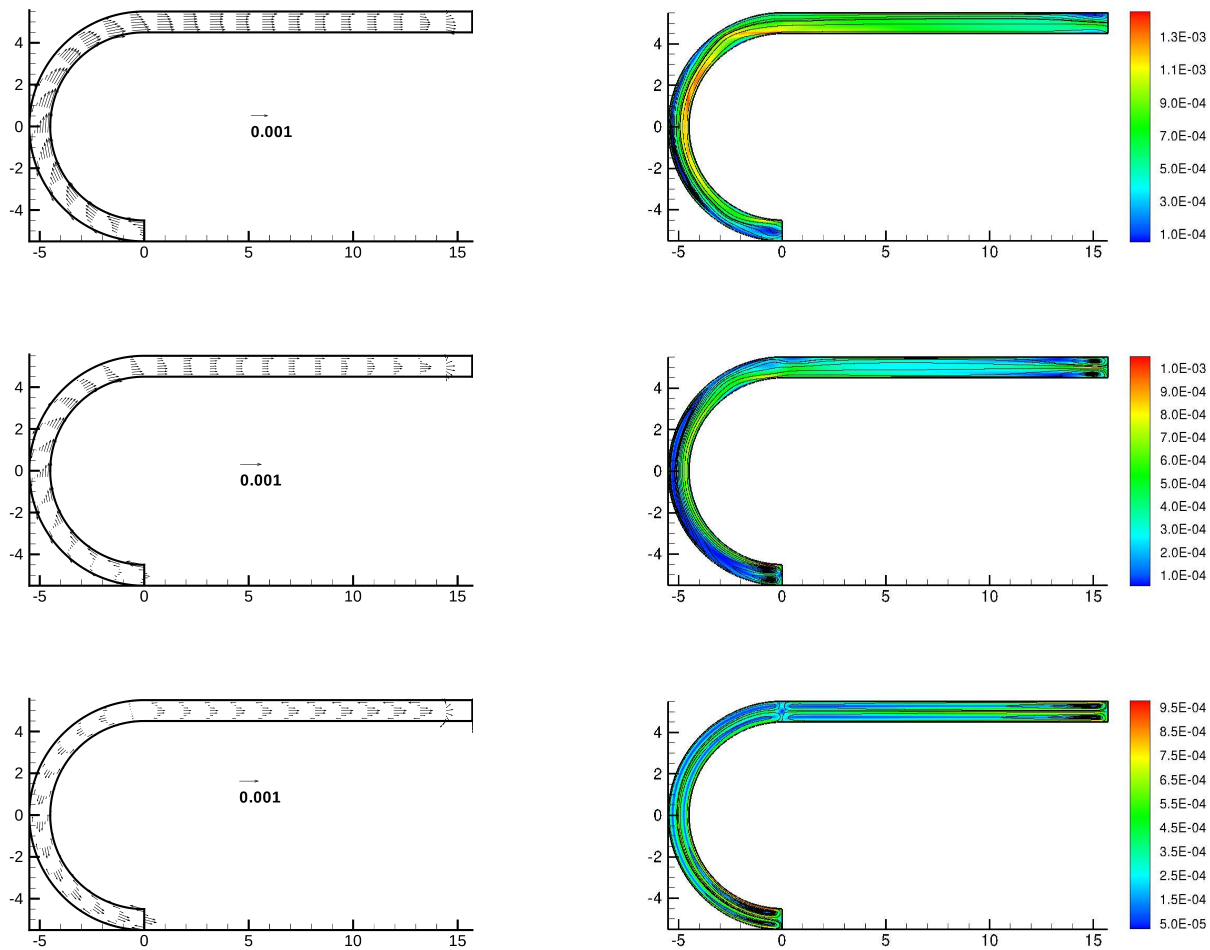




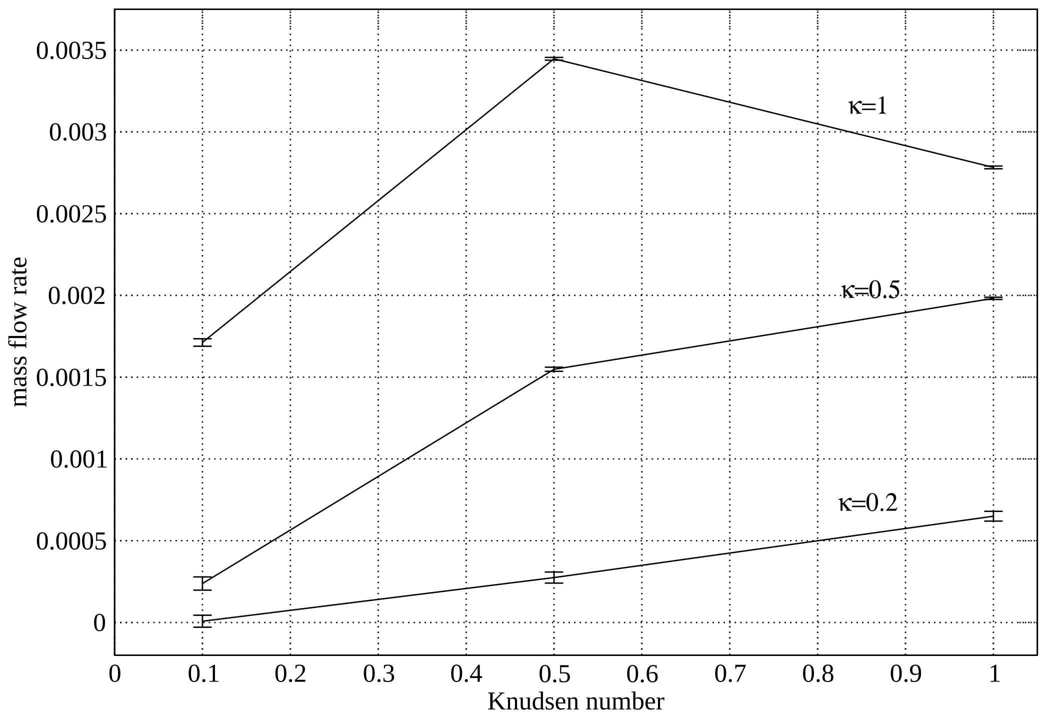
Numerical simulations: *Circulating flow*



Numerical simulations: *Circulating flow*



Numerical simulations: *Circulating flow*

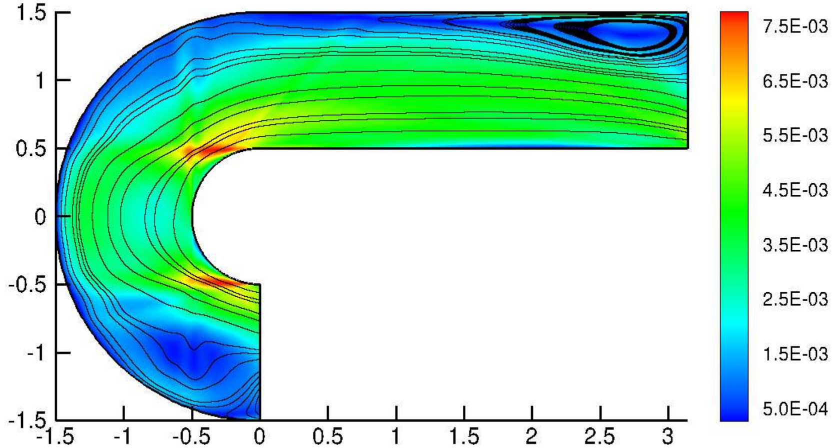


Mass fbw rate in the ring-shaped channel as a function of the Knudsen number.

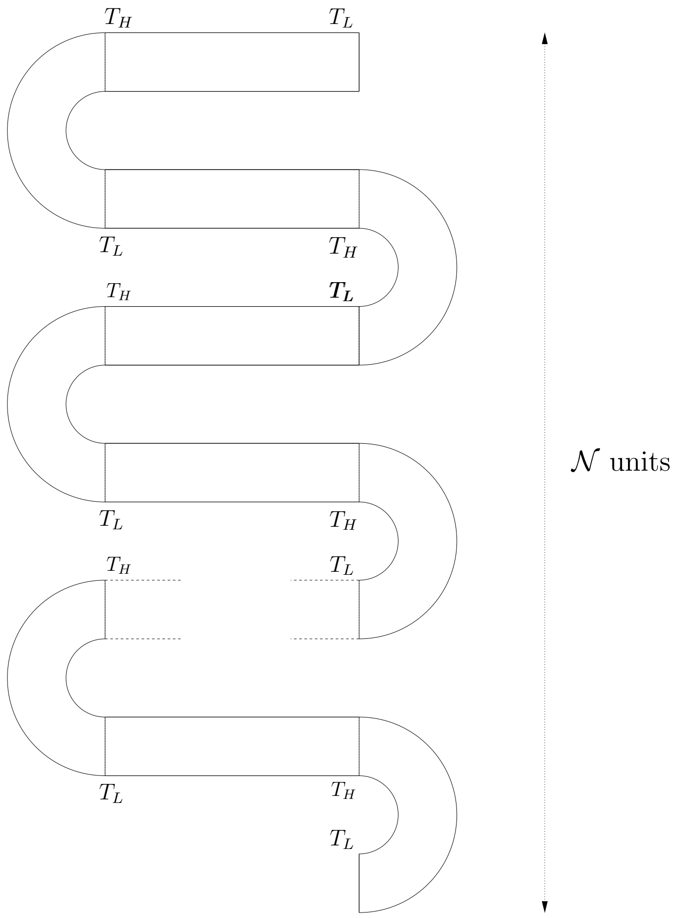
Each curve corresponds to one of the three different size of channel

Numerical simulations: *Circulating flow*

time evolution of the density and velocity fields + mass flow rate:

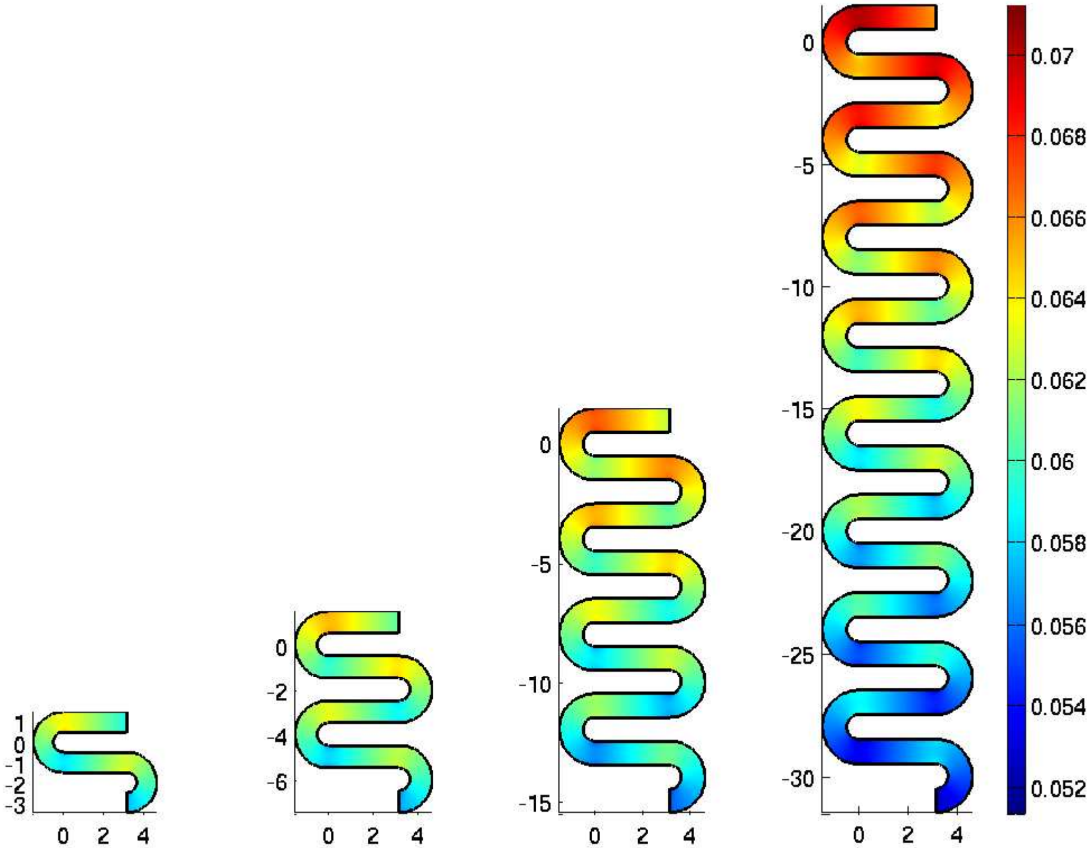


Numerical simulations: *Micro-Pump*



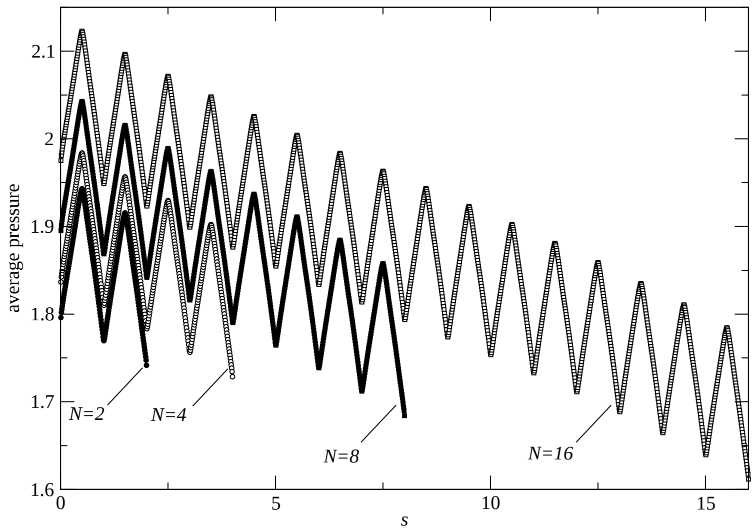
Closed cascade device to generate a pumping effect.

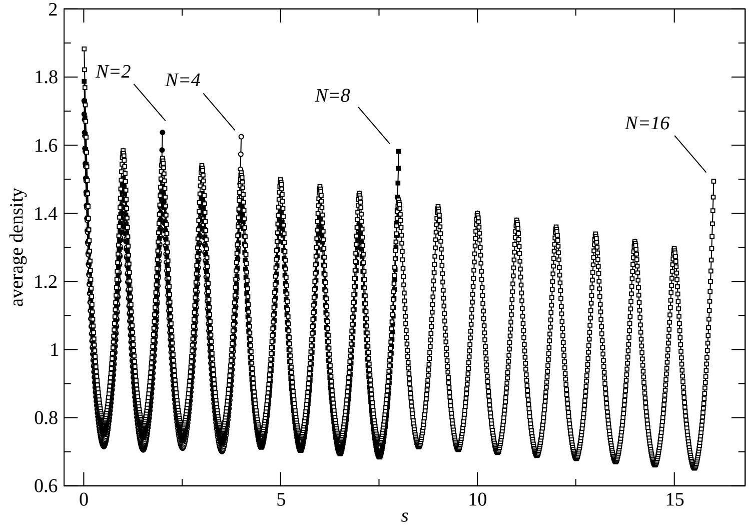
Numerical simulations: *Micro-Pump*



Pressure field in the closed cascade device: 2, 4, 8 and 16 units.

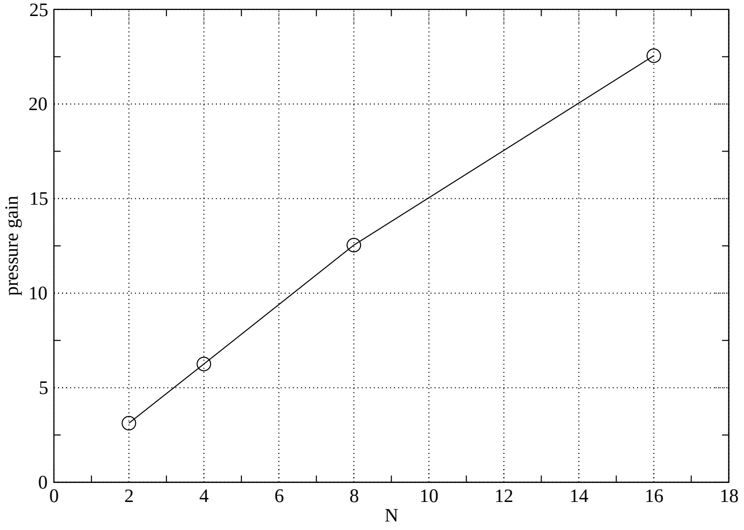
Numerical simulations: *Micro-Pump*

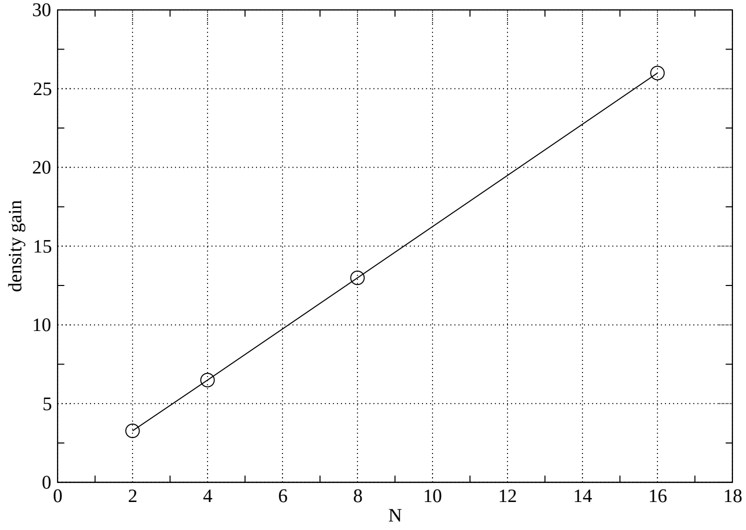




Non-dimensionalized average pressure (left) and density (right) profi les for the pumping device with several numbers N of units. Thick case with Kn $= 0.5$.

Numerical simulations: *Micro-Pump*

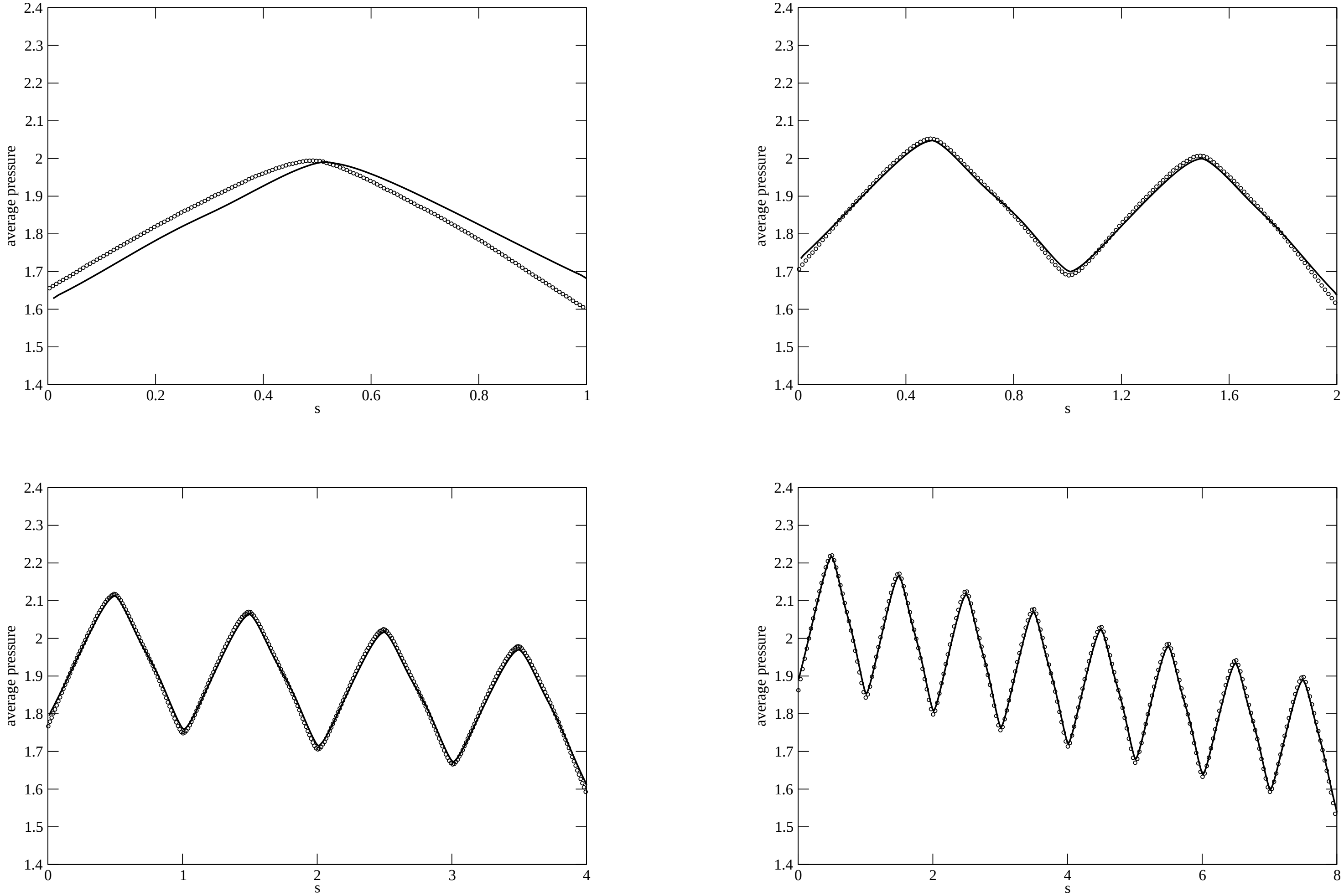




Pressure (left) and density gain (right) for the pumping device with several numbers N of units. Thick case with $\mathrm{Kn} = 0.5$.

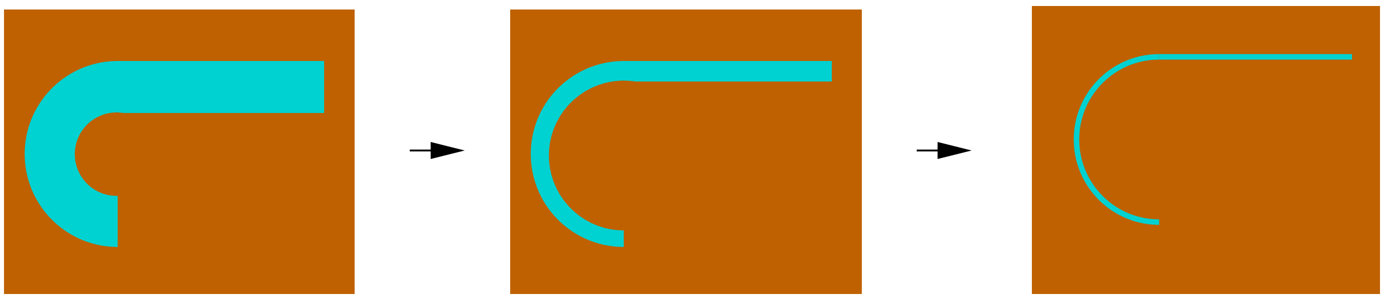
Numerical simulations: *Micro-Pump*

comparison BGK/DSMC



Asymptotic model

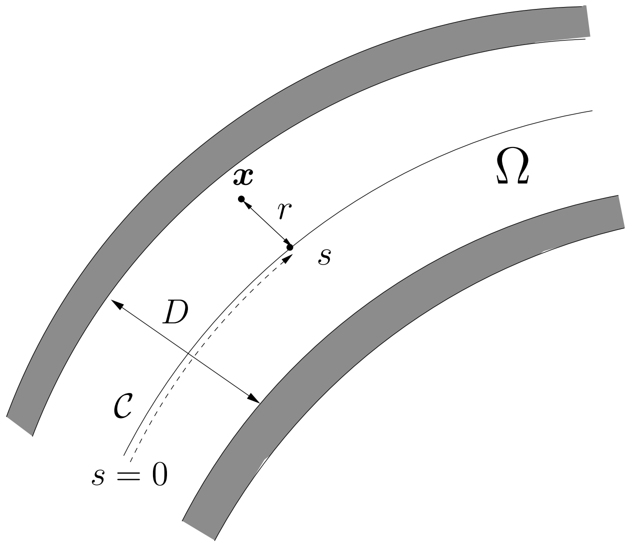
- problem: simulation impossible for a large number of units
- idea: develop a simplified mathematical model (asymptotic analysis)



- 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)]



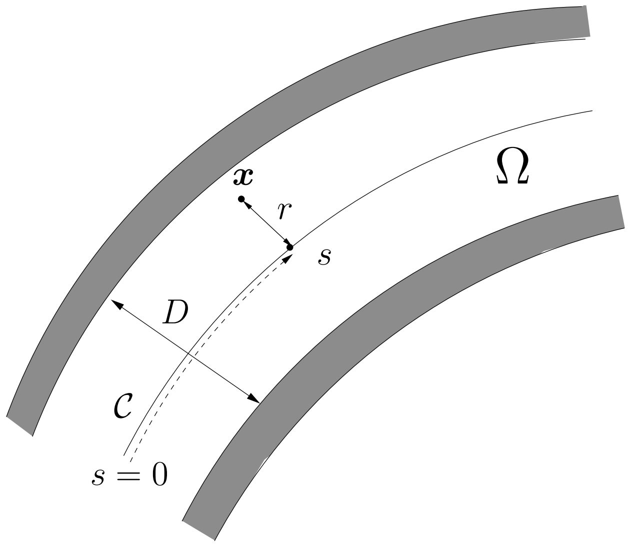
BGK equation:

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

Local coordinates:

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

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



BGK equation:

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

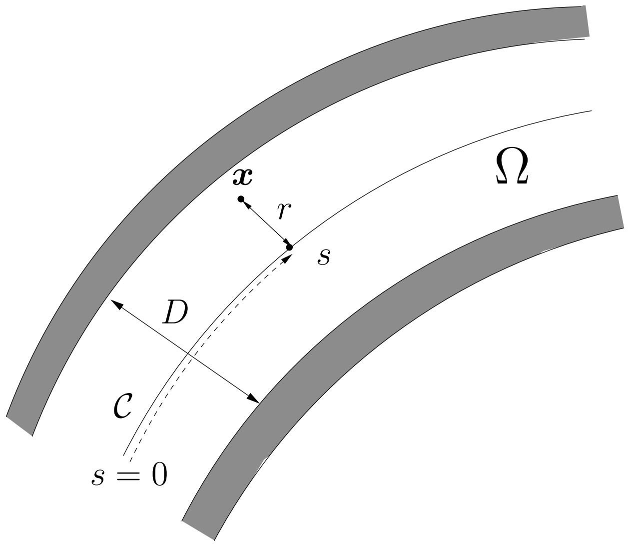
Local coordinates:

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

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

Asymptotic model

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



BGK equation:

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

Local coordinates:

$$\epsilon^2 \partial_t f + \epsilon (1 - \kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1 - \kappa r)^{-1} v_r v_s \partial_{v_s} f - \kappa (1 - \kappa r)^{-1} v_s^2 \partial_{v_r} f = \frac{1}{K_0} \rho (M[\rho, \boldsymbol{u}, T] - f)$$

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

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

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

Asymptotic model

Theorem (formal)

(i) $\varrho \longrightarrow \rho_0$, solution of

$$\partial_t \rho_0 + \partial_s j_1 = 0,$$

$$j_1 = \underbrace{\sqrt{T_w} M_P \partial_s \rho_0}_{\text{diffusion}} \quad + \quad \underbrace{\frac{\rho_0}{\sqrt{T_w}}(M_P + M_T)\partial_s T_w}_{\text{drift=thermal creep !}},$$

(where M_P and M_T are non-linear functions of ρ_0)

(original method: Babovski, Bardos, Platkowski (1991))

(ii) $M_P \leq 0$

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

Asymptotic model

$$\epsilon^2 \partial_t f + \epsilon (1-\kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1-\kappa r)^{-1} v_r v_s \partial_{v_s} f$$
$$- \kappa (1-\kappa r)^{-1} v_s^2 \partial_{v_r} f = \frac{1}{K_0} \rho (M[\rho, \boldsymbol{u}, T] - f)$$

Hilbert expansion: $f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \ldots$

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

$$\Downarrow$$

ρ_0 to be determined, and $j_0 = \dfrac{1}{\epsilon} \displaystyle\int_{-1/2}^{1/2} \int_{\mathbb{R}^3} v_s f_0 \, d\boldsymbol{v} dr = 0$

Asymptotic model

$$\epsilon^2 \partial_t f + \epsilon (1-\kappa r)^{-1} v_s \partial_s f + v_r \partial_r f + \kappa (1-\kappa r)^{-1} v_r v_s \partial_{v_s} f$$
$$- \kappa (1-\kappa r)^{-1} v_s^2 \partial_{v_r} f = \frac{1}{K_0} \rho (M[\rho, \boldsymbol{u}, T] - f)$$

Hilbert expansion: $f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \ldots$

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

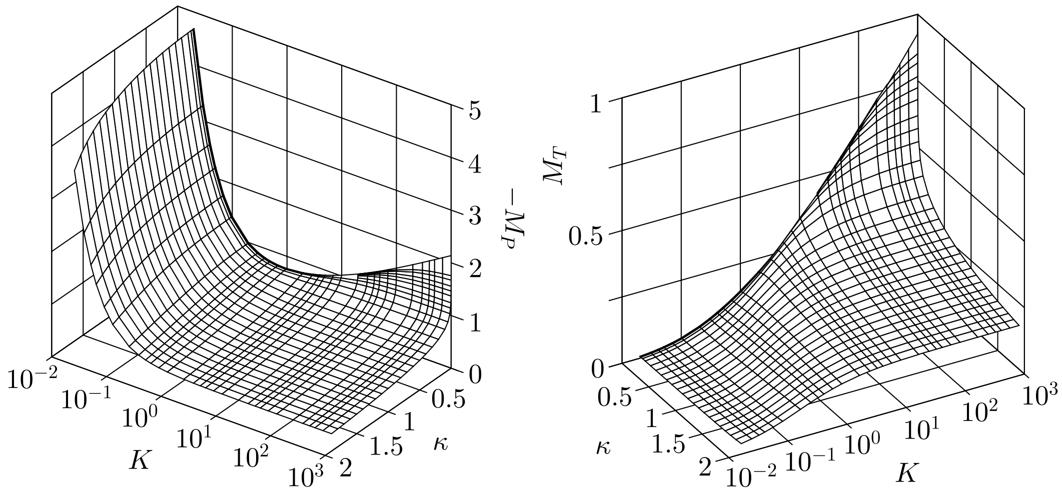
$$\Downarrow$$

$\rho_1 = 0$ and

$$j_1(s,t) = \int_{-1/2}^{1/2} \int_{\mathbb{R}^3} v_s f_1 \, d\boldsymbol{v} dr = \sqrt{T_w} M_P \partial_s \rho_0 + \frac{\rho_0}{\sqrt{T_w}} (M_P + M_T) \partial_s T_w$$

Numerical computations:

- M_P and M_T:
  - depend only on s through K and κ
  - 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 ε
  - construction of a database for M_P and M_T

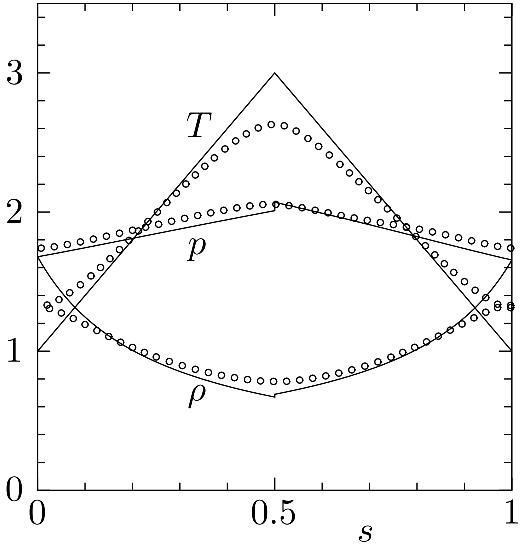


Asymptotic model

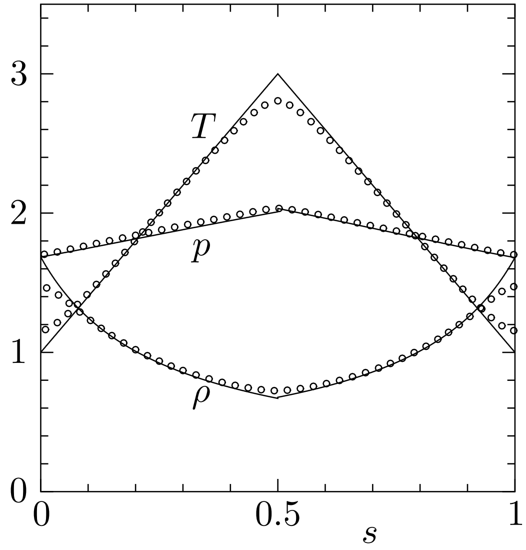
Numerical computations:

- 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

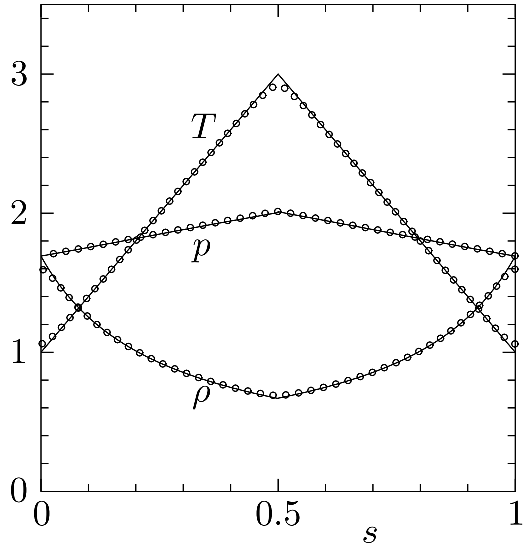
Comparison with 2D BGK: circulating flow



(a)



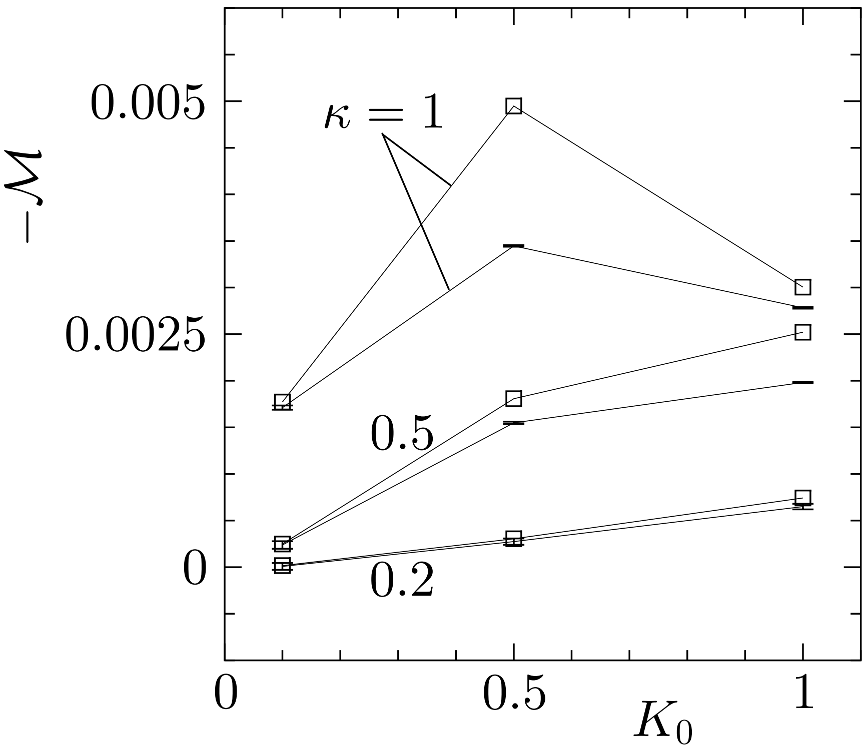
(b)



(c)

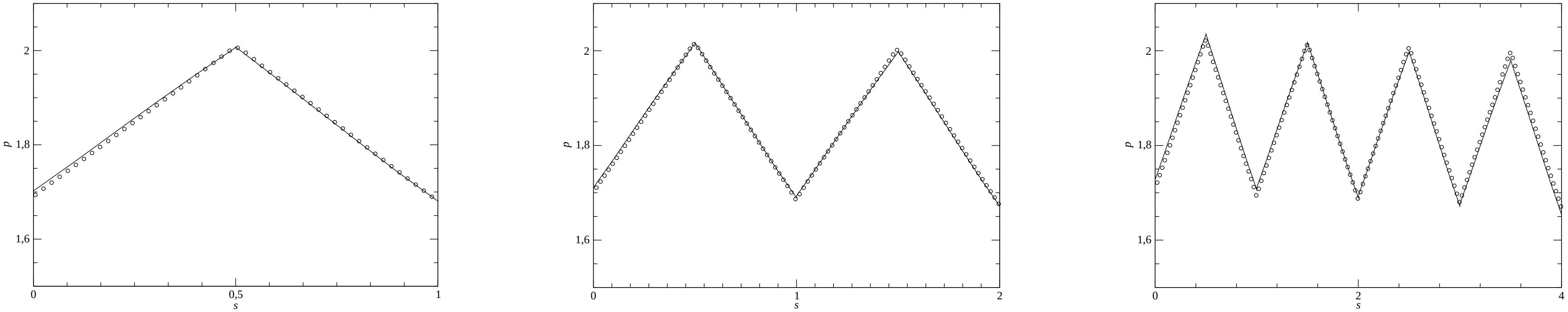
Asymptotic model

Comparison with 2D BGK: circulating flow

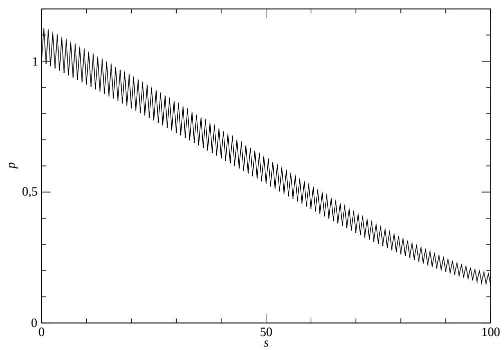


Asymptotic model

Comparison with 2D BGK: micro-pump



100 unit pump: pressure gain = factor 6



Perspectives

- 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