Modeling and calculations of rarefied gas flows: DSMC vs kinetic equation

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Main problems of vacuum technology:

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Gas dynamics is a basis of vacuum technology

Gas rarefaction

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$$\mathrm{Kn} = \frac{\textit{molecular mean free path}}{\textit{characteristic size}}$$

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Gas rarefaction

Free molecular regime

$$\text{Kn} \gg 1$$

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- Test particle Monte Carlo method

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- Test particle Monte Carlo method
- Method of angle elements

Gas rarefaction

Hydrodynamic regime

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Continuum mechanics equations are solved

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- The methods are well developed and well known.

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Hydrodynamic regime

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Continuum mechanics equations are solved

- The methods are well developed and well known.
- There are many commercial codes.

Gas rarefaction

Transition regime

$$\mathrm{Kn} \sim 1$$

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Navier-Stokes eq. is not valid
Intermolecular collision cannot be neglected

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- Direct simulation Monte Carlo method is applied

Gas rarefaction

Transition regime

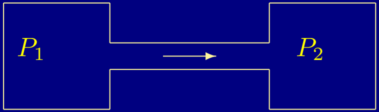
$$\mathrm{Kn} \sim 1$$

Navier-Stokes eq. is not valid
Intermolecular collision cannot be neglected

- Direct simulation Monte Carlo method is applied
- Kinetic Boltzmann equation is solved

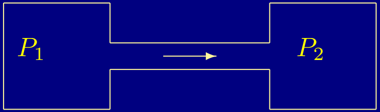
TYPICAL PROBLEMS

Poiseuille flows



$P_1 > P_2$

Poiseuille flows



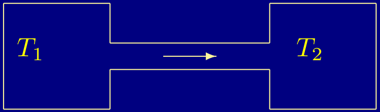
$P_1 > P_2$

To be calculated:

$\dot{M}$ mass flow rate

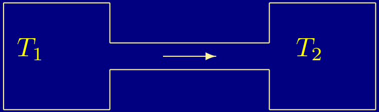
density (or pressure) distribution

Non-isothermal flows, thermal creep



$T_1 < T_2$

Non-isothermal flows, thermal creep



$T_1 < T_2$

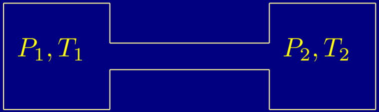
To be calculated:

$\dot{M}$ mass flow rate

Q heat flow rate

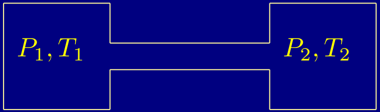
density (or pressure) distribution

Thermomolecular pressure difference



$\dot{M} = 0$ no mass flow

Thermomolecular pressure difference



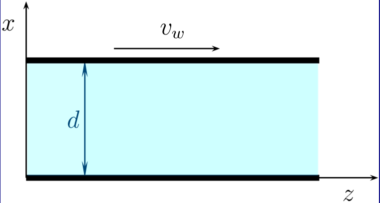
$\dot{M} = 0$ no mass flow

To be calculated:

What is the pressure ratio

$$\frac{P_2}{P_1} = \left(\frac{T_2}{T_1}\right)^{\gamma} \qquad 0 \geq \gamma \geq 0.5$$

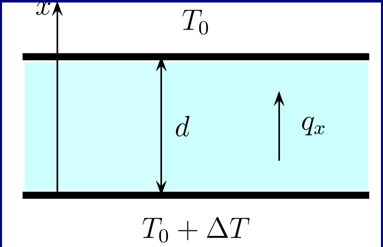
Couette flow



To be calculated:

P_{xz} shear stress

Heat transfer between two plates

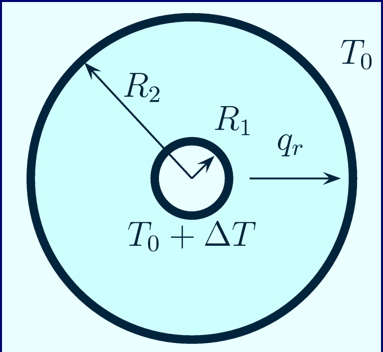


To be calculated:

q_x Heat flux

Heat transfer between two cylinders

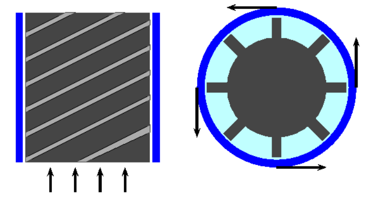
Pirani sensor



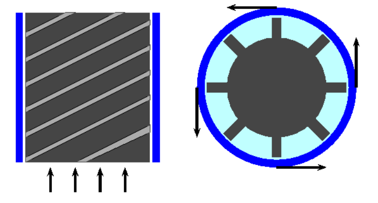
To be calculated:

q_r Heat flux

Holweck pump



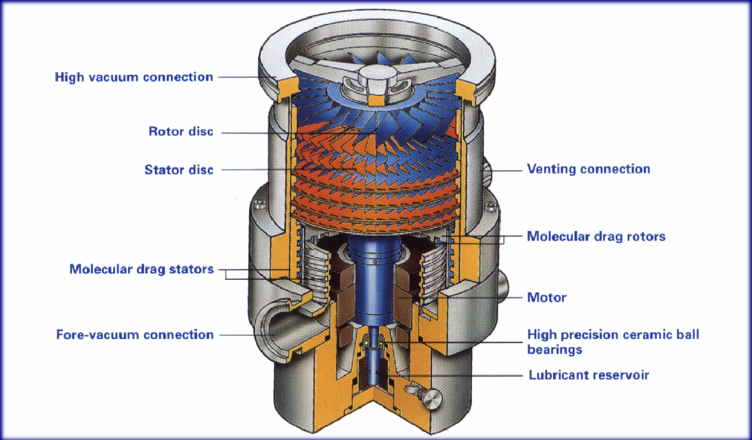
Holweck pump



To be calculated:

- Compression ratio
- Pumping speed
- Torque

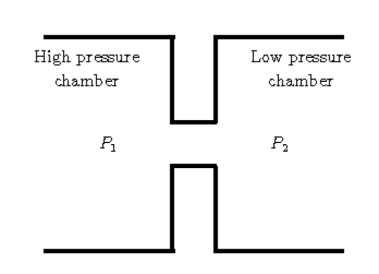
Combination Holweck and turbomolecular pumps



Direct Simulation Monte Carlo method

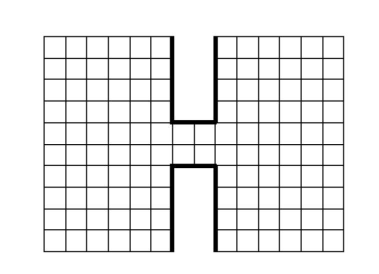
DSMC

DSMC, Main ideas



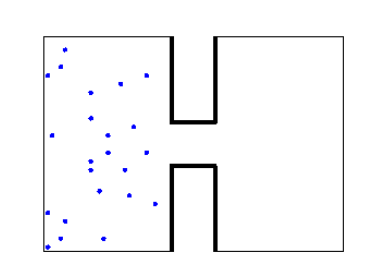
Gas flow through a short tube.

DSMC, Main ideas



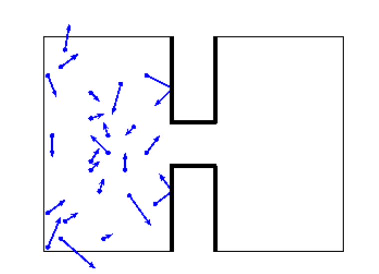
Flow region is divided into cells

DSMC, Main ideas



M model particles are considered.
Their positions $\boldsymbol{r}_i$ and velocities $\boldsymbol{v}_i$ are saved.

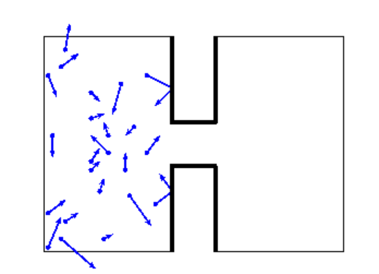
DSMC, Main ideas



Time is advanced in steps Δt.
New positions are calculated

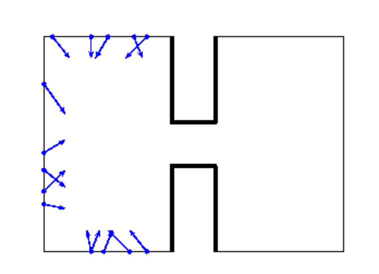
$$\boldsymbol{r}_{i,new} = \boldsymbol{r}_{i,old} + \boldsymbol{v}_i \Delta t$$

DSMC, Main ideas



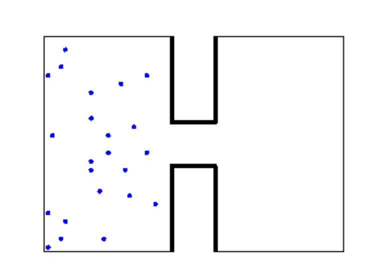
Gas-surface interaction is simulated.
Some particles are removed.

DSMC, Main ideas



New particles are generated.

DSMC, Main ideas

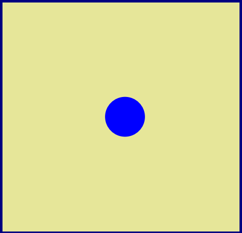


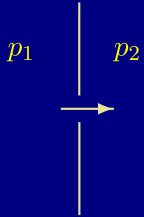
Intermolecular interactions are simulated.
Macroscopic quantities are calculated.

DSMC, Main ideas

All steps are repeated many times in order to reduce the statistical noise.

DSMC, Orifice flow into vacuum





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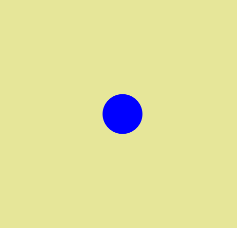

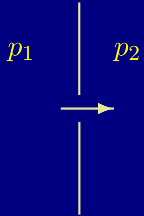

Reduced flow rate

$$W = \frac{\dot{M}}{\dot{M}_0}, \qquad \dot{M}_0 = \frac{\sqrt{\pi}a^2}{v_m} p_1$$

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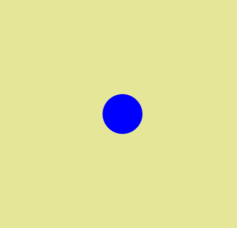

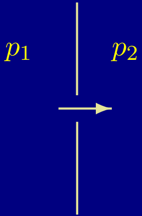

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Rarefaction parameter

$$\delta = \frac{PR}{\mu v_m} \propto \frac{1}{\text{Kn}}, \qquad v_m = \sqrt{\frac{2R_g T}{M}}$$

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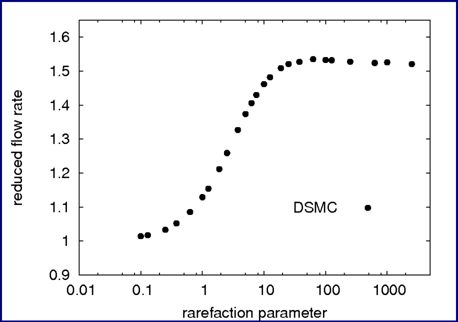

Sharipov, AIAA Journal (2002); J. Fluid Mech. (2004)

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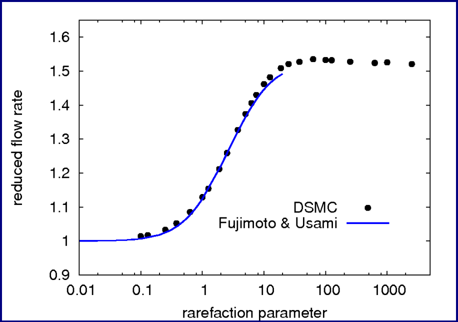

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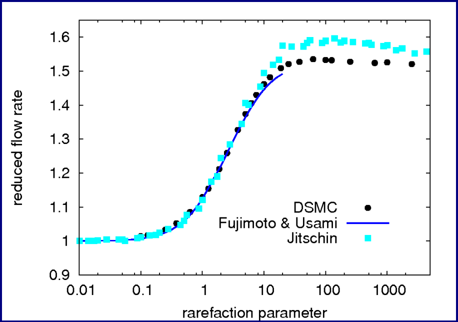

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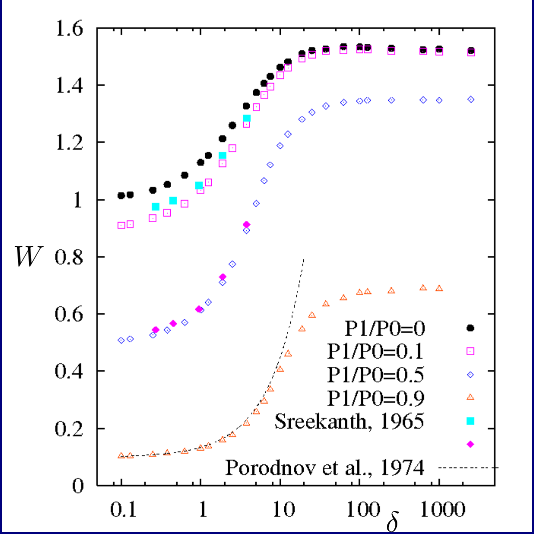
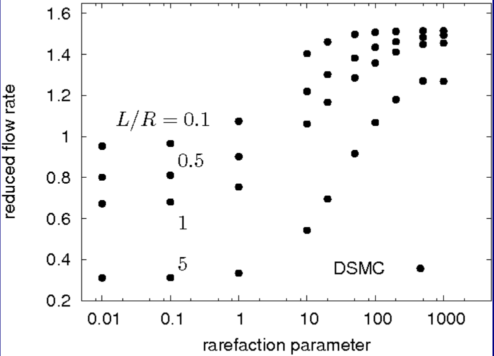
Jitschin et al., Vacuum (1995)

DSMC, Orifice flow into background gas



Sharipov, J. Fluid Mech. (2004)

DSMC, Flow into vacuum through a short tube



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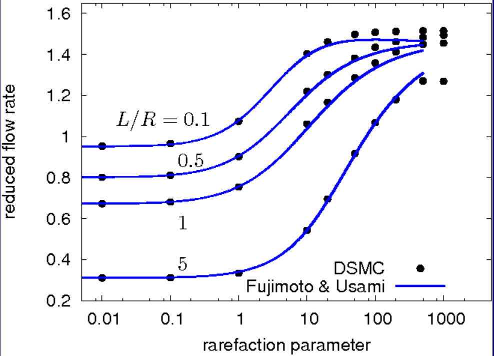
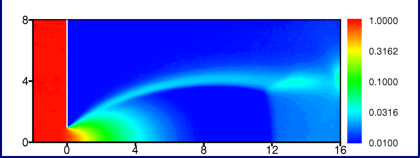


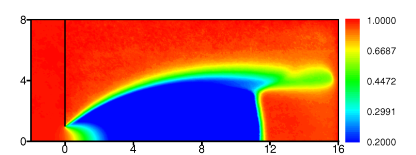
Fujimoto & Usami (1984)

DSMC, Orifice flow into background gas

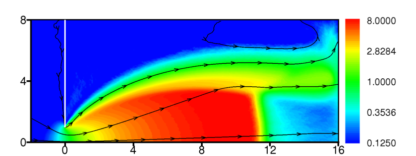
Flow-field at $p_2/p_1 = 100$ and $\delta = 1000$



ϱ/ϱ_0 density



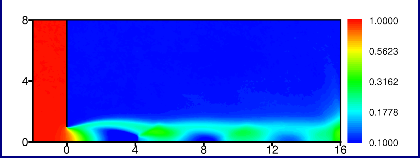
T/T_0 temperature



Local Mach number

DSMC, Orifice flow into background gas

Flow-field at $p_2/p_1 = 10$ and $\delta = 1000$



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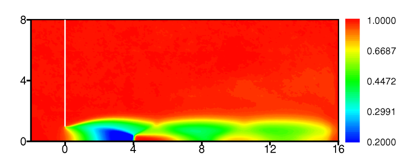

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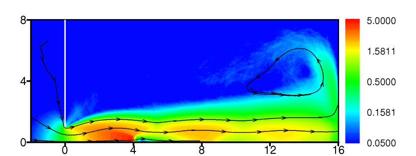

Mach number

DSMC

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DSMC

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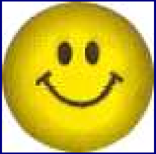
- The physical cells can be easily adapted to any geometrical configuration
- It is easy to simulate non-elastic collisions occurring in polyatomic gases
- Even more complicated phenomena like dissociation, ionization etc. are considered without effort.
- The books by G.A. Bird contain numerical codes that can be modified and used in engineer calculations.

DSMC

NICE!



DSMC

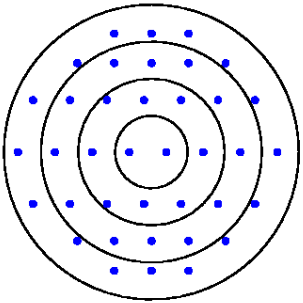
IS IT UNIVERSAL REMEDY?

DSMC, disadvantages

UNFORTUNATELY NOT

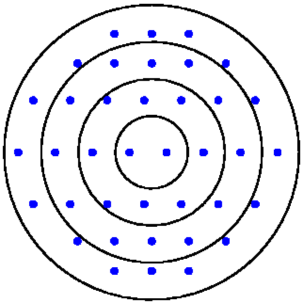
DSMC, disadvantages

Axisymmetrical flows:



DSMC, disadvantages

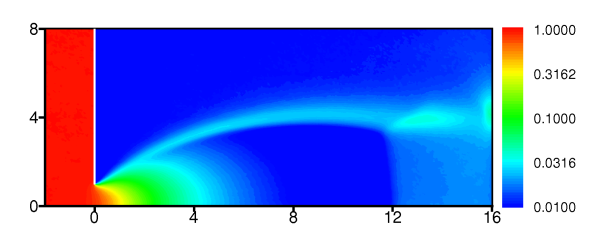
Axisymmetrical flows:



It is necessary to use the radial weighting factor.

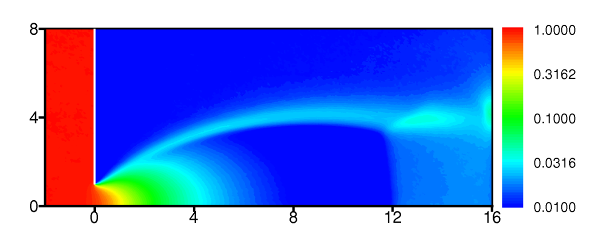
DSMC, disadvantages

Flow with high variation of density



DSMC, disadvantages

Flow with high variation of density

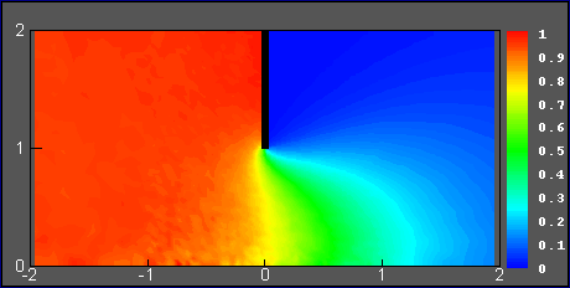


It is necessary to use the longitudinal weighting factor.

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0$

Density distribution

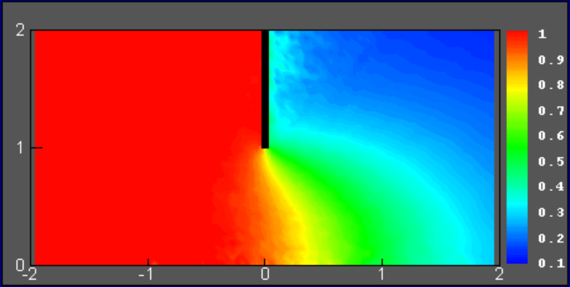


Number of samples 10^4
Calculation time - few hours

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0$

Temperature distribution



Number of samples 10^4
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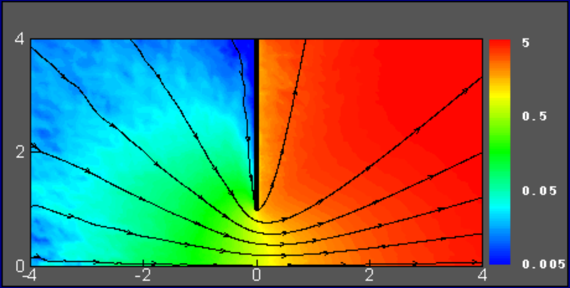
DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0$

Local Ma distribution

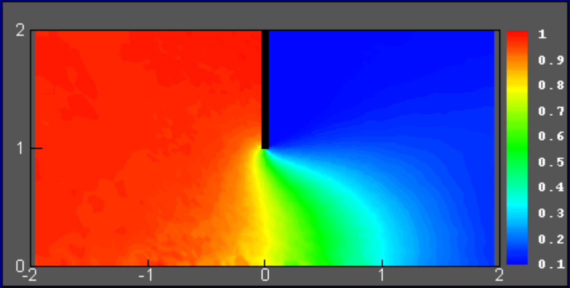


Number of samples 10^4
Calculation time - few hours

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.1$

Density distribution



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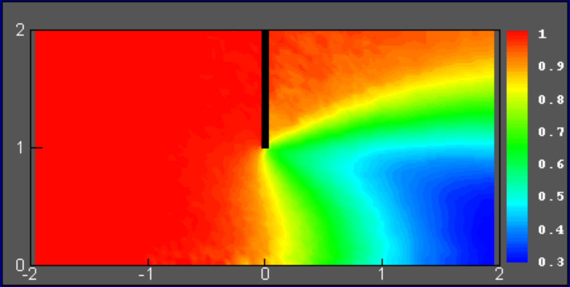

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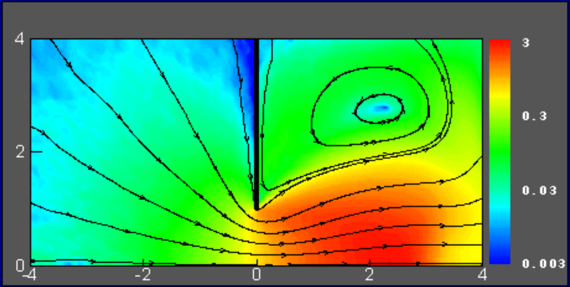
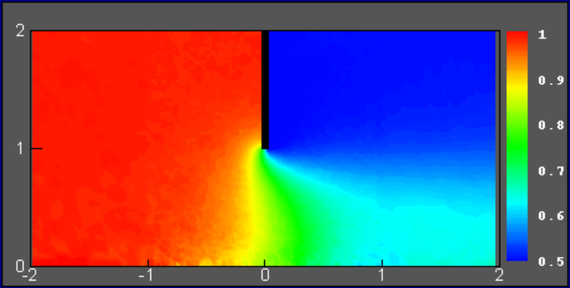


Number of samples 10^4
Calculation time - few hours

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.5$

Density distribution

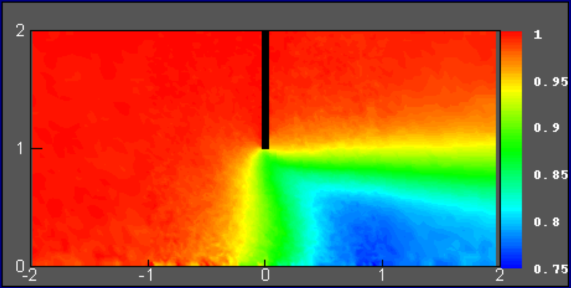


Number of samples 10^5
Calculation time - few days

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.5$

Temperature distribution

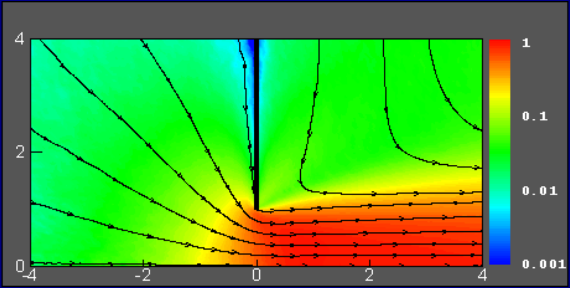


Number of samples 10^5
Calculation time - few days

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.5$

Local Ma distribution



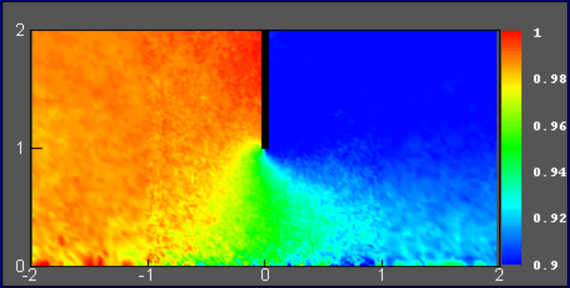
Number of samples 10^5

Calculation time - few days

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.9$

Density distribution

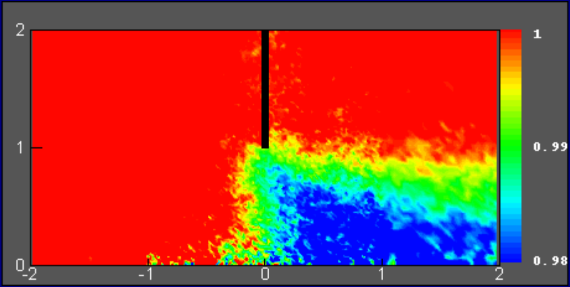


Number of samples 10^6
Calculation time - few weeks

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.9$

Temperature distribution

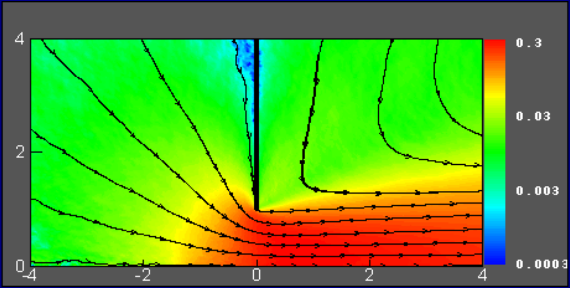


Number of samples 10^6
Calculation time - few weeks

DSMC, Statistical noise

Kn=0.01 and $P_2/P_1 = 0.9$

Local Ma distribution



Number of samples 10^6
Calculation time - few weeks

DSMC, statistical noise

Statistical noise is very significant
at low Mach number

DSMC

disadvantages

DSMC

disadvantages

- A large computer memory

DSMC

disadvantages

- A large computer memory
- Significant non-uniformity of model particle distribution

DSMC

disadvantages

- A large computer memory
- Significant non-uniformity of model particle distribution
- Significant statistical noise

Kinetic equation

Velocity distribution function

$f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}$ number of molecules in $\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}$

$n(t, \boldsymbol{r}) = \int f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - number density

$\boldsymbol{u}(t, \boldsymbol{r}) = \frac{1}{n} \int \boldsymbol{v} f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - bulk velocity

$P(t, \boldsymbol{r}) = \frac{m}{3} \int V^2 f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - pressure

$T(t, \boldsymbol{r}) = \frac{m}{3nk} \int V^2 f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - temperature

$\boldsymbol{q}(t, \boldsymbol{r}) = \frac{m}{2} \int V^2 \boldsymbol{V} f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - heat flux vector

$\boldsymbol{V} = \boldsymbol{v} - \boldsymbol{u}$

Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} = Q(f f_*)$$

$$Q(f f_*) = \int \left(f' f'_* - f f_* \right) |\boldsymbol{v} - \boldsymbol{v}_*| b \mathrm{d}b \, \mathrm{d}\varepsilon \, \mathrm{d}\boldsymbol{v}_*$$

$\boldsymbol{v}'$ and $\boldsymbol{v}_*{}'$ - pre-collision molecular velocities

$\boldsymbol{v}$ and $\boldsymbol{v}_*$ - post-collision molecular velocities

Boltzmann equation

Discrete velocity method:

$$\boldsymbol{v}_1,\ \boldsymbol{v}_2,\ \dots,\boldsymbol{v}_N,$$

The BE is split into N differential eqs. coupled via the collisions integral

Model equations

The collision integral is simplified

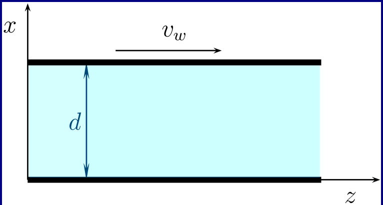
BGK model

$$Q(f\,f_*) = \nu\left(f^M - f\right)$$

S model

$$Q(f\,f_*) = \nu\left\{f^M\left[1 + \frac{2m(\boldsymbol{q}\cdot\boldsymbol{V})}{15n(kT)^2}\left(\frac{mV^2}{2kT} - \frac{5}{2}\right)\right] - f\right\}$$

Couette flow



P_{xz} shear stress?

Couette flow

Input equation

$$c\frac{\partial\phi}{\partial x} = \delta(u-\phi), \quad u = \frac{1}{\sqrt{\pi}}\int \mathrm{e}^{-c^2}\phi(x,c)\mathrm{d}c$$

$$\delta = \frac{Pd}{\mu v_m} \propto \frac{1}{\mathrm{Kn}}$$

Couette flow

Input equation

$$c\frac{\partial \phi}{\partial x} = \delta(u - \phi), \quad u = \frac{1}{\sqrt{\pi}} \int \mathrm{e}^{-c^2} \phi(x, c) \mathrm{d}c$$

$$\delta = \frac{Pd}{\mu v_m} \propto \frac{1}{\mathrm{Kn}}$$

Free-molecular regime, $\delta = 0$

analytical solution

$$P_{xz}^{fm} = \frac{p}{\sqrt{\pi}} \frac{v_w}{v_m}, \quad v_m = \sqrt{2kT/m}$$

Couette flow

Transitional regime, $\delta \sim 1$

Equation is solved numerically in few seconds

Couette flow

Transitional regime, $\delta \sim 1$

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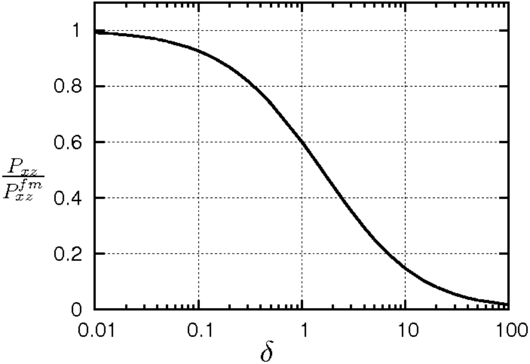
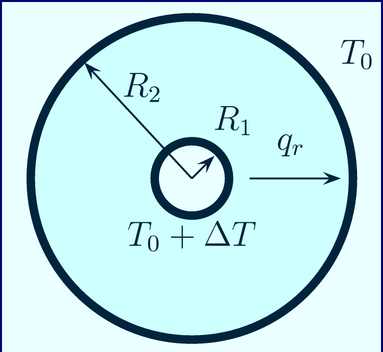


Heat transfer between two cylinders

Pirani sensor



To be calculated:

q_r Heat flux

Heat transfer between two cylinders

Input equation

$$c_r \frac{\partial h}{\partial r} - \frac{c_\varphi}{r}\frac{\partial h}{\partial \theta} = \delta\left[\upsilon + \tau\left(c^2 - \frac{3}{2}\right) + \frac{4}{15} q c_r \left(c^2 - \frac{5}{2}\right) - h\right],$$

$$\upsilon(r) = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(r, \boldsymbol{c}) \, \mathrm{d}\boldsymbol{c},$$

$$\tau(r) = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(r, \boldsymbol{c}) \left(\frac{2}{3}c^2 - 1\right) \mathrm{d}\boldsymbol{c},$$

$$q(r) = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(r, \boldsymbol{c}) \left(c^2 - \frac{5}{2}\right) c_r \, \mathrm{d}\boldsymbol{c}.$$

Heat transfer between two cylinders

Free-molecular regime, $\delta = 0$

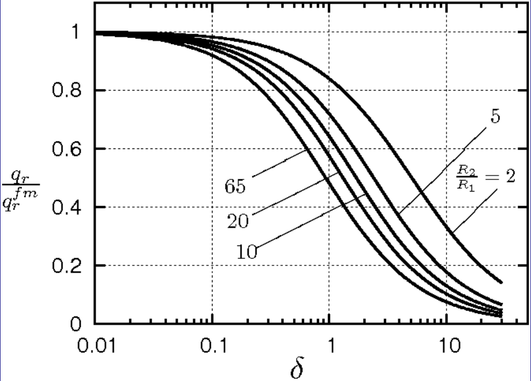
analytical solution

$$q_r^{fm}(r) = \frac{p\,v_m\,R_1}{\sqrt{\pi}r}\frac{\Delta T}{T_0},$$

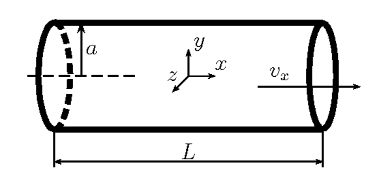
Heat transfer between two cylinders

Transitional regime, $\delta \sim 1$

Equation is solved numerically in few minutes



Flow through a long tube



$$\dot{M} = \frac{\pi a^2 P}{v_m}\left(-G_P \frac{a}{P}\frac{\mathrm{d}P}{\mathrm{d}x} + G_T \frac{a}{T}\frac{\mathrm{d}T}{\mathrm{d}x}\right)$$

$$G_P = G_P(\delta) \qquad G_T = G_T(\delta)$$

$$\delta = \frac{Pa}{\mu v_m} \sim \frac{1}{\mathrm{Kn}}$$

Flow through a long tube

Input equation to obtain G_P

$$c_r \frac{\partial \phi}{\partial r} - \frac{c_\theta}{r} \frac{\partial \phi}{\partial \theta} = \delta(u - \phi) - \frac{1}{2}, \quad u = \frac{1}{\sqrt{\pi}} \int \mathrm{e}^{-c^2} \phi(x, c) \mathrm{d}c$$

Flow through a long tube

Input equation to obtain G_{P}

$$c_r \frac{\partial \phi}{\partial r} - \frac{c_\theta}{r}\frac{\partial \phi}{\partial \theta} = \delta(u-\phi) - \frac{1}{2}, \quad u = \frac{1}{\sqrt{\pi}} \int \mathrm{e}^{-c^2} \phi(x,c) \mathrm{d}c$$

Free-molecular regime, $\delta = 0$

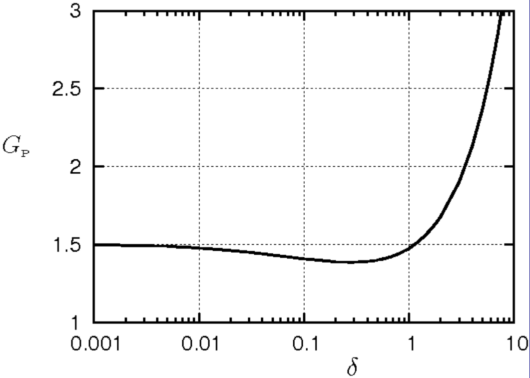
analytical solution

$$G_{\mathrm{P}} = \frac{8}{3\sqrt{\pi}}$$

Flow through a long tube

Transitional regime $\delta \sim 1$

Equation is solved numerically in few minutes



Flow through a long tube

Transitional regime $\delta \sim 1$

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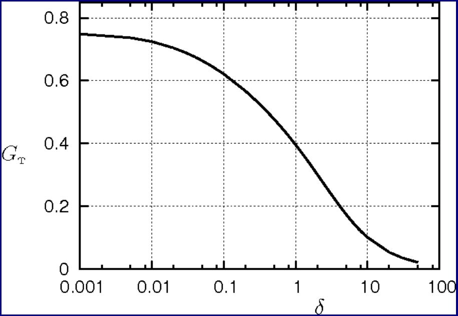
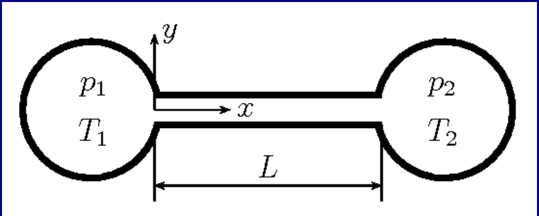


Flow through a long tube

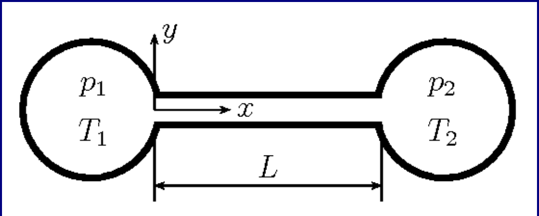


If $p_1 \gg p_2$ and/or $T_1 \gg T_2$ then Eq.

$$\dot{M} = \frac{\pi a^2 P}{v_m}\left(-G_P \frac{a}{P}\frac{\mathrm{d}P}{\mathrm{d}x} + G_T \frac{a}{T}\frac{\mathrm{d}T}{\mathrm{d}x}\right)$$

is integrated along x

Flow through a long tube



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is integrated along x

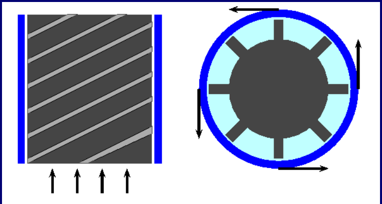
Numerical calculations of $\dot{M}$

can be carried out on-line

http://fisica.ufpr.br/sharipov

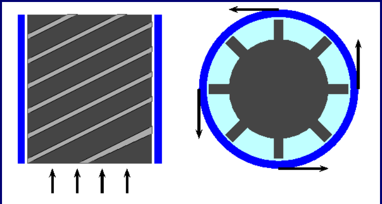
Modelling of Holweck pump

Scheme of pump

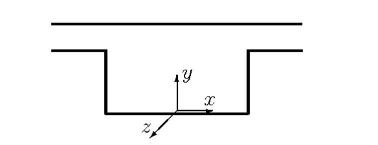


Modelling of Holweck pump

Scheme of pump



Scheme of single groove



Modeling of Holweck pump

First stage

Four problems are solved for a single groove

Modeling of Holweck pump

First stage

Four problems are solved for a single groove

- Longitudinal Poiseuille flow

Modeling of Holweck pump

First stage

Four problems are solved for a single groove

- Longitudinal Poiseuille flow
- Transversal Poiseuille flow

Modeling of Holweck pump

First stage

Four problems are solved for a single groove

- Longitudinal Poiseuille flow
- Transversal Poiseuille flow
- Longitudinal Couette flow

Modeling of Holweck pump

First stage

Four problems are solved for a single groove

- Longitudinal Poiseuille flow
- Transversal Poiseuille flow
- Longitudinal Couette flow
- Transversal Couette flow

Solution is determined by geometrical parameters of groove and by local rarefaction parameter.
This stage takes few days of computation.

Modeling of Holweck pump

Second stage stage

Compression ratio and pumping speed are calculated as a linear combinations of the four solutions.

Modeling of Holweck pump

Second stage stage

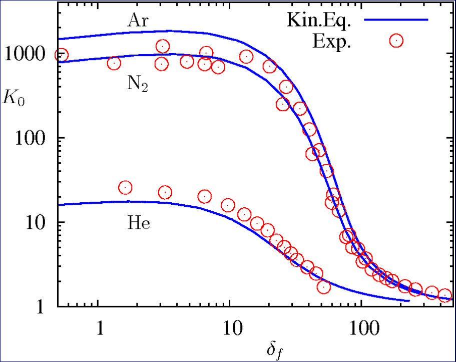
Compression ratio and pumping speed are calculated as a linear combinations of the four solutions.

This stage takes few seconds of computation.

Modelling of Holweck pump

Comparison numerical and experimental results

Compression ratio

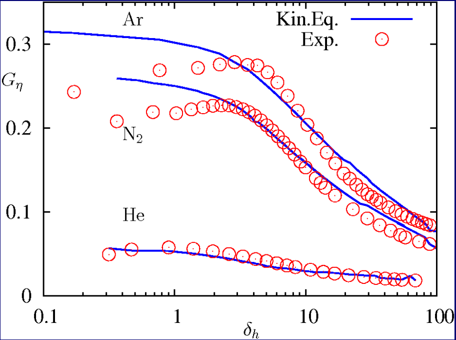


Sharipov, Fahrenbach, and Zipp, JVSTA, Vol. 23, P.1331 (2005).

Modelling of Holweck pump

Comparison numerical and experimental results

Dimensionless pumping speed



Sharipov, Fahrenbach and Zipp, JVSTA, Vol. 23 (1331).

Kinetic equation

Advantages

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- No statistical noise.

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- Short computational time (model equations)

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Advantages

- No statistical noise.
- Small computational memory
- Short computational time (model equations)
- Possibility to apply already obtained results

Kinetic equation

Disadvantages

Kinetic equation

Disadvantages

- Grids in both physical and velocity spaces must be carefully chosen

Kinetic equation

Disadvantages

- Grids in both physical and velocity spaces must be carefully chosen
- Discontinuity of the distribution function

Kinetic equation

Disadvantages

- Grids in both physical and velocity spaces must be carefully chosen
- Discontinuity of the distribution function
- Difficult generalization for gaseous mixtures and polyatomic gases

DSMC is recommended for:

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- Flows with high Mach number

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- Small (compact) region of gas flows

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- Small (compact) region of gas flows
- Complicated geometrical configurations

DSMC is recommended for:

- Flows with high Mach number
- Small (compact) region of gas flows
- Complicated geometrical configurations
- Flows with dissociation, recombinations, ionization etc.

Kinetic equation is recommended for:

Kinetic equation is recommended for:

- Flows with low Mach number

Kinetic equation is recommended for:

- Flows with low Mach number
- Extended region of gas flows

Kinetic equation is recommended for:

- Flows with low Mach number
- Extended region of gas flows
- Simple geometrical configurations

Kinetic equation is recommended for:

- Flows with low Mach number
- Extended region of gas flows
- Simple geometrical configurations
- Flows without dissociation, recombinations, ionization etc.

Thank you for your attention

http://fisica.ufpr.br/sharipov/