Lomonosov Moscow State University
Faculty of Mechanics and Mathematics

Gas separation effect induced by filaments with different temperatures

Artem Yakunchikov, *Vasily Kosyanchuk*

31st International Symposium on Rarefied Gas Dynamics
July 23 – 27, 2018, Glasgow, UK

Mechanics & Mathematics Faculty
Department of Engineering Mechanics and Applied Mathematics

Institute of Mechanics
Laboratory of Nanomechanics

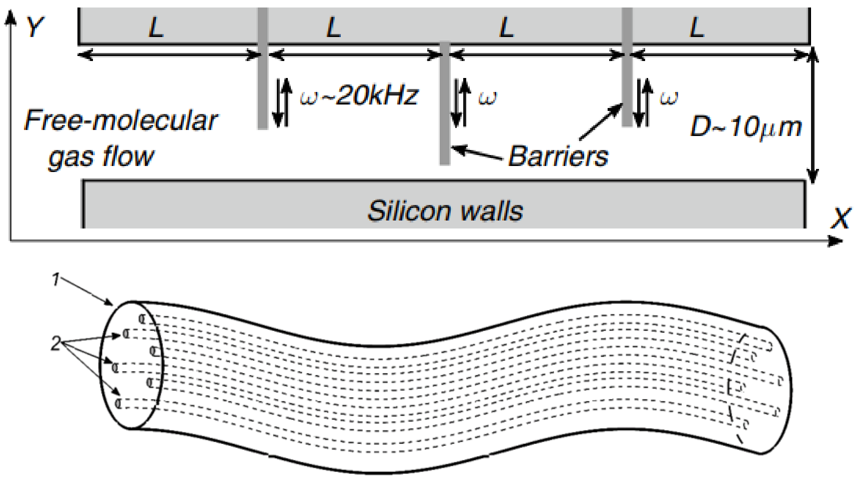
Multiscale Simulation Laboratory

Mechanical Engineering Research Institute of the RAS

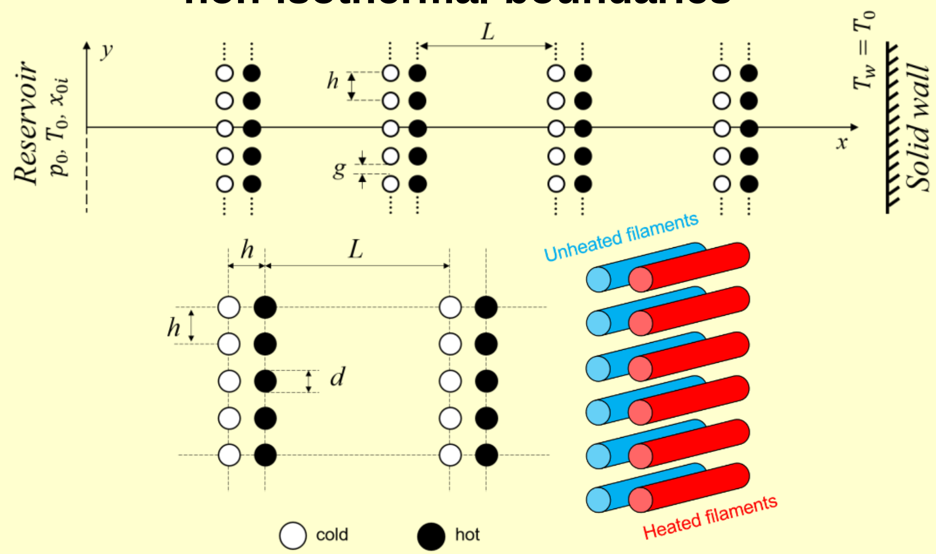
enmech.ru **multiscale.ru** **imash.ru**

Development of new energy efficient methods for gas separation in membranes and microelectromechanical systems

1. Simulation of free-molecular flows in regions with a moving and deforming boundary



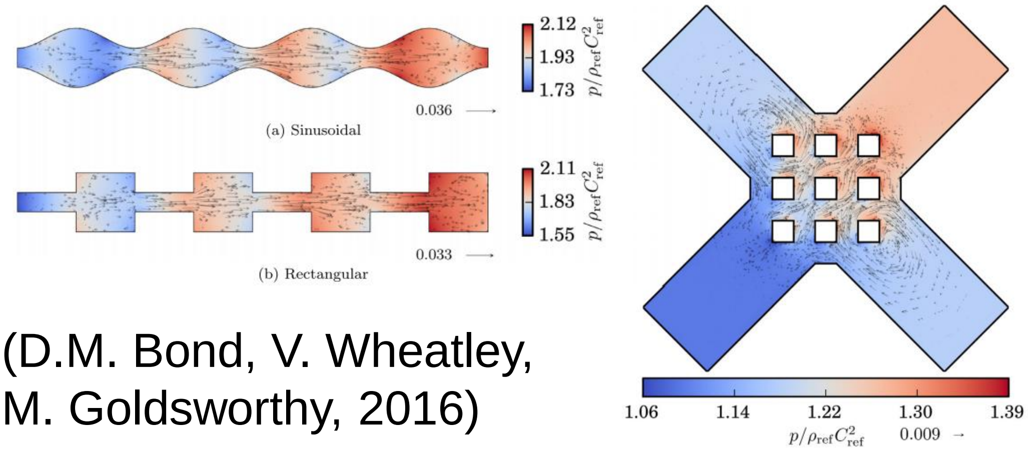
2. Flow of a mixture of three or more gases in the transitional regime in a regions with non-isothermal boundaries



(June 2019)

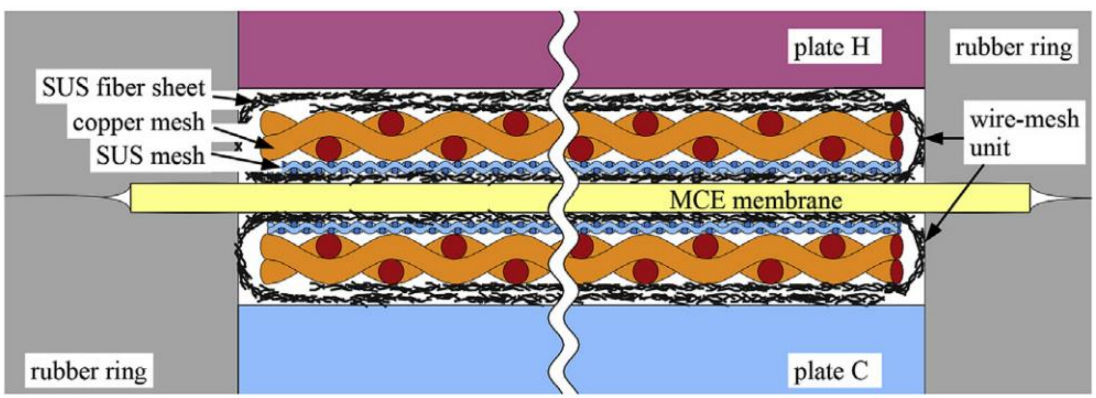
3. Transitional gas flow of mixture of gases in a region with moving boundaries and non-isothermal boundary conditions

Alternative Knudsen pump designs



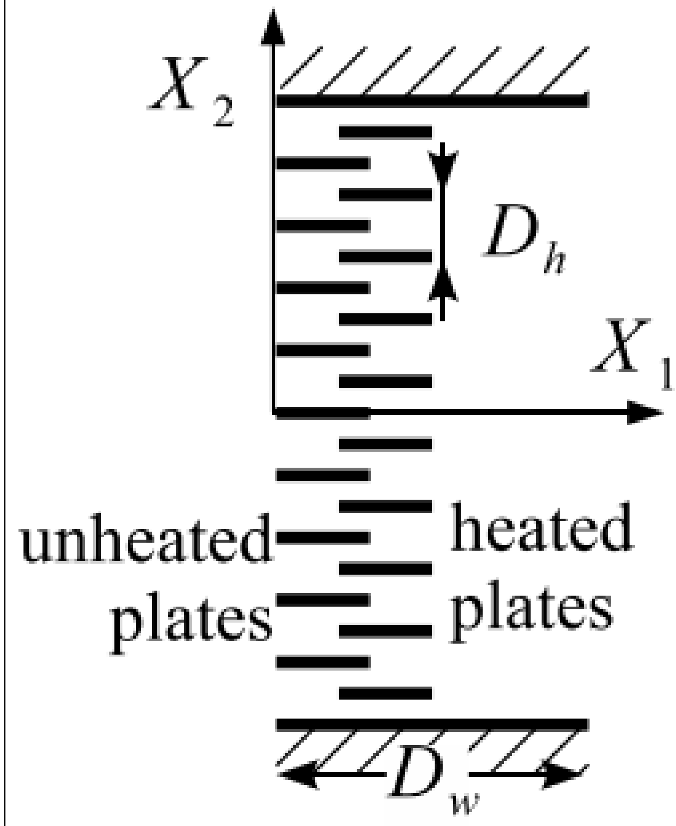
(D.M. Bond, V. Wheatley, M. Goldsworthy, 2016)

Membrane Knudsen pump as a gas separator



(S. Nakaye, H. Sugimoto, 2016)

Thermal edge flow

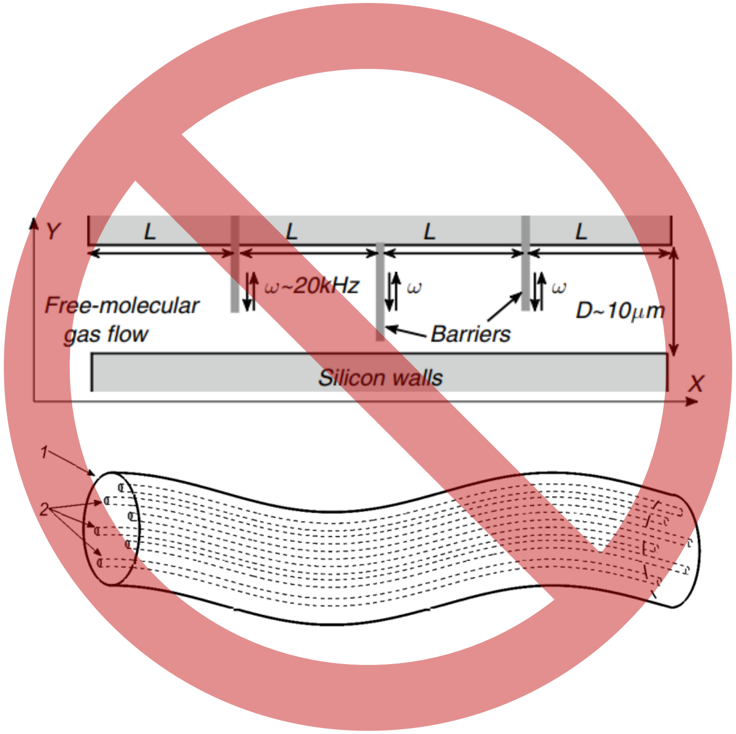


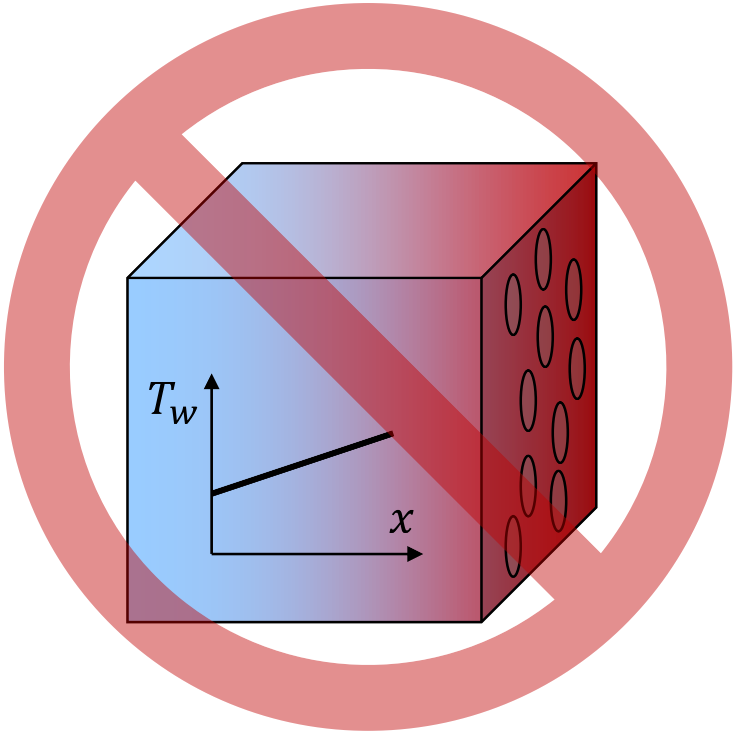
(H. Sugimoto, S. Takata, S. Kosuge, 2007)

and a large number of others…

Separation device

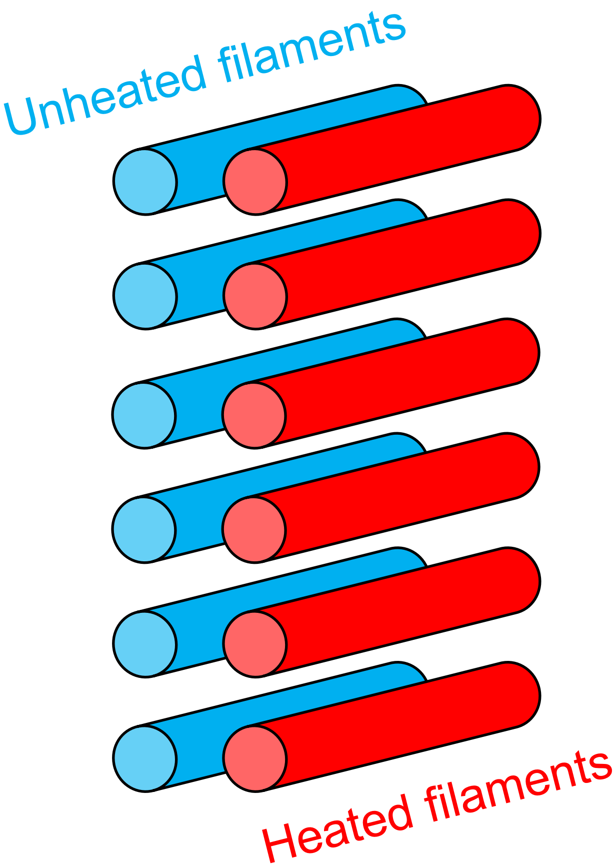
- Without movable elements
- Without temperature gradients in a solid
- Simple geometry



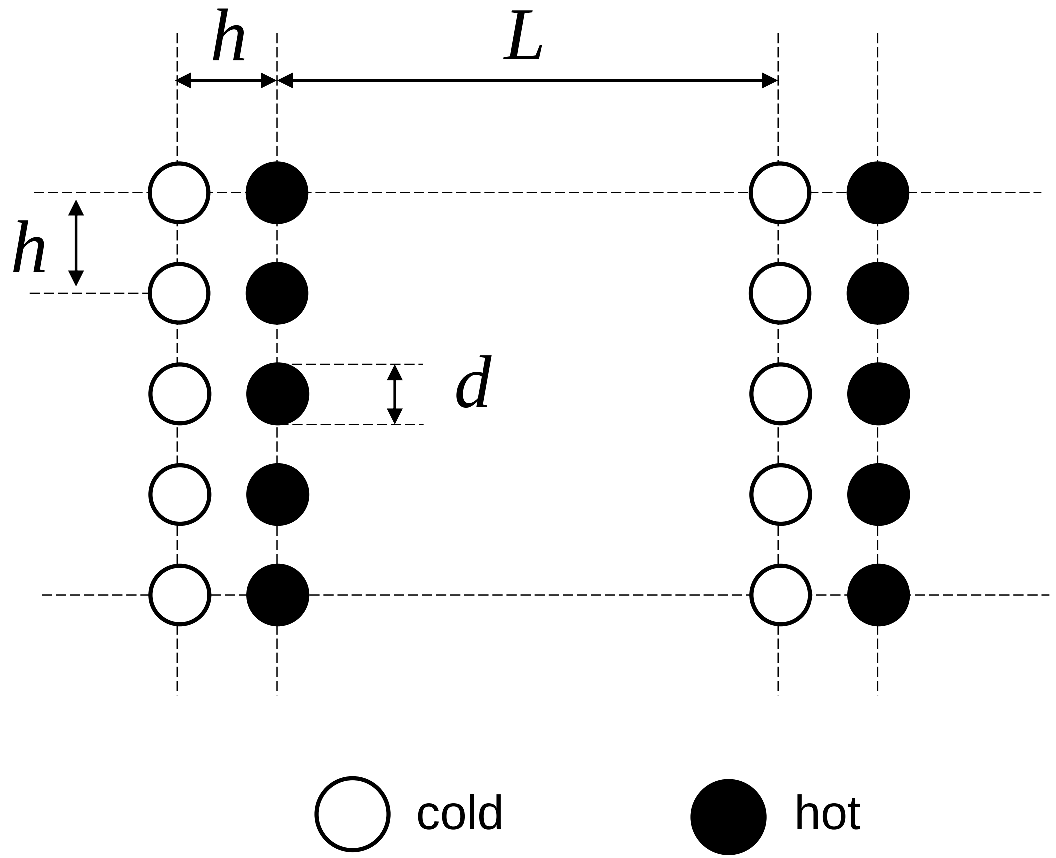


Problem statement

One stage



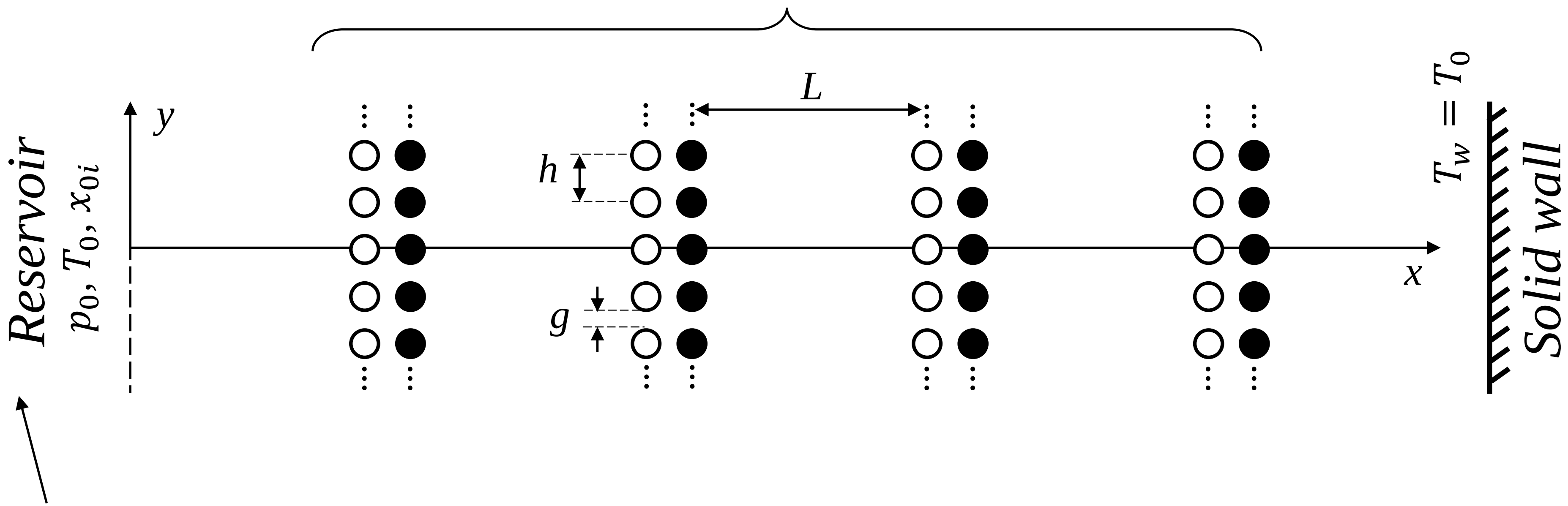
Geometric parameters



$$g = h - d$$

Problem statement

Four stages



Initial mixture composition:

(He, Ne, Ar, Kr, Xe)

$x_{0i} = 0.2$

○ – Cold filament: $T_w = T_0$

● – Hot filament: $T_w = \boldsymbol{T_1 = 2T_0}$

Knudsen numbers:

$Kn_L = \lambda/L = 0.1, 0.15, 0.2, 0.4$

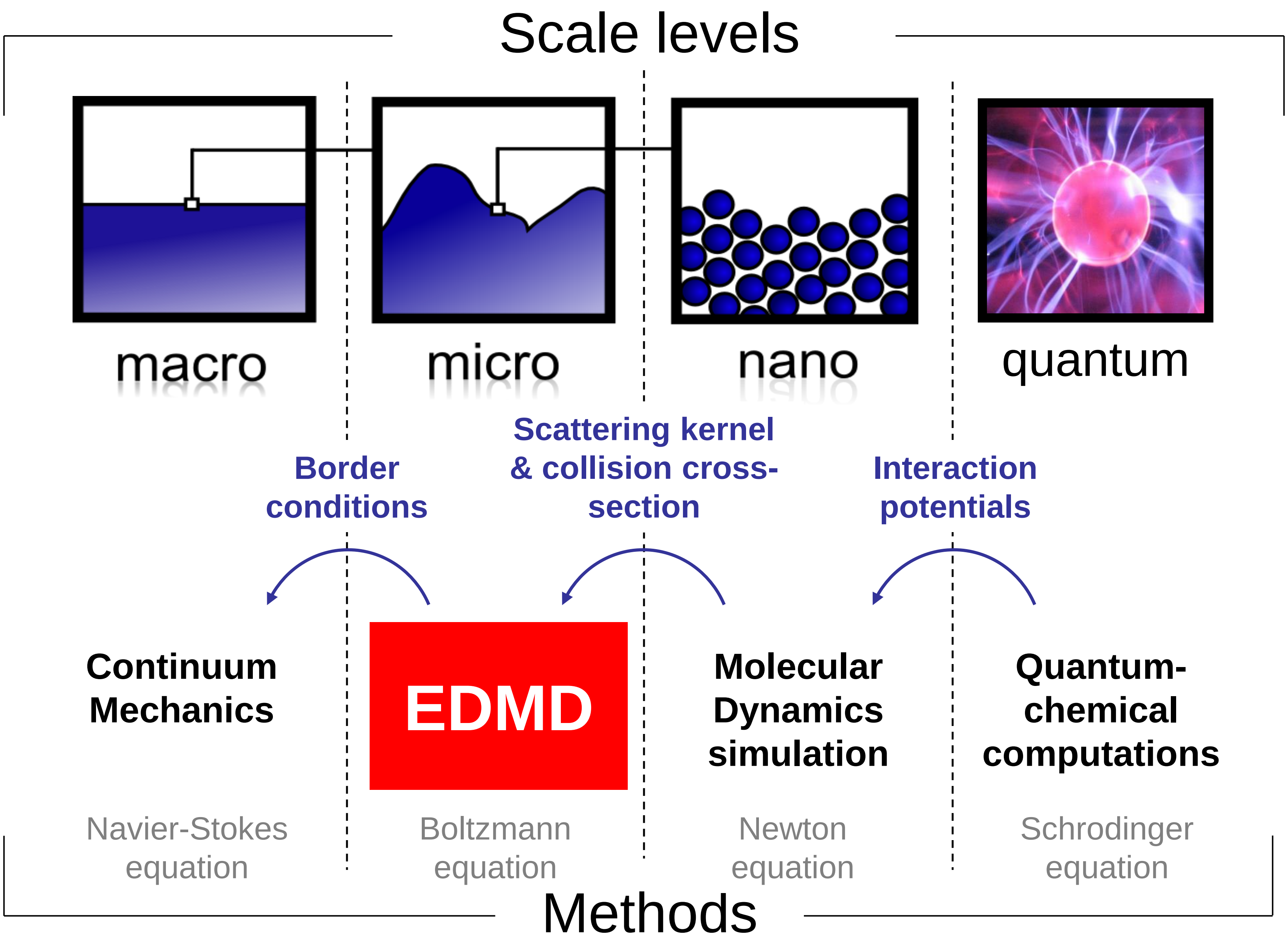
$Kn_g = \lambda/g = 5, 10, 20, 40$

Geometries:

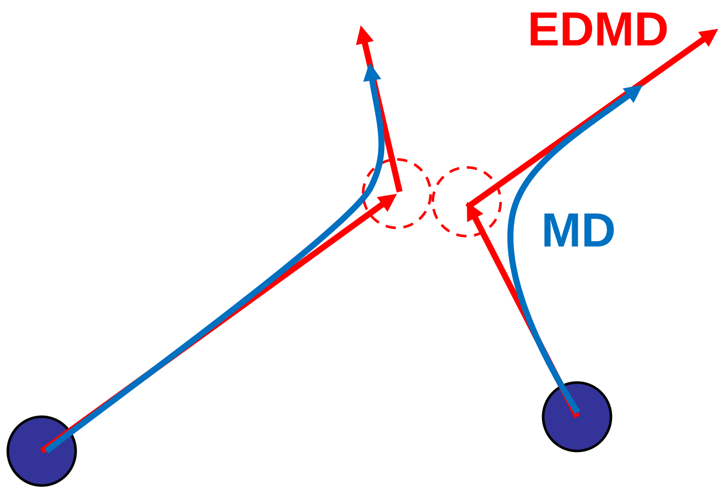
$\frac{h}{d} = 1.25, 1.5, 2, 3$

64 cases

Methods


Scale levels
macro
micro
nano
quantum
Border conditions
Scattering kernel & collision cross-section
Interaction potentials
Continuum Mechanics
EDMD
Molecular Dynamics simulation
Quantum-chemical computations
Navier-Stokes equation
Boltzmann equation
Newton equation
Schrodinger equation
Methods

Event-driven Molecular Dynamics



Trajectories of gas molecules between collisions – **straight lines**

- Intermolecular collisions,
- Collisions with solid surface,
- … other interactions in the simulation system

called "**events**"

The **time** in the simulation system **is changed discretely – via times of events**

References

- **B.J. Alder, T.E. Wainwright**, Studies in molecular dynamics. General method, J. Chem. Phys. 31 (**1959**) 459. doi:10.1063/1.1730376.
- **S. Miller, S. Luding**, Event-driven molecular dynamics in parallel, J. Comput. Phys. 193 (**2004**) 306–316. doi:10.1016/j.jcp.2003.08.009.
- **A. Donev, A.L. Garcia, B.J. Alder**, Stochastic Event-Driven Molecular Dynamics, J. Comput. Phys. 227 (**2008**) 2644–2665. doi:10.1016/j.jcp.2007.11.010.
- **P. Valentini, T.E. Schwartzentruber**, A combined Event-Driven/Time-Driven molecular dynamics algorithm for the simulation of shock waves in rarefied gases, J. Comput. Phys. 228 (**2009**) 8766–8778. doi:10.1016/j.jcp.2009.08.026. RGD
- **M.N. Bannerman, R. Sargant, L. Lue**, DynamO: A free O(N) general event-driven molecular-dynamics simulator, J. Comput. Chem. 32 (**2011**) 3329– 3338. doi:10.1002/jcc.21915.
- **V.R. Akkaya, I. Kandemir**, Event-driven molecular dynamics simulation of hard-sphere gas flows in microchannels, Math. Probl. Eng. 2015 (**2015**). doi:10.1155/2015/842837. RGD
- **A. Yakunchikov, V. Kosyanchuk**, Application of event-driven molecular dynamics approach to rarefied gas dynamics problems // Computers and Fluids 170 (**2018**) 121–127. RGD

Why EDMD?

Meshless – no mesh, no time step

Fully deterministic – no adjustment parameters

Without stochastic collision pair selection

Without simplification of the collision integral

Our interest in the EDMD approach is caused by the possibility of its application to the problems of **separation of multicomponent gas mixtures in devices with oscillating elements**, because EDMD unlike the most of existing particle and mesh methods **can be naturally generalized to the case of moving boundaries** without significant complications of algorithm.

EDMD is a compromise between DSMC and classical (time-driven) MD

Molecule state

- **x, y, z** - Coordinates
- **vx, vy, vz** - Velocity
- **t** - **time when molecule obtained these coordinates and velocity**

Between collisions molecule moves along a straight line

$$\vec{x}(t) = \vec{x}' + \vec{v}'(t - t')$$

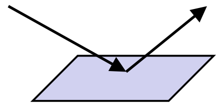
where $\vec{x}'$ – coordinates of molecule after last collision, $\vec{v}'$ – velocity of molecule after last collision, t' – time of last collision

Collisions with solid surface:

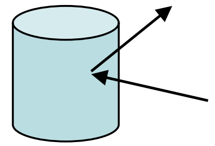
The time of i-th molecule collision with k-th boundary flat element can be found from linear equation:

$$\vec{x}_i(t) \cdot \vec{n}_k = R_k$$

Boundary element types:

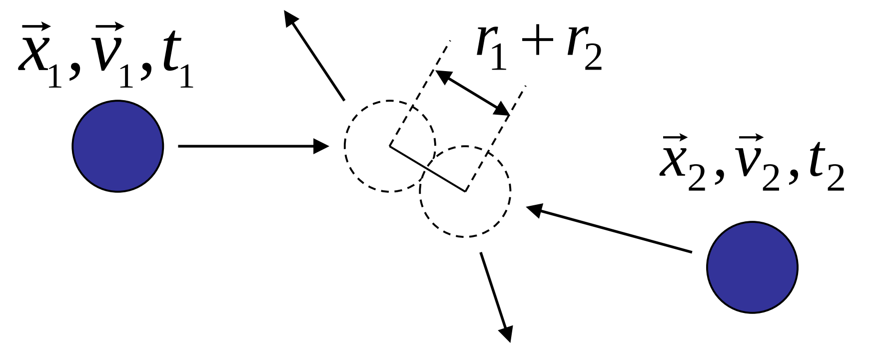


flat element



cylinder

Hard spheres (HS) model was used:



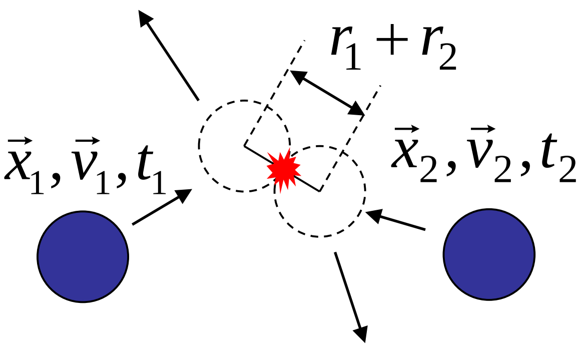
The time of i-th and j-th molecules collision can be found from this quadratic equation

$$\left(\vec{x}_i(t) - \vec{x}_j(t)\right)^2 = \left(\frac{d_i}{2} + \frac{d_j}{2}\right)^2$$

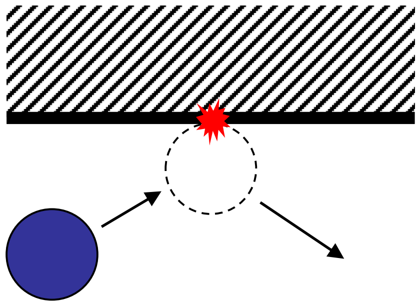
Event-driven Molecular Dynamics

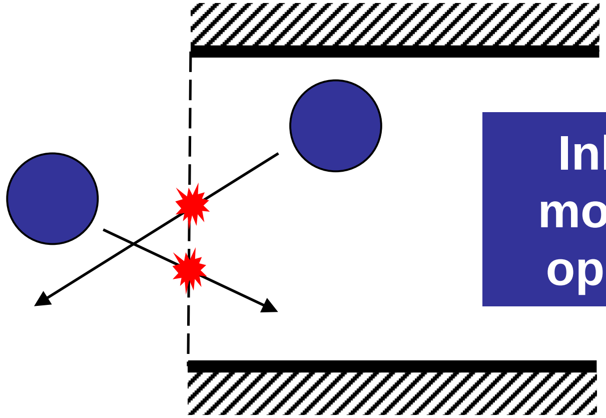
Events

Intermolecular collisions



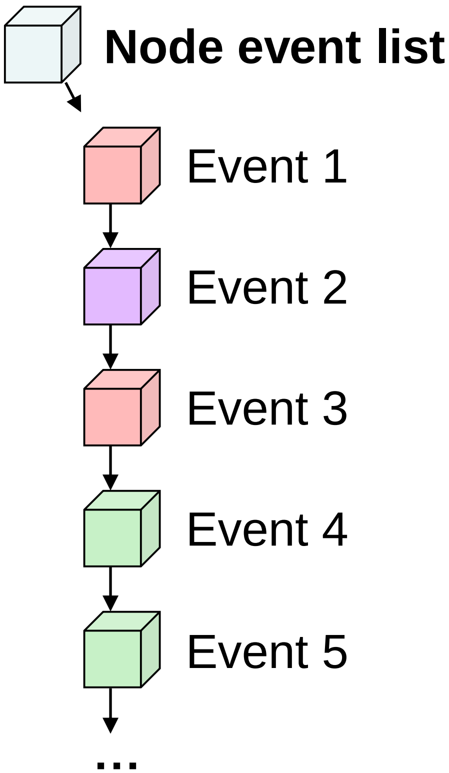
Collisions with solid surface





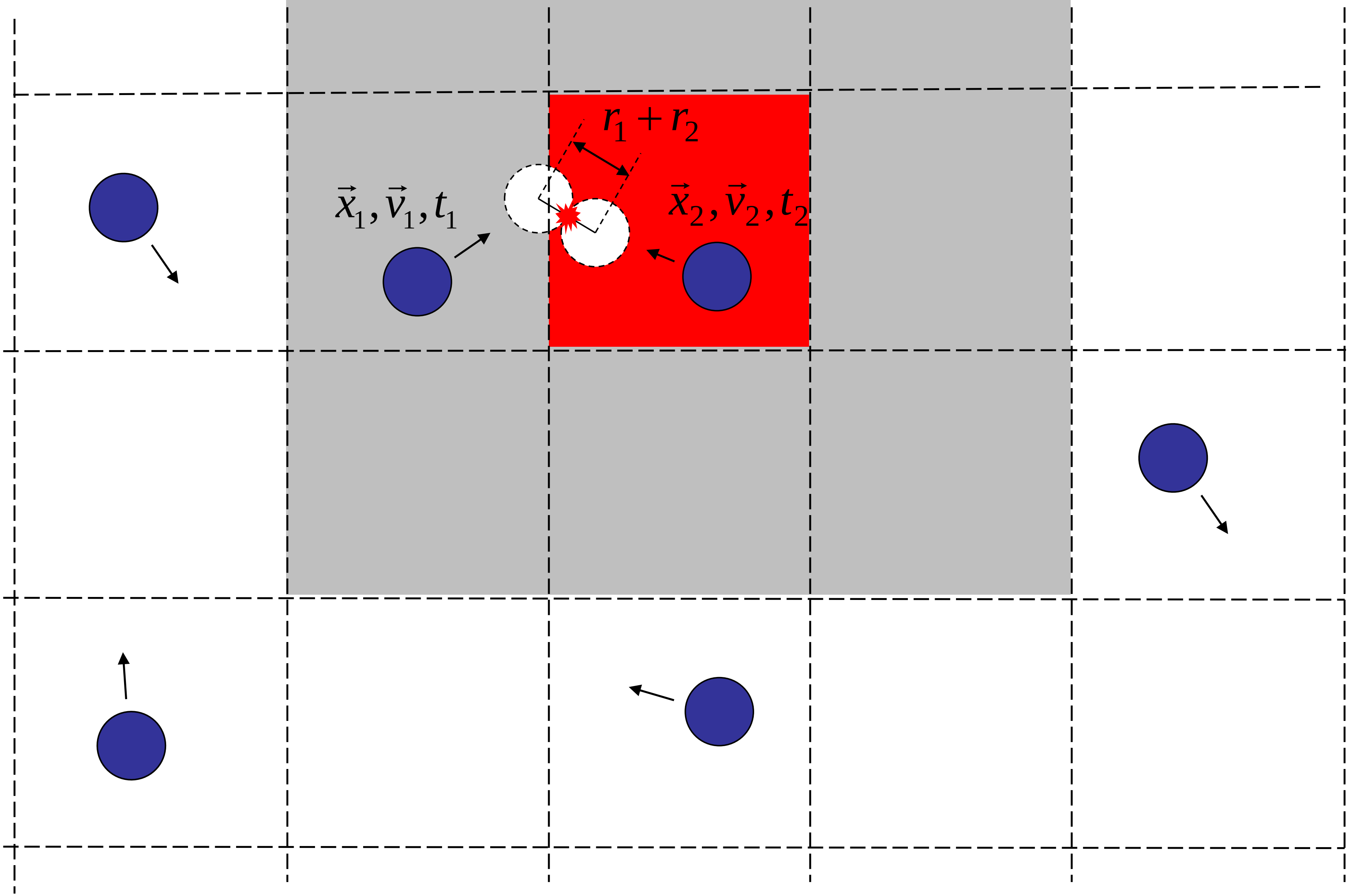
Inlet or outlet of molecule through open boundaries

Event list



Size of event list will be greater than number of molecules

Many-body problem

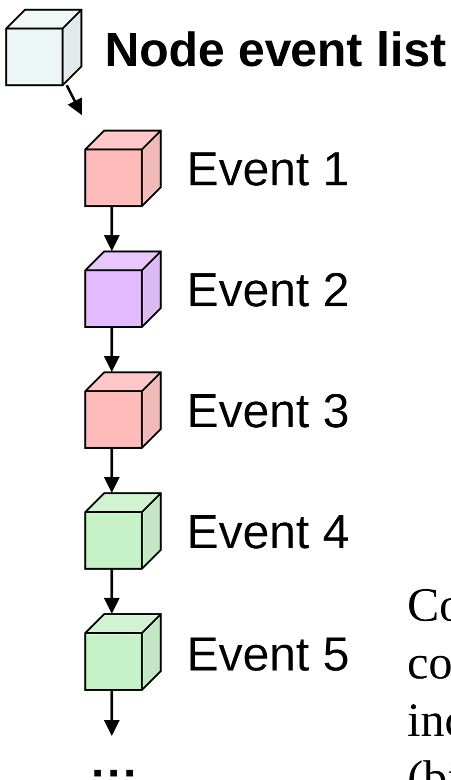


Event-driven Molecular Dynamics

The most expensive operation during the simulation is search of place for insertion of new event!

Variants of the event list implementation

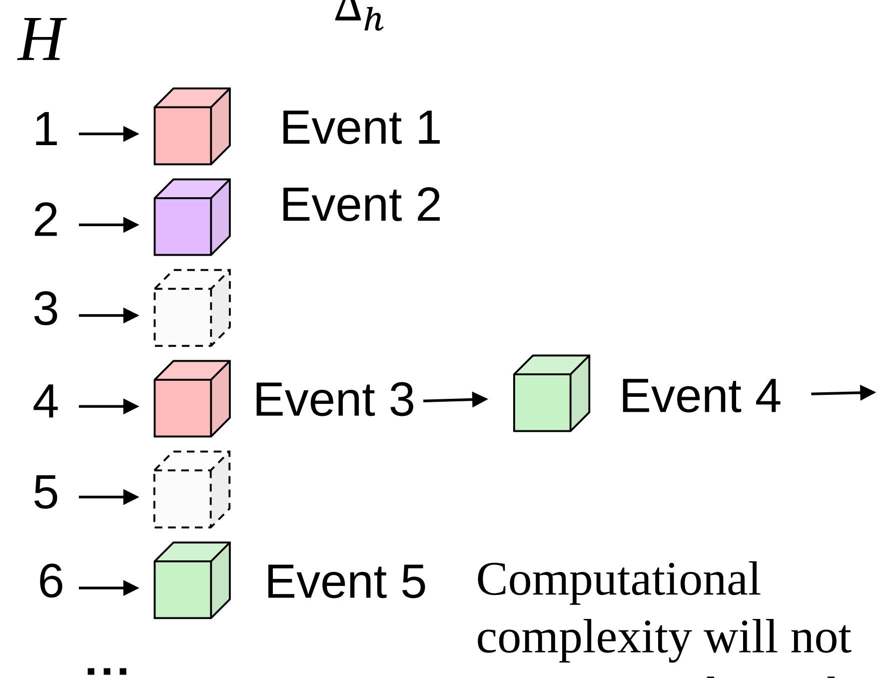
Sorted list



Computational complexity will increase as lnN (binary tree algorithm)

Hash-table

$$H(t) = \frac{t}{\Delta_h} \ mod \ N_h$$

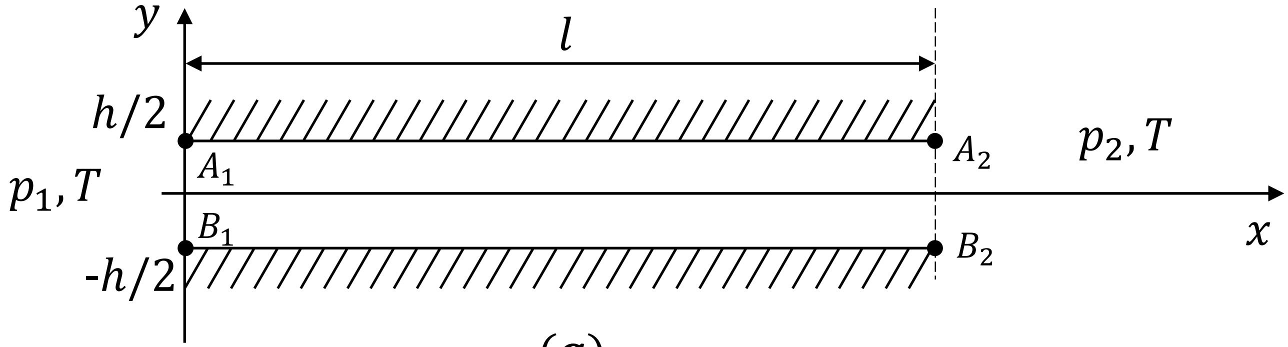


Computational complexity will not increase with number of event list items

Benchmark computation #1 – Flow in plane channel of finite length

Problem statements

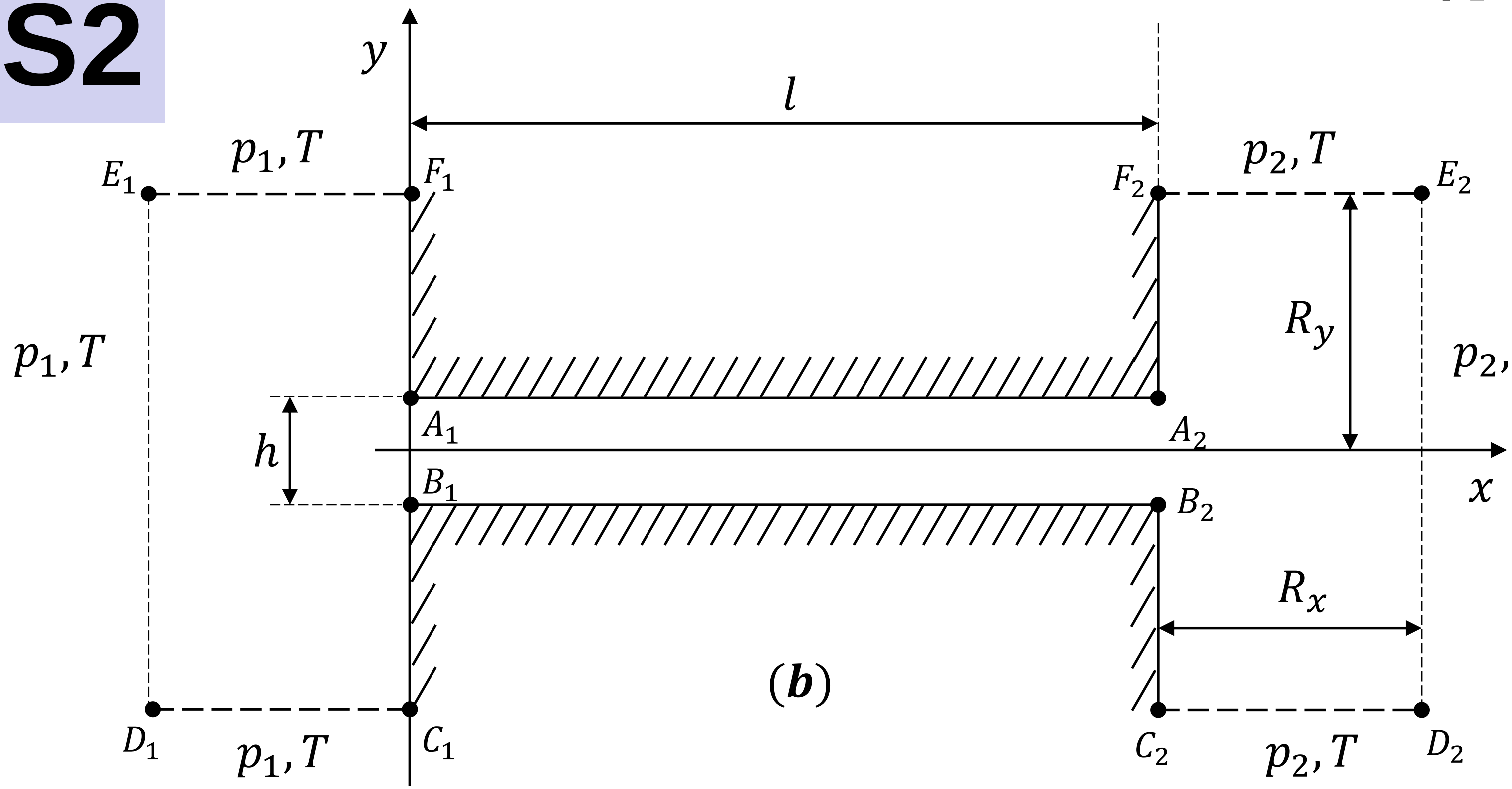
S1



$(\boldsymbol{a})$

$p_1/p_2 = 1.1$

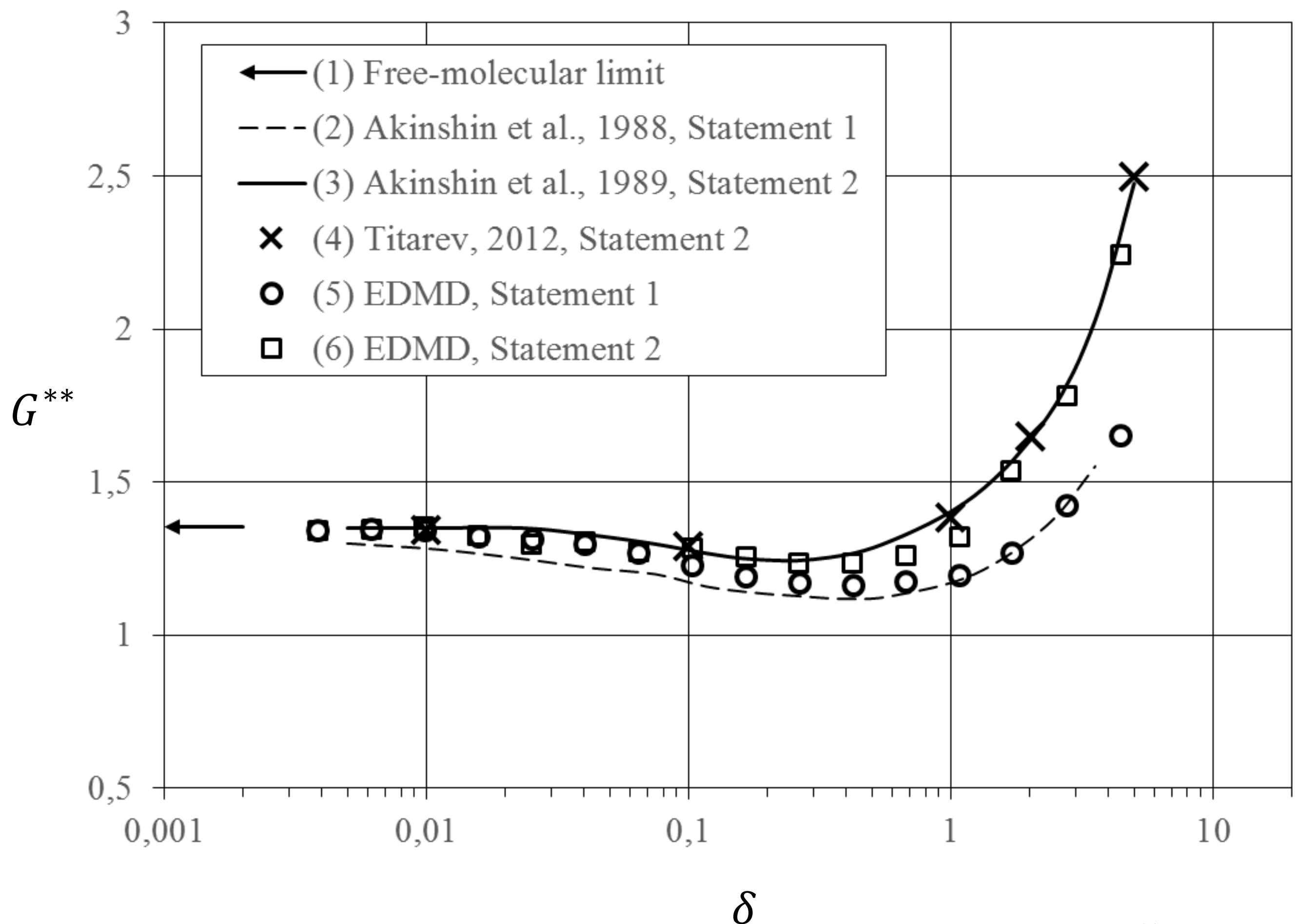
S2



$(\boldsymbol{b})$

A. Yakunchikov, V. Kosyanchuk, Computers and Fluids 170 (2018) 121–127

Benchmark computation #1 – Flow in plane channel of finite length



$$G = -\frac{(p_2 - p_1)}{l}\frac{h^2}{\sqrt{2RT}}G^{**}$$

$$\delta = h\sqrt{\pi}/(4\lambda)$$

$$p_1/p_2 = 1.1$$

S1 – $0.5 \cdot 10^6$ molecules
S2 – $2 \cdot 10^6$ molecules
(per core)

Relative statistical error of mass flow

$$e = \frac{\sigma}{a\sqrt{N}} = \frac{2}{N_+ - N_-}\sqrt{\frac{N_+N_-}{N}} < 1\%$$

Supercomputer "Lomonosov"
(based on Intel Xeon X5570 2.93GHz)

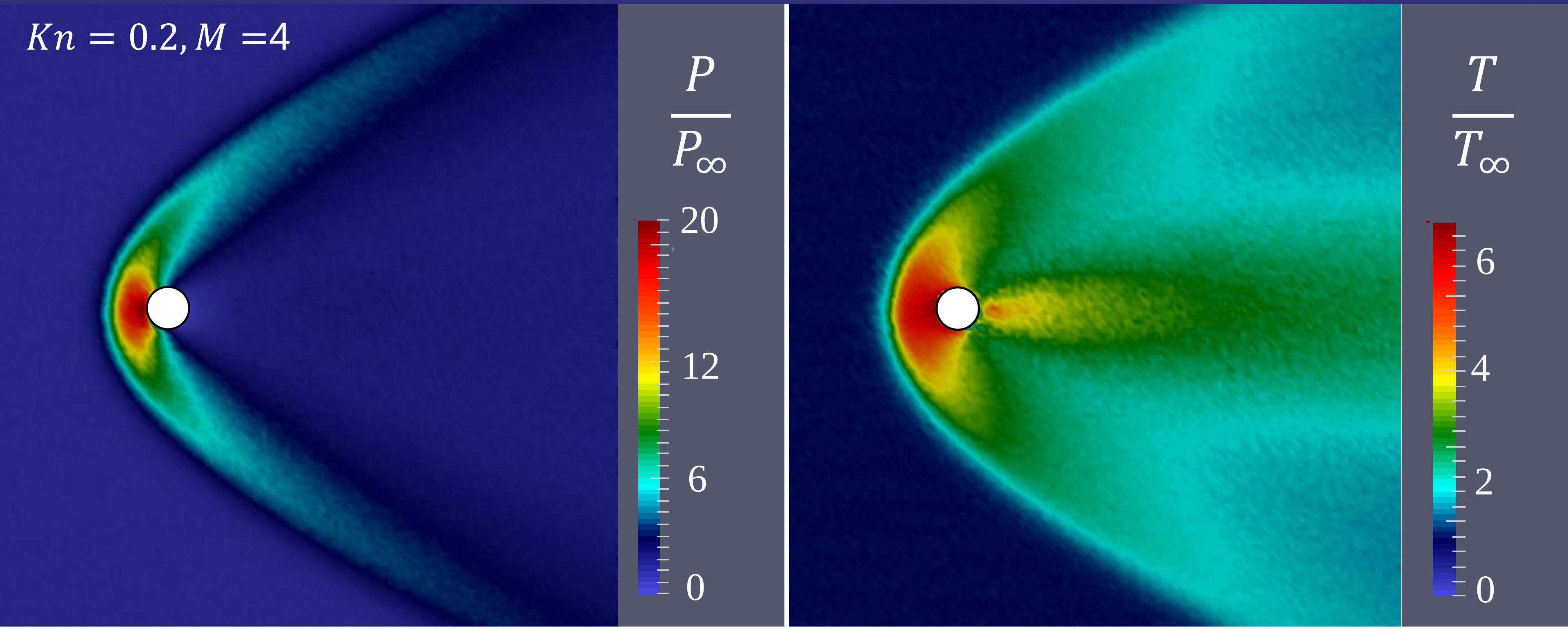
Statement 1 – used less than **400MB RAM per core**

Statement 2 – used less than **1.3GB RAM per core**

Computation time = 50 hours

A. Yakunchikov, V. Kosyanchuk, Computers and Fluids 170 (2018) 121–127

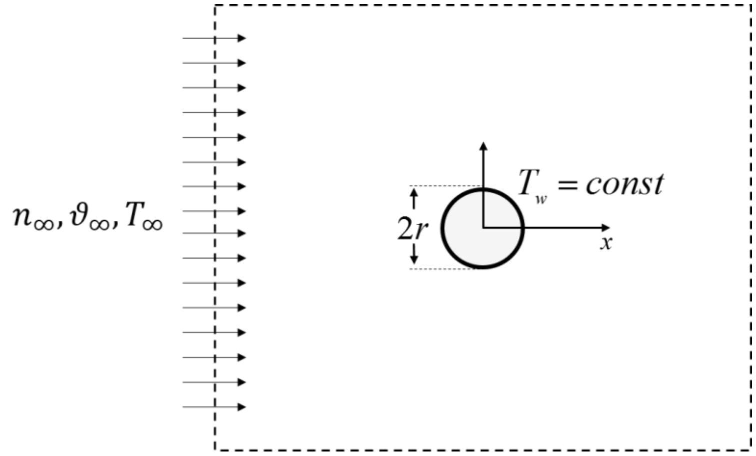
Benchmark computation #2 – Supersonic flow past cylinder



$$Kn = \lambda_\infty / 2\,r$$

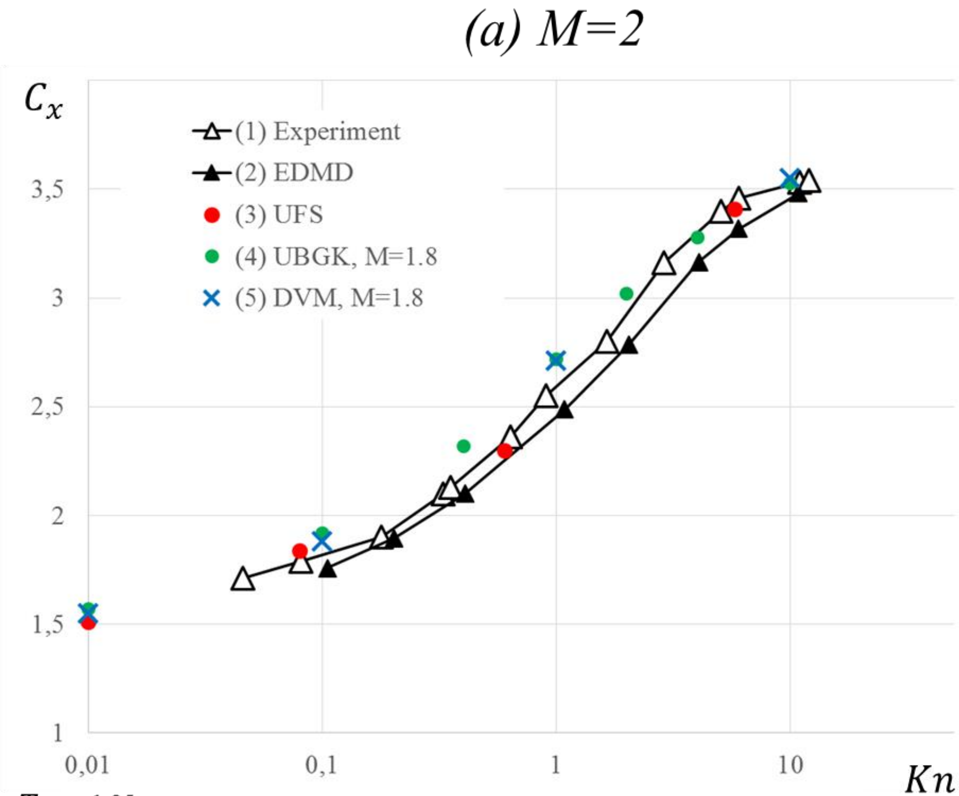
$$M_\infty = \vartheta_\infty / \sqrt{\gamma R T_\infty}$$

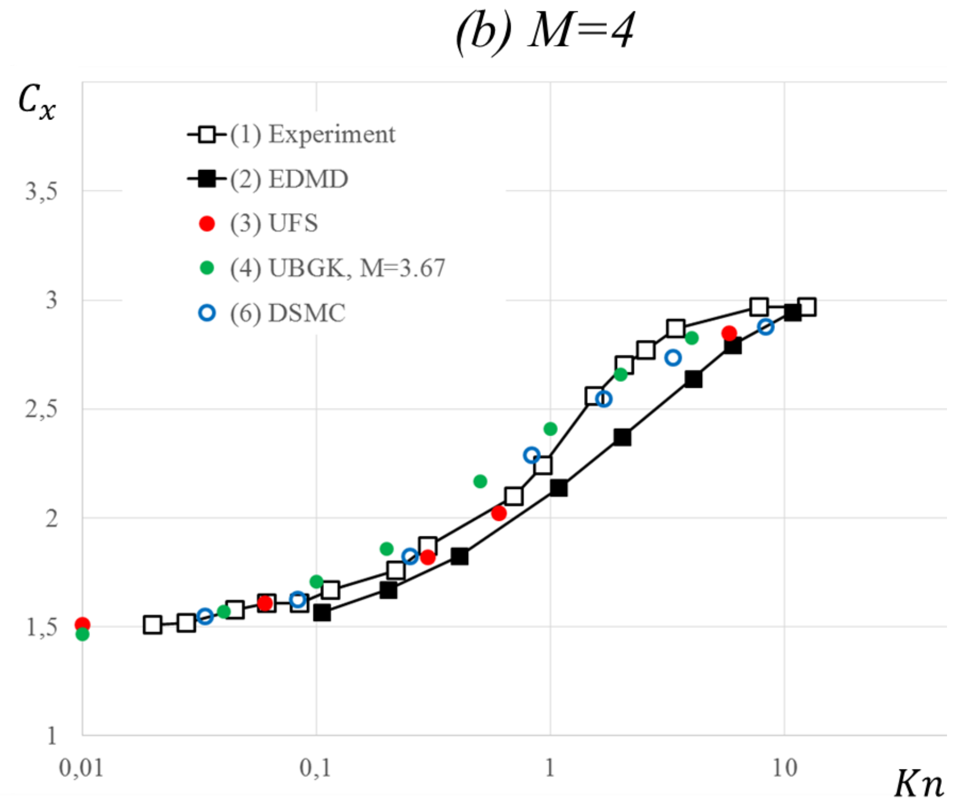
$$Re = \sqrt{\gamma\,\pi/2}\,M_\infty / K\,n$$

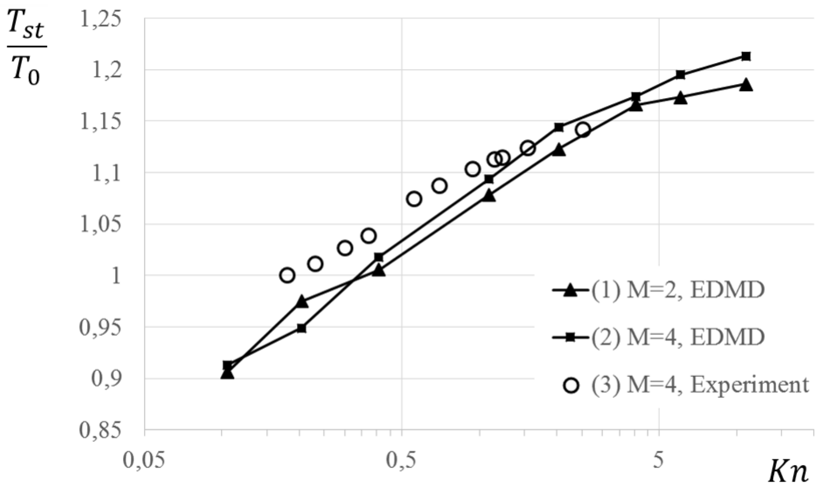


50x40x10 cylinder radii

Benchmark computation #2 – Supersonic flow past cylinder







$\sim 10^6$ molecules per core

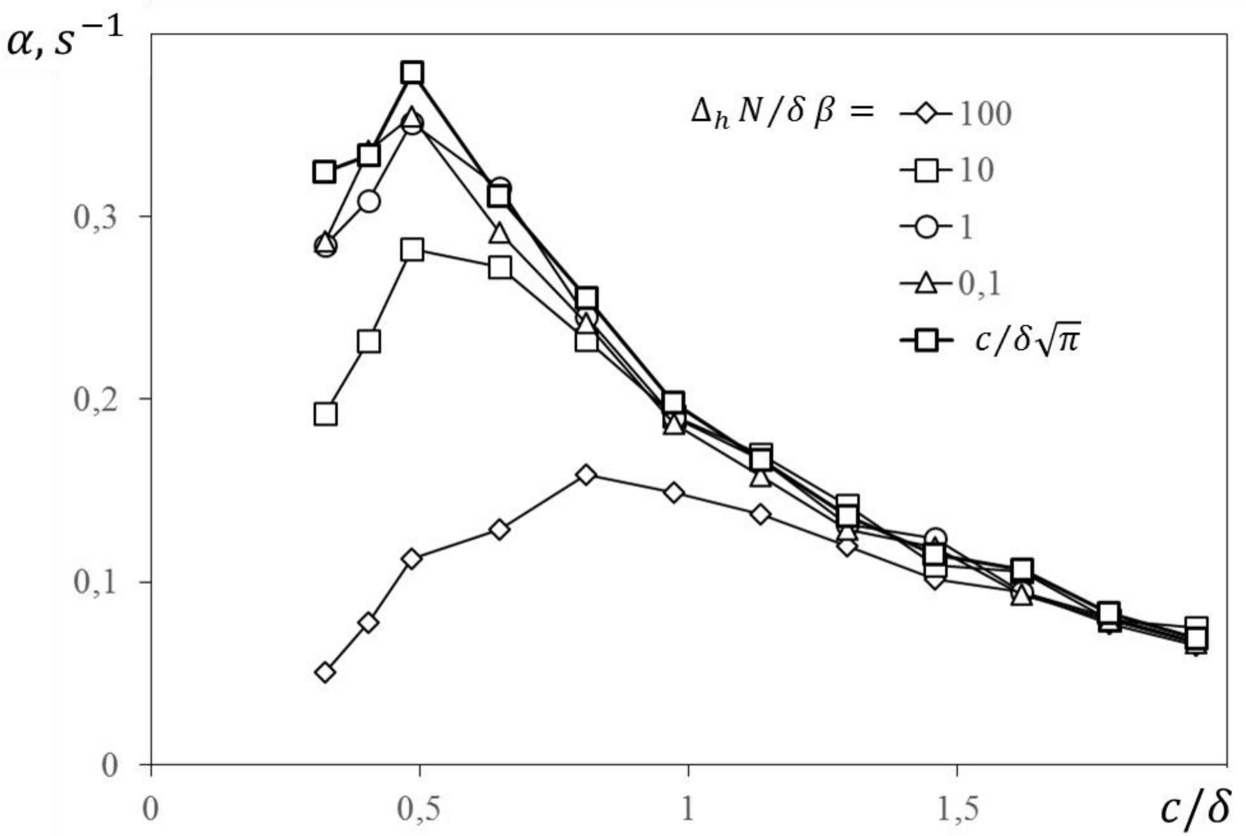
Supercomputer "Lomonosov"

(based on Intel Xeon X5570 2.93GHz)

Computation time = 10 hours

A. Yakunchikov, V. Kosyanchuk, Computers and Fluids 170 (2018) 121–127

Before EDMD computation **three parameters should be preset:**
hash-table parameters (Δ_h and N_h) and **cell size c**.
(result of simulation doesn't depend on these parameters – only speed of calculation)



$$\Delta_h = c\,\beta/\sqrt{\pi}\,N$$

$$\frac{c}{\delta} = \frac{1}{2}$$

$$\Downarrow$$

The optimal number of cells should be approximately 8 times greater than the number of particles!

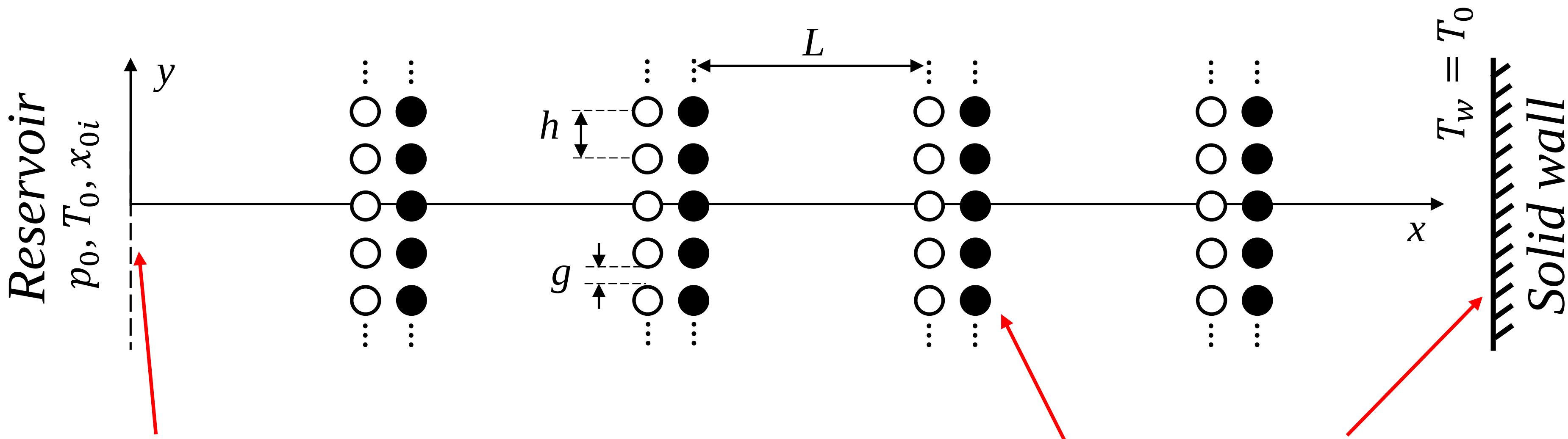
$\tau = t/\delta\beta,$

t – dimensional time, $\delta = n^{-1/3}$,

$\alpha = \Delta\tau/\Delta t_c$

This confirms the result obtained in S. Miller, S. Luding, J. Comput. Phys. 193 (2004) 306–316.

Border conditions



Open border

Equilibrium state with certain numerical density n, mean velocity $\vec{\vartheta}$ and temperature T:

$$\rho(\vec{u}) = \frac{n}{J_1}\left(\frac{\beta}{\sqrt{\pi}}\right)^3 u_n exp\left(-\beta^2\left(\vec{u}-\vec{\vartheta}\right)^2\right),$$

$$J_1 = n\left(\frac{\beta}{\sqrt{\pi}}\right)^3 \int_0^{\infty}\iint_{-\infty}^{\infty} u_n exp\left(-\beta^2\left(\vec{u}-\vec{\vartheta}\right)^2\right) d\vec{u} =$$

$$= \frac{n}{2\sqrt{\pi}\beta}\left(exp(-\beta^2\vartheta_n^2) + \sqrt{\pi}\beta\vartheta_n erfc(-\beta\vartheta_n)\right)$$

Solid wall and filaments surface

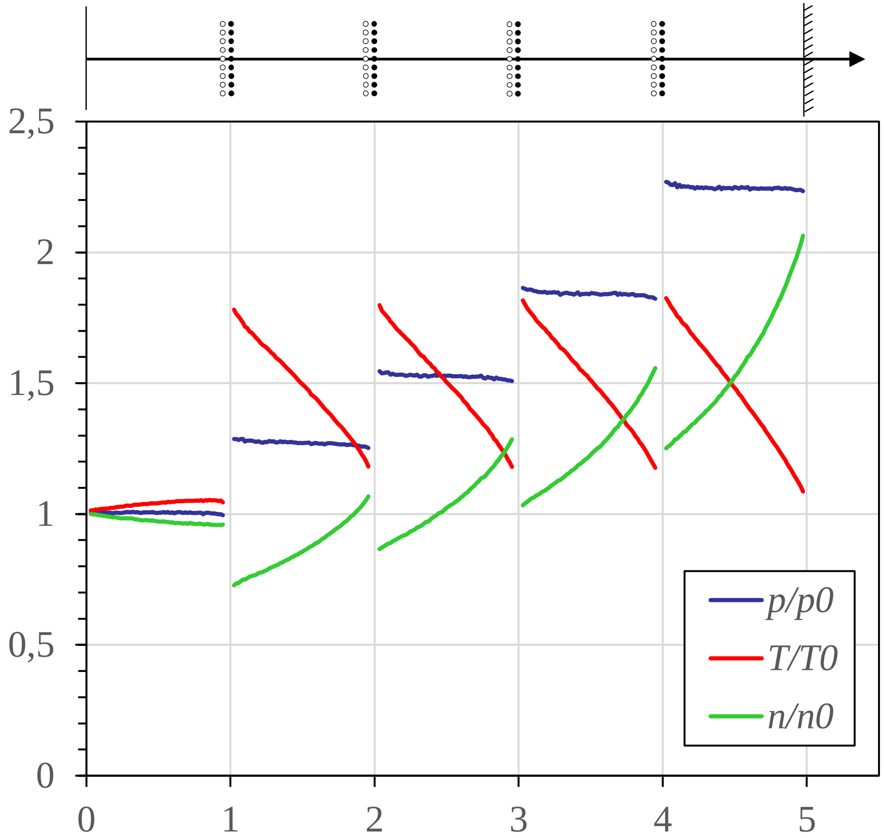
Maxwell scattering kernel with full accommodation:

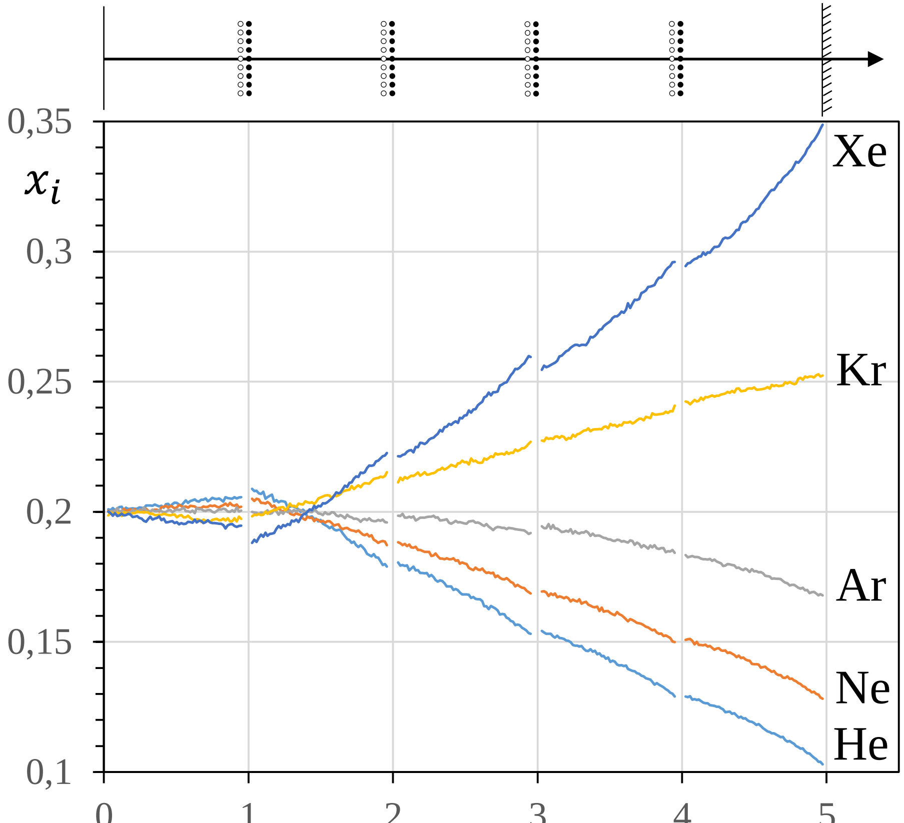
$$\rho(\vec{u}) = \frac{2\beta_w^4 u_n}{\pi} exp(-\beta_w^2 u^2),$$

$$\beta_w = \sqrt{m/2\,kT_w}$$

Results

$Kn_L = \lambda/L = \mathbf{0.15}$ $Kn_g = \lambda/g = \mathbf{40}$ $\frac{h}{d} = \mathbf{1.25}$ ***(case #13)***





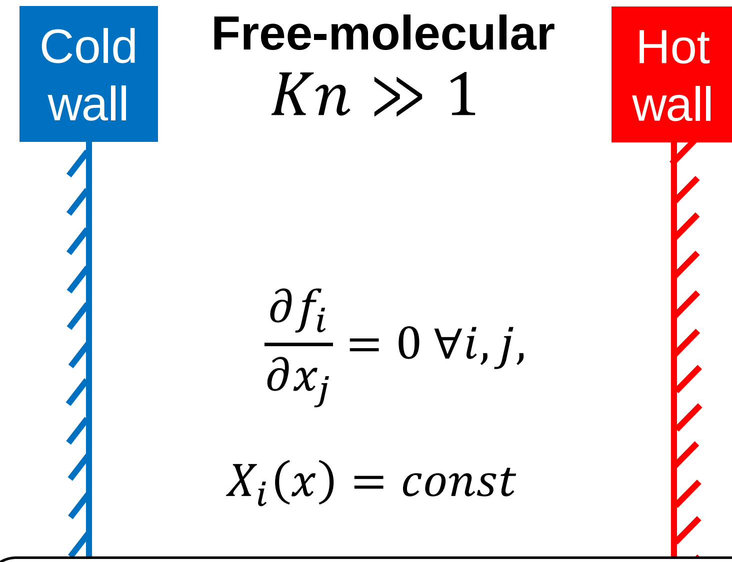
Separation takes place in chambers **between stages!**

Qualitative physical explanation

Heat transfer between two walls

Free-molecular

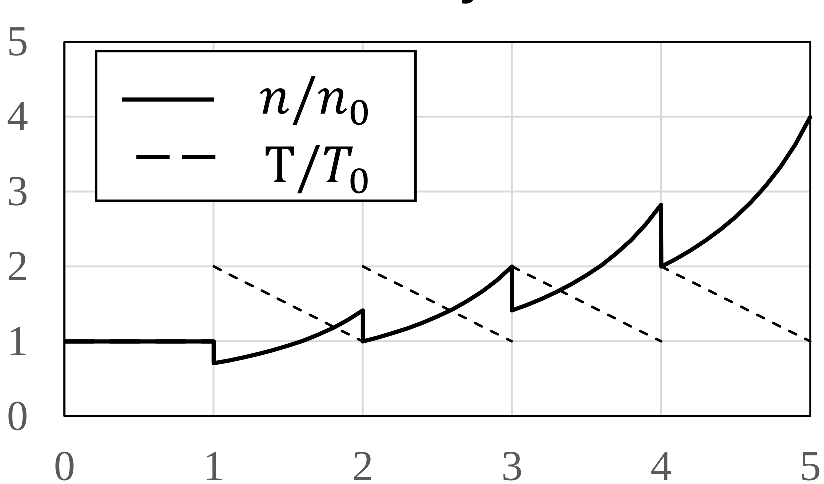
$Kn \gg 1$



$$\frac{\partial f_i}{\partial x_j} = 0 \ \forall i, j,$$

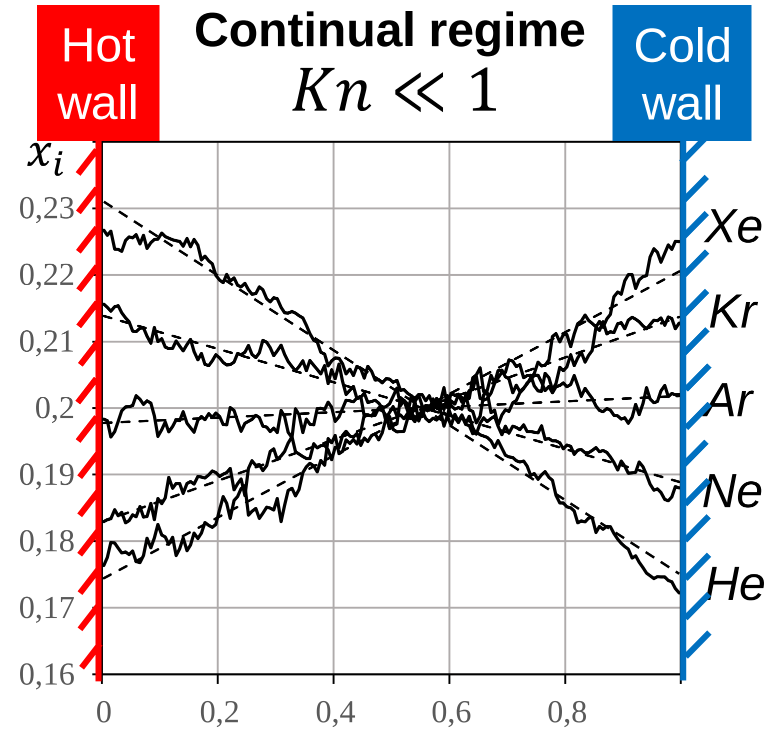
$$X_i(x) = const$$

Idealized system



Continual regime

$Kn \ll 1$

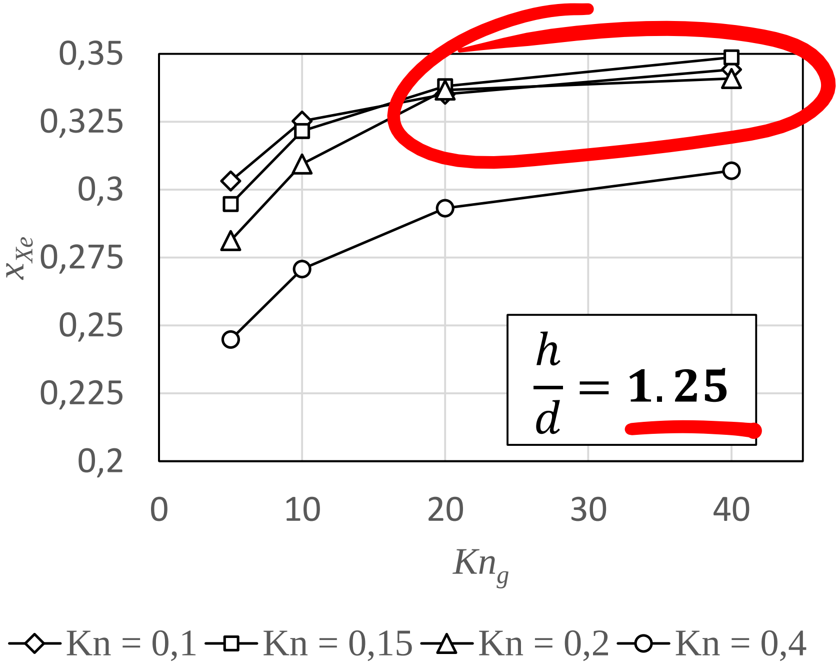


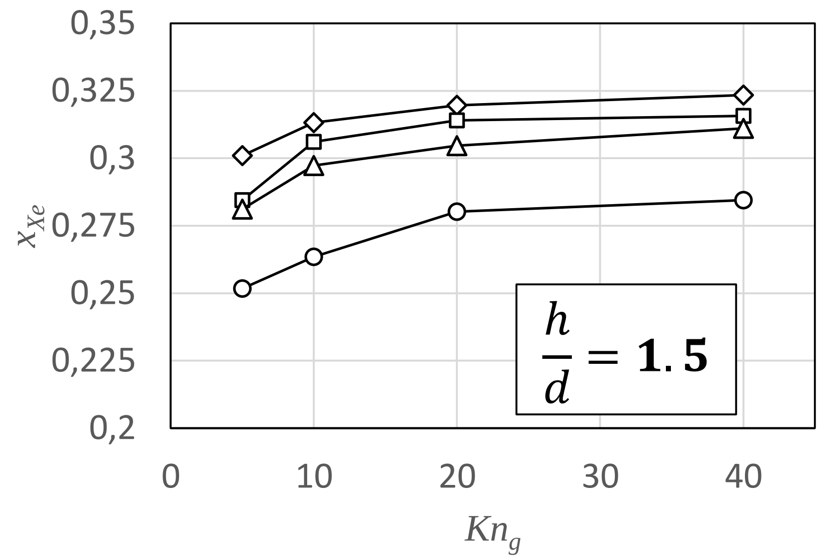
$$p(x) = const,$$

$$T(x) = T_1 + \frac{T_2 - T_1}{L} x,$$

$$n(x) = \frac{p(x)}{kT(x)}$$

Xe molar concentration at the closed end of the system



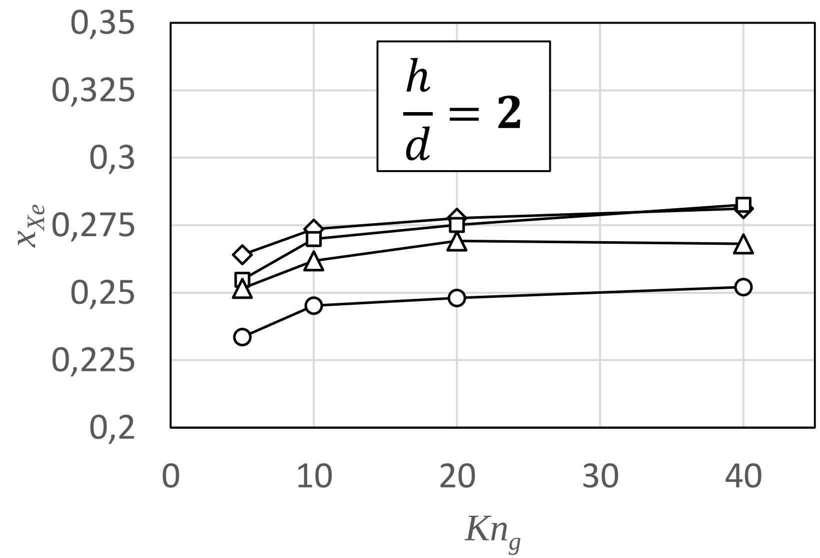


There is no sense in increasing the

$$Kn_g \geq 20$$

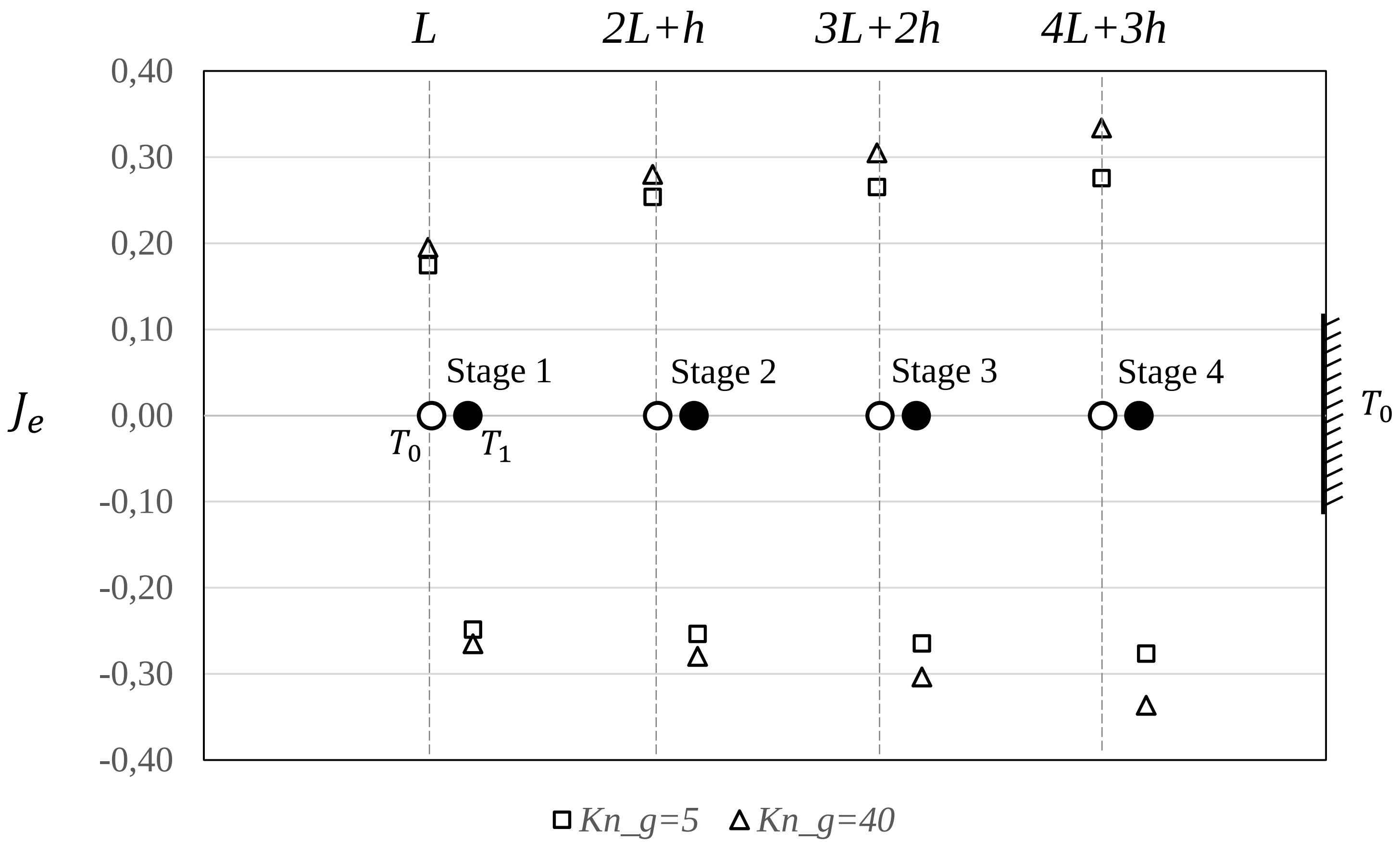
and decreasing the

$$Kn_L \leq 0.2$$



Heat flux

$Kn_L = 0.15$



$$J_e = Q / \sum Q_i^*$$

$$Q_i^* = d\sqrt{\frac{2\pi k T_1}{m_i}} p x_{0i} \left(1 - \left(\frac{T_2}{T_1}\right)^{\frac{3}{2}}\right) h_z$$

Conclusion

A plane problem about the transitional flow of a mixture of five noble gases in a system consisting of several rows of stretched filaments having different temperatures was studied.

It was obtained that **separation takes place exactly in chambers between stages due to regular thermal diffusion, rather than inside stages**.

It also means that **geometry of filaments doesn't play significant role in separation**. The main requirement is that flow between filaments has to be in near free-molecular regime, while flow in chambers has to be in near continual regime.

Also found that for $Kn_g \geq 20$ and $Kn_L \leq 0.2$ further oncoming to the free-molecule limit inside stage and to the continuum limit between stages insignificantly increases the separation effect.

This work is supported by the Russian Science Foundation
Grant № 17-71-10227

The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University and Joint Supercomputer Center of the Russian Academy of Sciences

Thank you for attention!

Lomonosov Moscow State University

Faculty of Mechanics and Mathematics

Department of Engineering Mechanics and Applied Mathematics

www.multiscale.ru, www.enmech.ru