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Micro and Nano Mechanics

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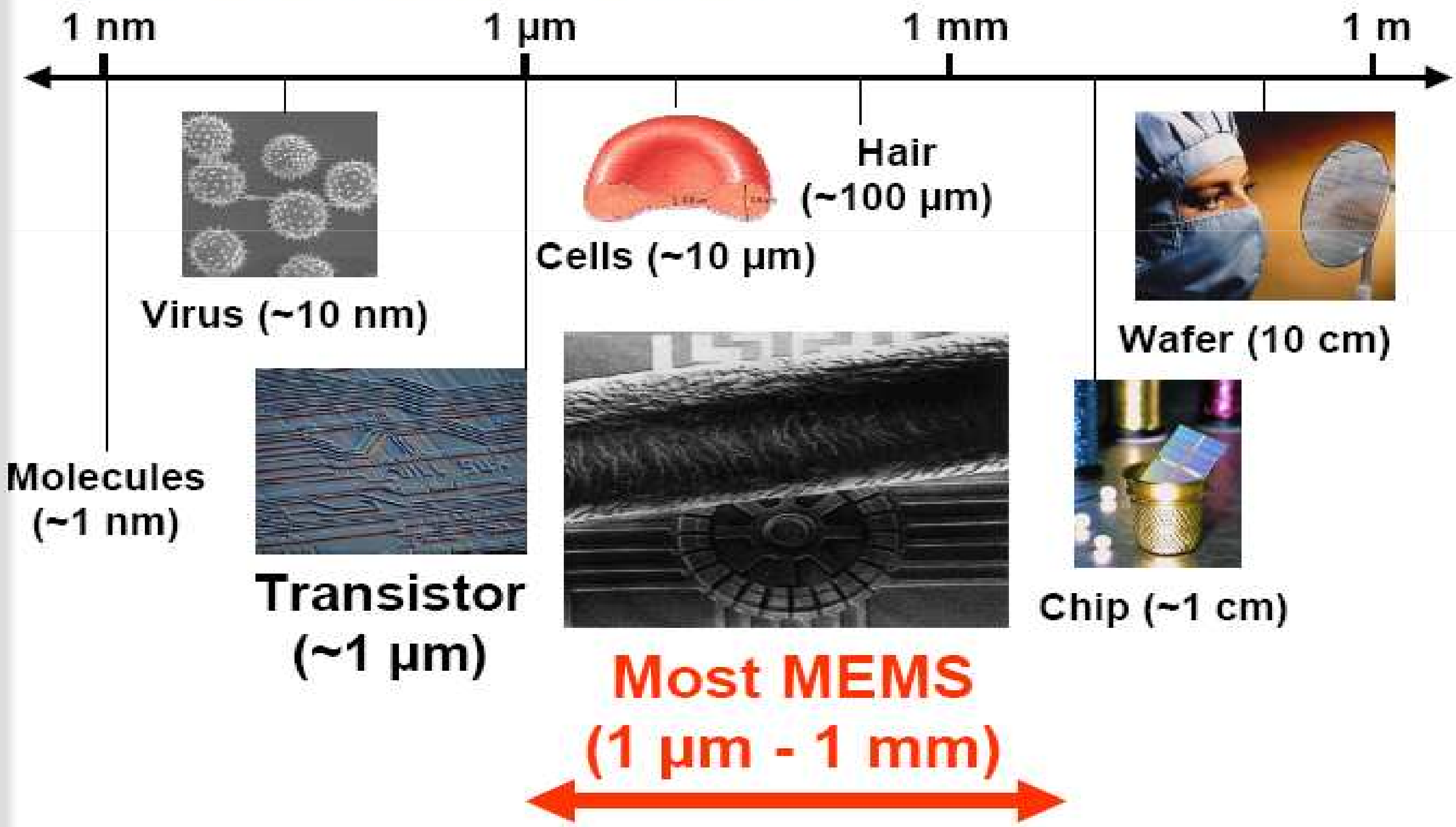
ERCOFTAG Spring Festival 2011, Gdansk, Poland

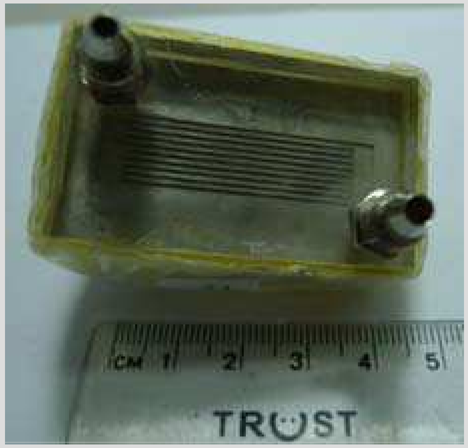
Topics

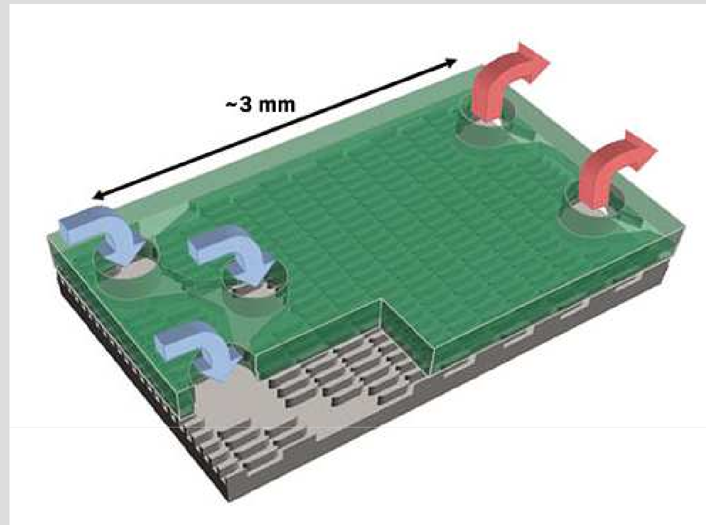
- Micromechanics basic
- Micro and nanomechanics research
- Results
- Initiatives

Manufacturing scales

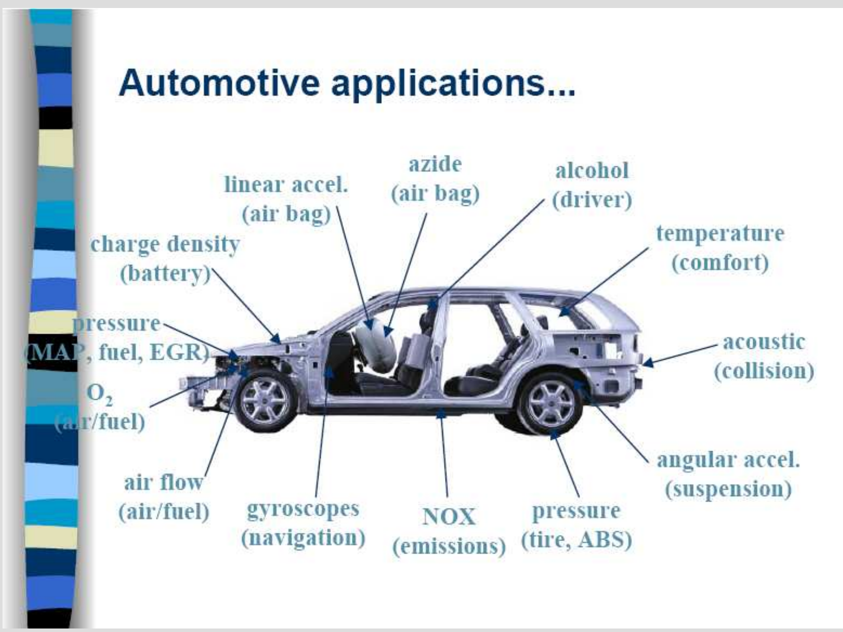


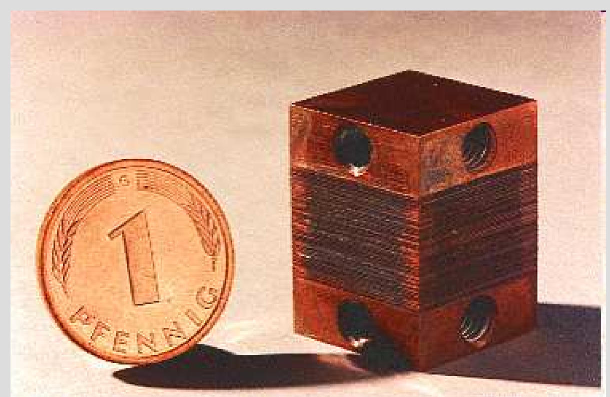
Products





35 micron channels on a 60 micron pitch
with 6 heat exchanger zones

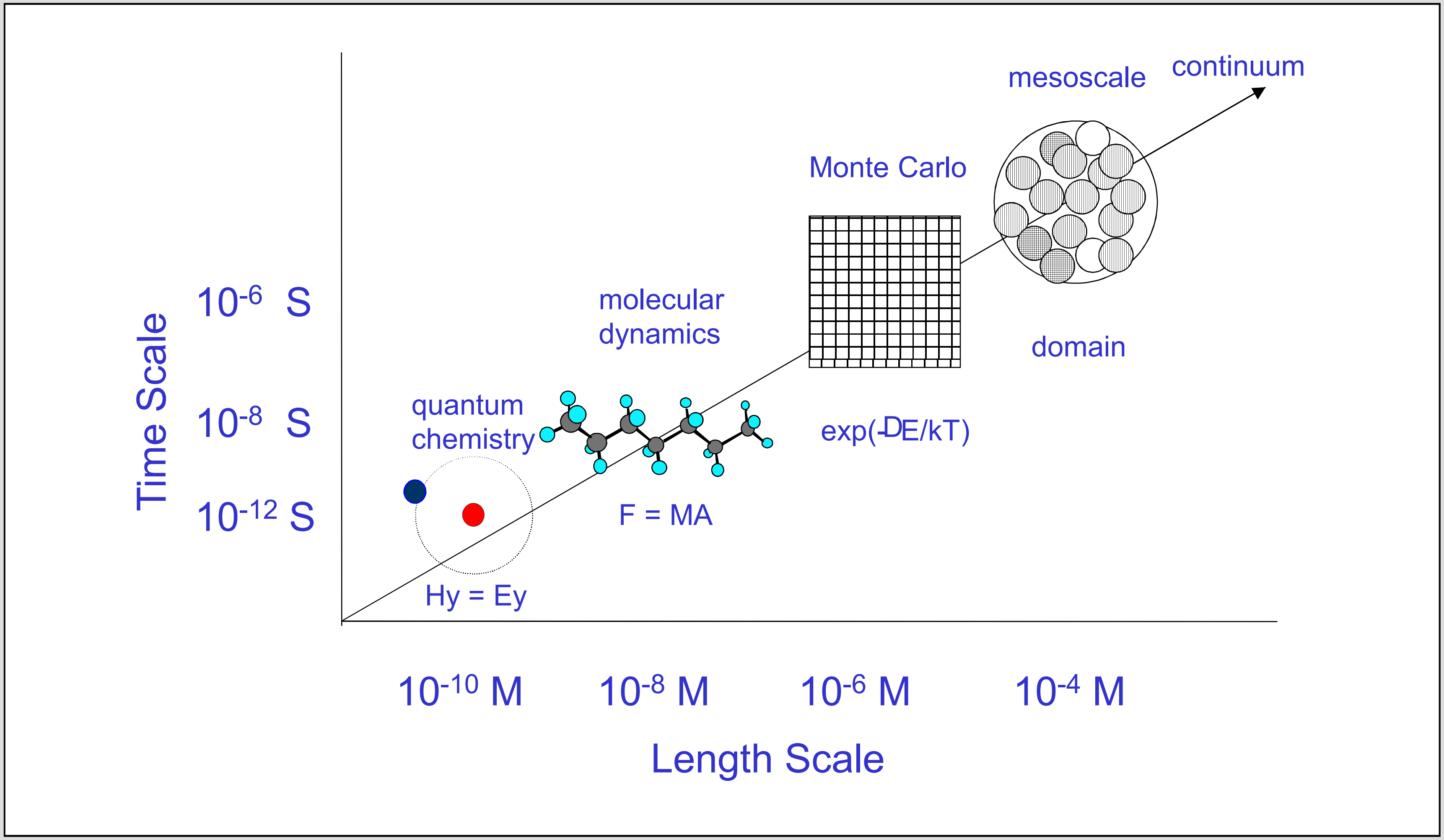




Micro and nanomechanics research

- Molecular dynamics
  - nano and microflows flow calculation
  - influence of wall material on the flow in nanochannels
    (with Walenta , Peradzynski)
  - verification and validation of the MD in terms of modeling the real materials *(with J. Bytnar PhD Student)*
- Microdevices calculations
  - micromixer optimisation *(with A. Mamrou PhD Student)*
  - effect of obstacle geometry on the image flow in microchannels *(with M.Kmiotek PhD Student)*
- Biomechanics: influence of microstructure on the properties bioliquids
-

Scale in Simulations



Molecular dynamics - Introduction

- *Molecular dynamics (MD)* is a computer simulation technique:

  the time evolution of interacting atoms is followed
  by integrating their equations of motion.

- We follow the laws of classical mechanics, and most notably Newton's law:

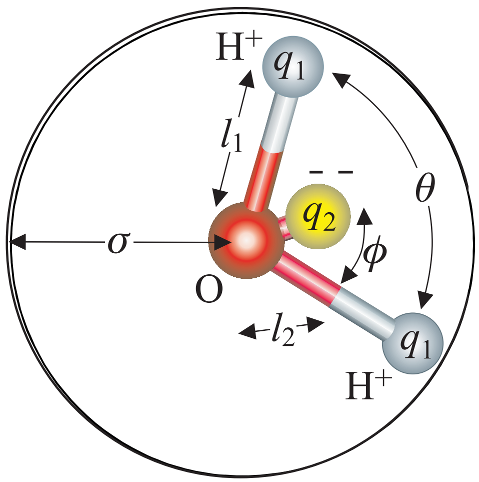
$$F_i = m_i a_i$$

$$a_i = d^2 r_i = dt^2$$

Procedure of Molecular dynamics

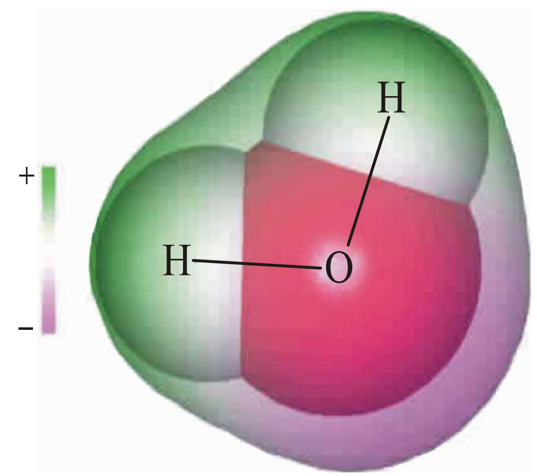
1. Give atoms initial positions $\boldsymbol{r}^{(t=0)}$, choose short Δt
2. Get forces $\boldsymbol{F} = - \nabla V(\boldsymbol{r}^{(i)})$ and $\boldsymbol{a} = \boldsymbol{F}/m$
3. Move atoms: $\boldsymbol{r}^{(i+1)} = \boldsymbol{r}^{(i)} + \boldsymbol{v}^{(i)} \Delta t + {}^{1}\!/_{2}\, \boldsymbol{a}\, \Delta t^{2} + \ldots$
4. Move time forward: $t = t + \Delta t$
5. Repeat as long as you need

Water



TIP4P molecular model of a water molecule

$l_1 = 0.9572 \cdot 10^{-10}$ m
$l_2 = 0.15 \cdot 10^{-10}$ m
$q_1 = +0.5200$
$q_2 = -1.0400$
$\theta = 104.52°$
$\phi = 52.26°$

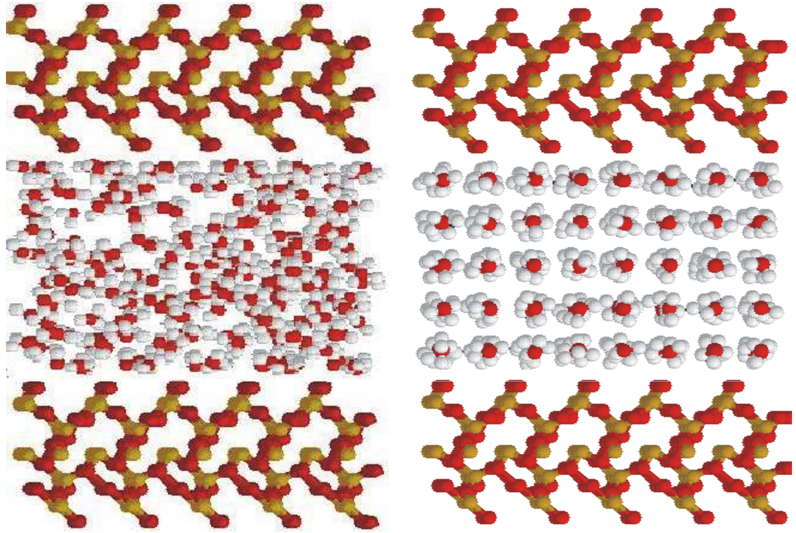


Water molecule

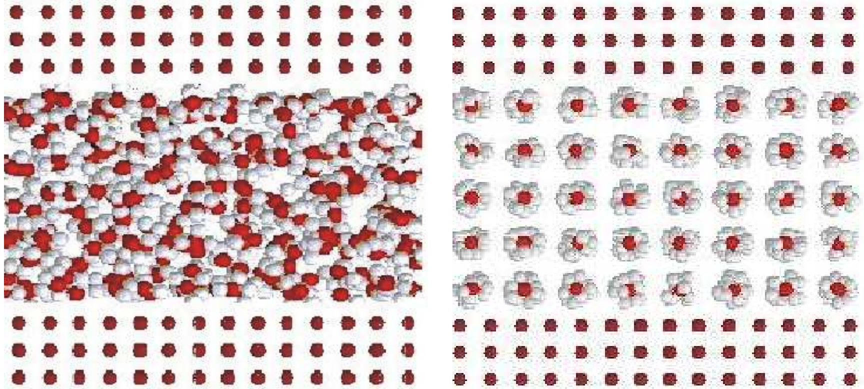
$$\Phi(r_{\alpha\beta}) = \begin{cases} \varepsilon\left(\left(\frac{\sigma}{r_{\alpha\beta}}\right)^{12} - \left(\frac{\sigma}{r_{\alpha\beta}}\right)^{6}\right) & r_{\alpha\beta} < r_c \\ 0 & \end{cases}$$

$\varepsilon = 0.6480$ kJ/mol, $\sigma = 3.15 \cdot 10^{-10}$ m:

Nanoflows MD simulation snapshots

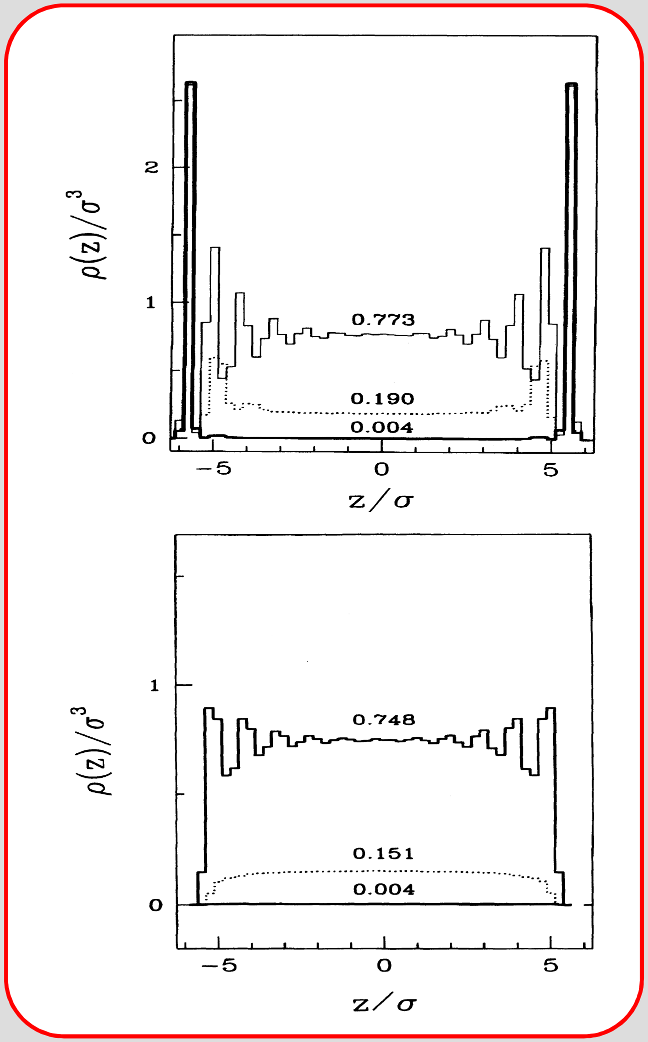


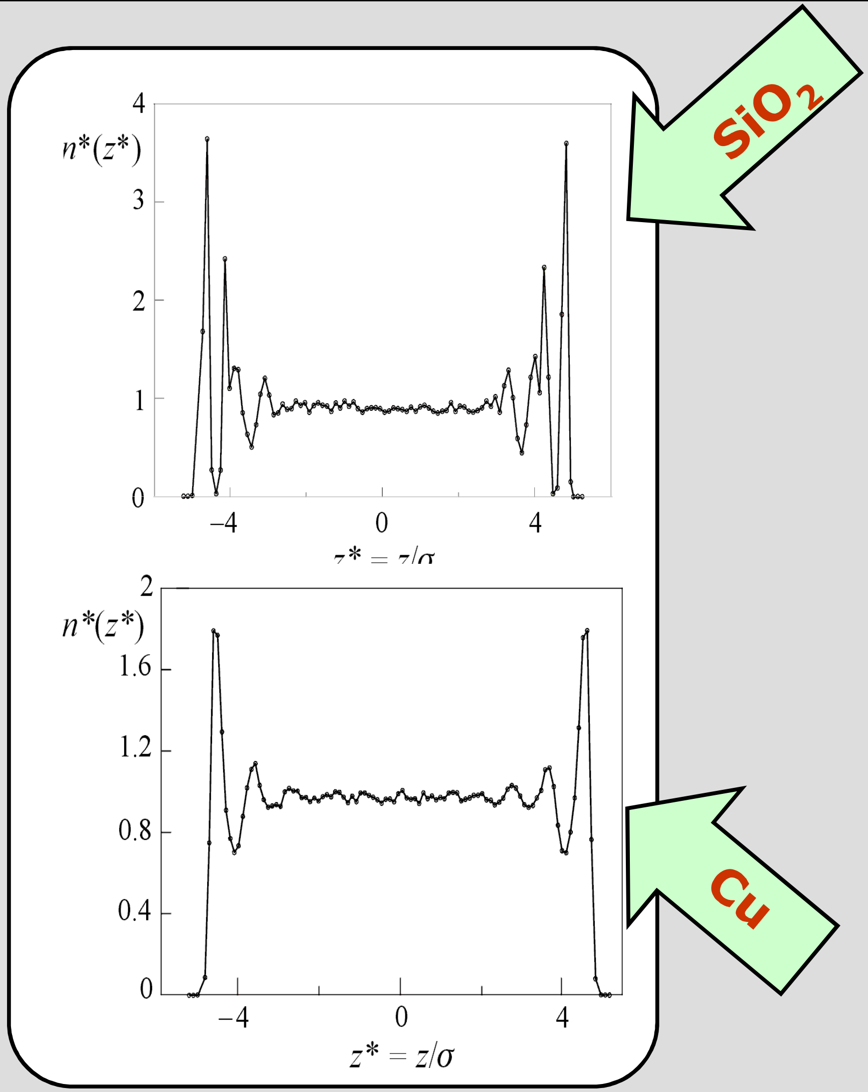
SiO_2



Cu

Density in nanochannels

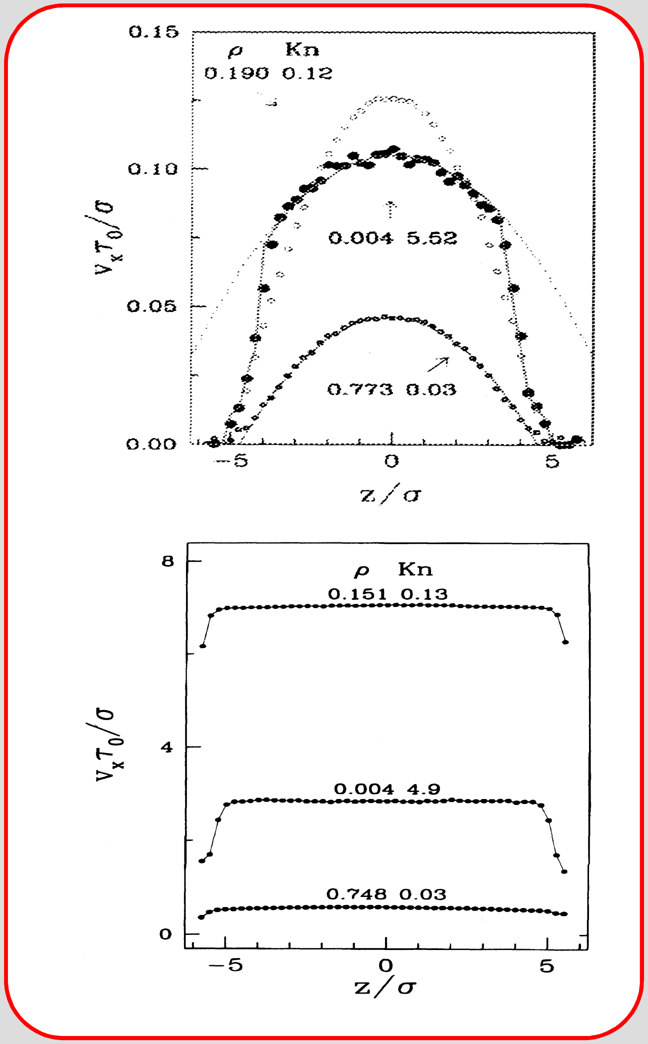


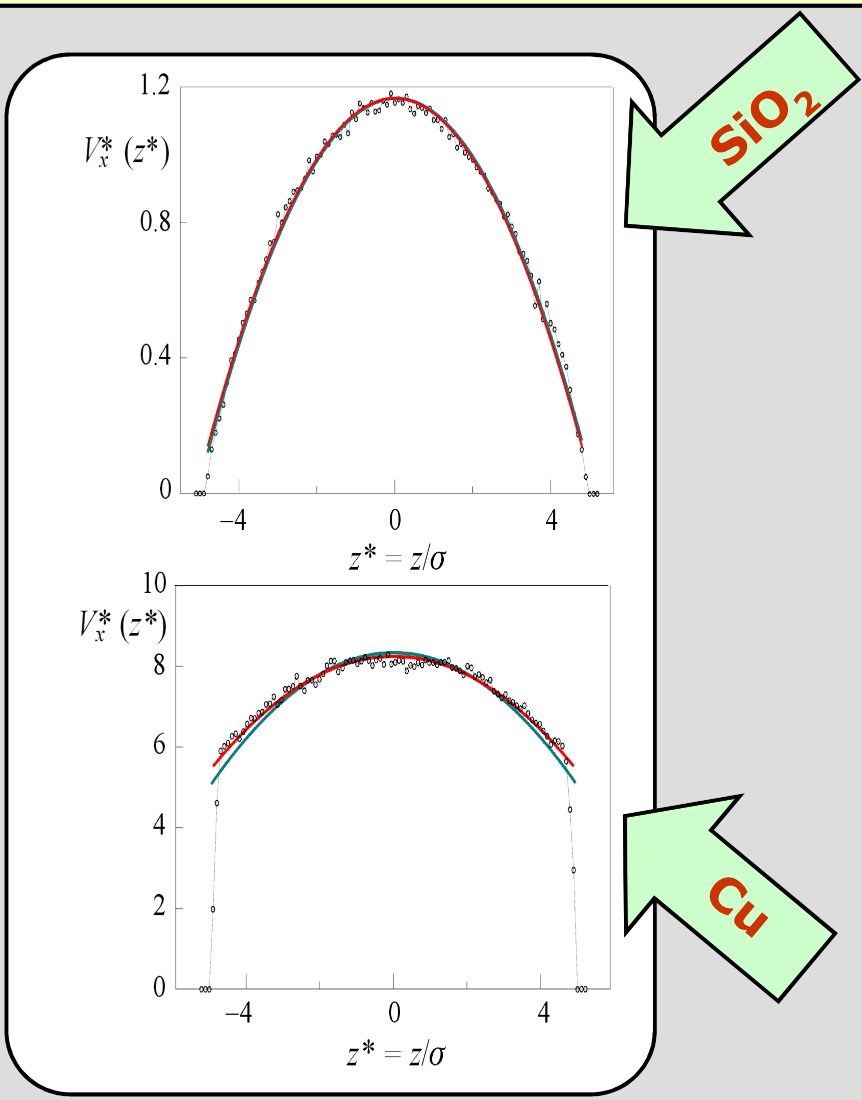


Cieplak 2002

Kucaba-Pietal, Walenta, Peradzyński 2002

Velocity in nanochannels

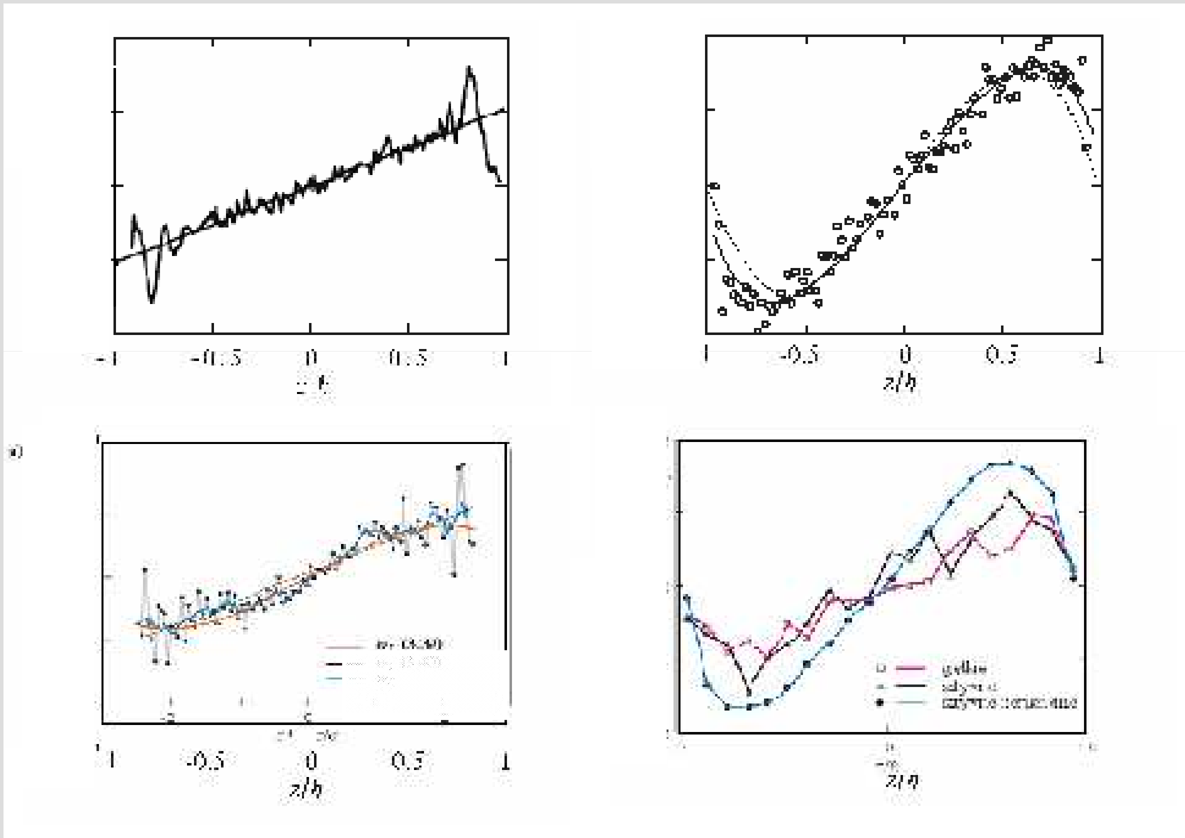




Cieplak 2002 Kucaba-Pietal, Walenta, Peradzyński 2002

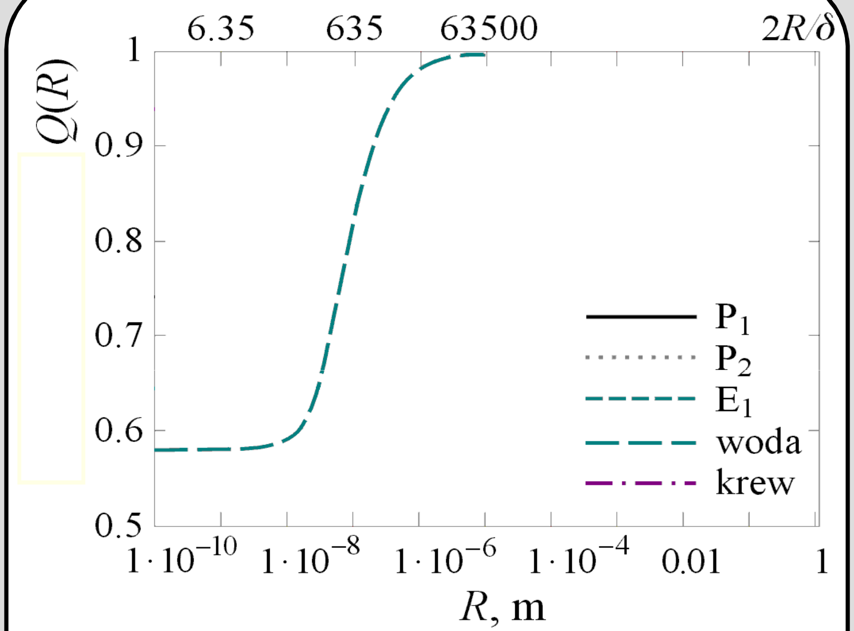
Microrotation in nanoflows exists*

*however, it can NOT be described in the frame of classical continuum model



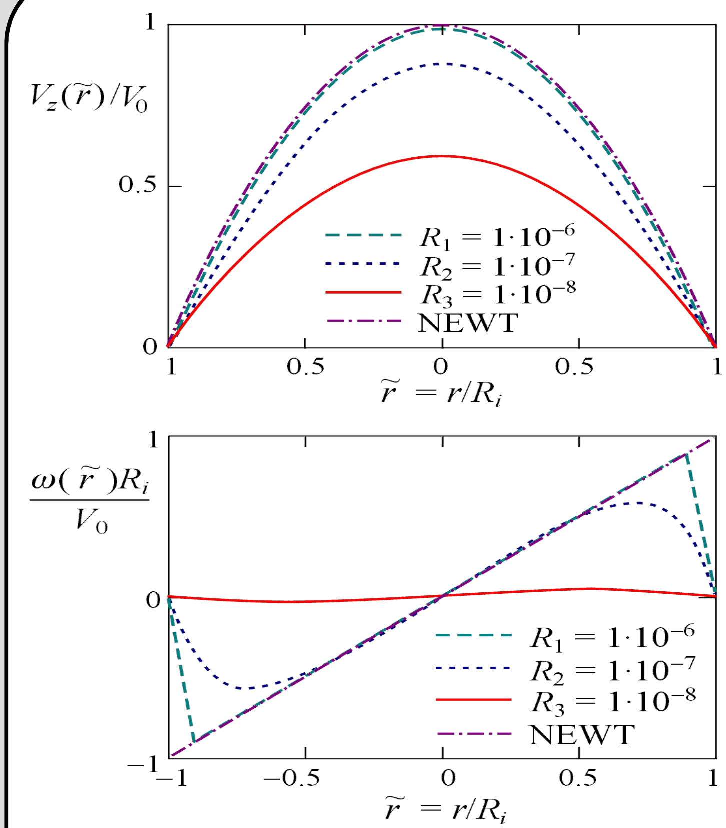
Results of MD nanoflows simulation (Poiseuillea flow):a) argon, h=5 (*Todd1998)* h=5,
b) Argon h=15 *(Duhammel 2000),* c) water, **h=5** *(Kucaba-Pietal, Walenta, Peradzyński, 2002),*
d) Dlugie molekuly, h=15, (*Rapaport,1998)*

Water flows in microchannels

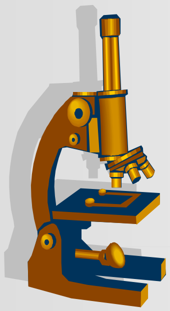


Q (R) in microchannels.

δ –linear dimension of water molecule



Water velocity
and microrotation distributions

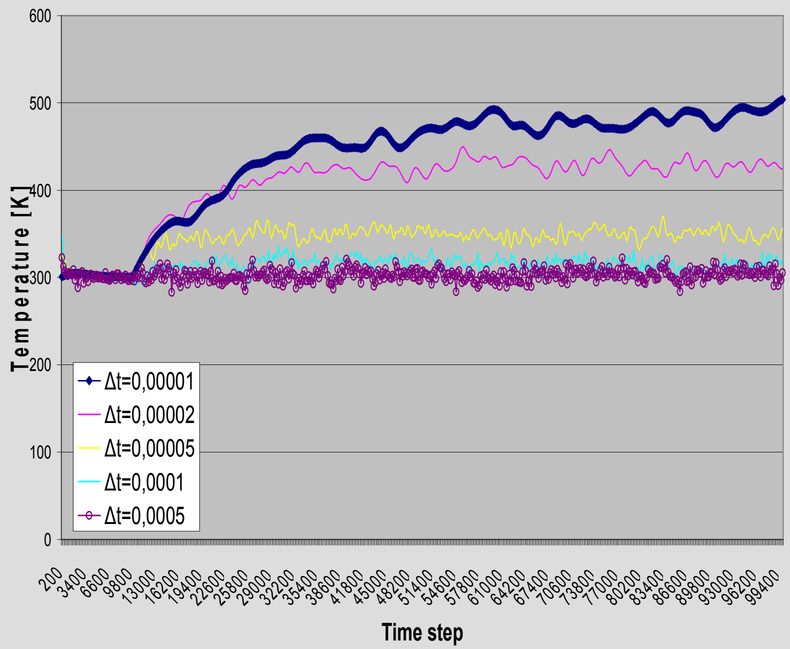


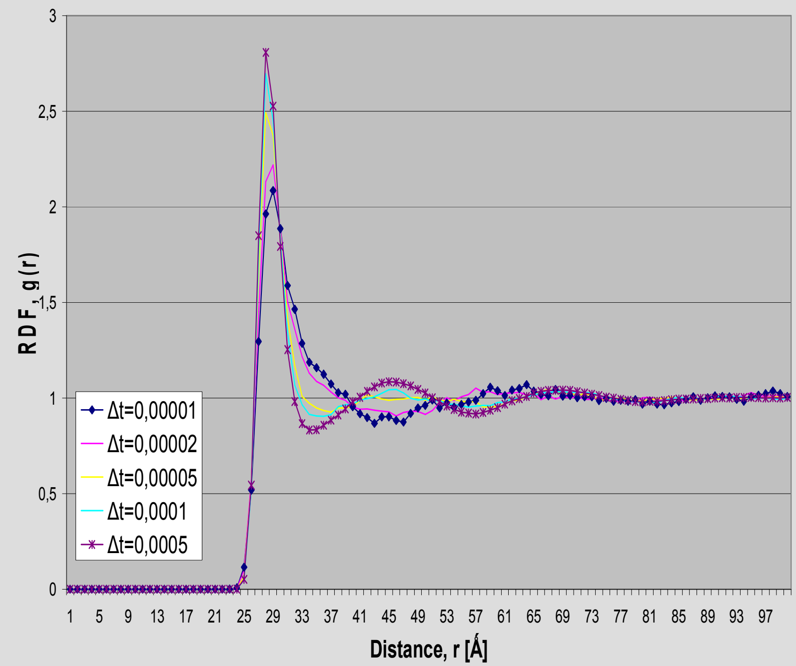
Werification and Walidation of MD method

Time Step δt in MD simulation

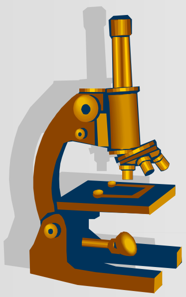
- Time step δt should be as large as possible to still get accurate trajectories (on the time scale needed) and conserve of energy
- In general, δt should be ≈0.01 x the fastest behavior of real system (e.g., atoms oscillate about once every 10^{-12} s in a solid ⇒ MD time steps are ≈ 10^{-14} s in simulations of solids)

Time Step δt in MD simulation



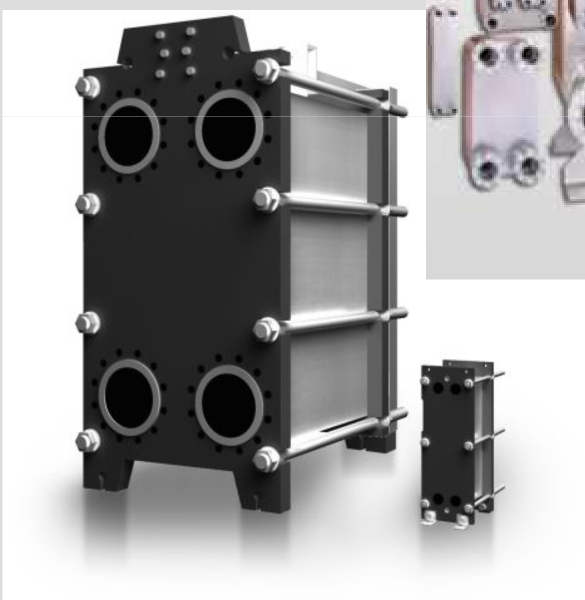


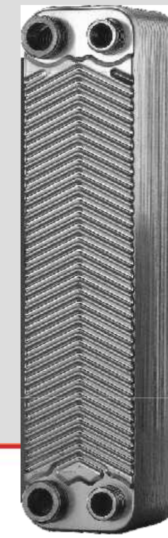
J.Bytnar 2011

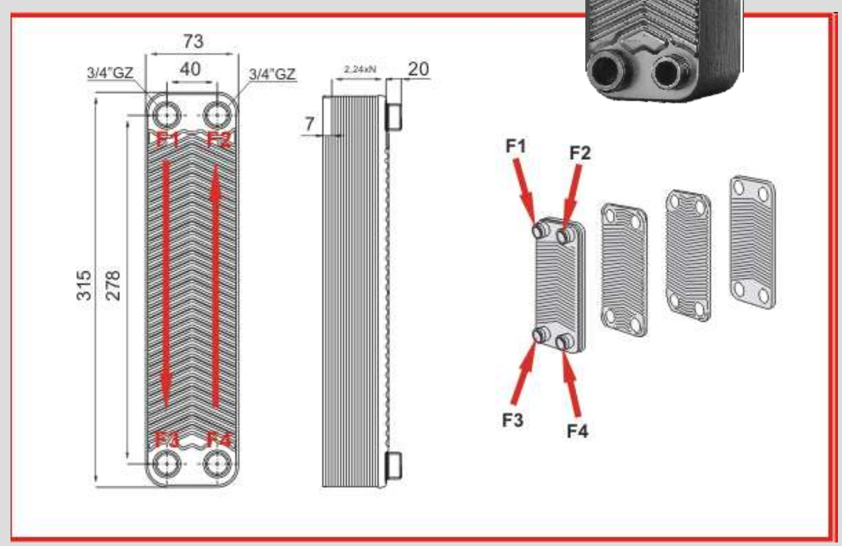


Effect obstacle geometry on flow in microchannel

Motivation – heats exchanger

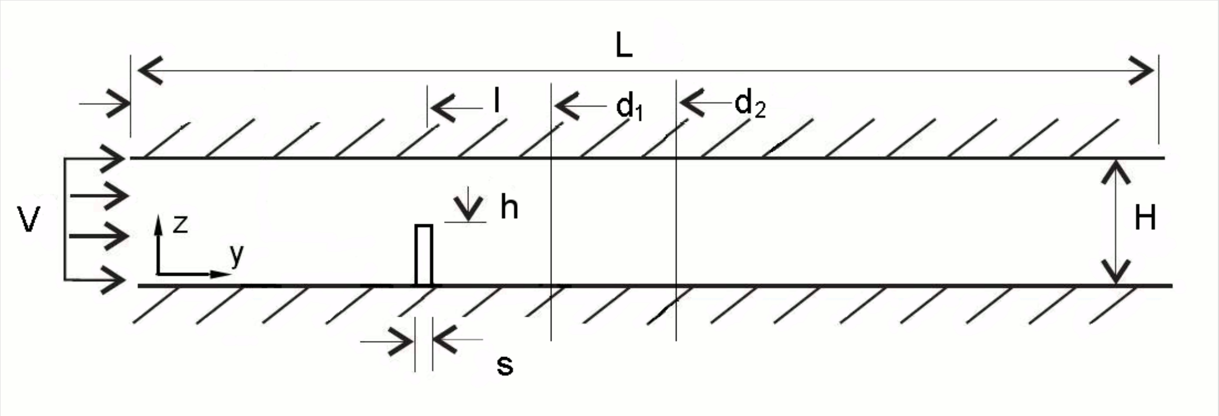




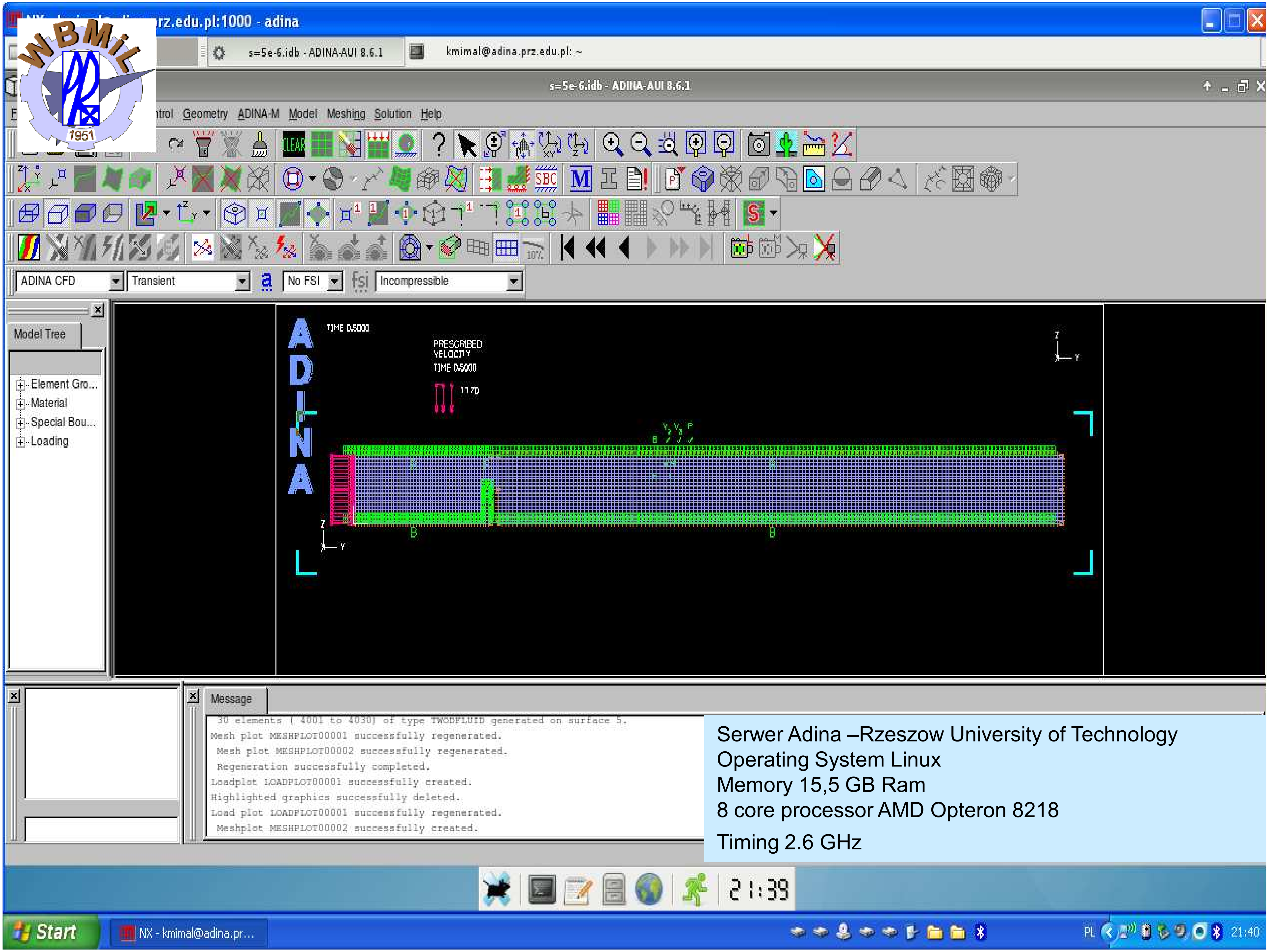


Problem description

- an obstacle was immersed in the l distance from inlet of the channel_of the H height (see Fig.)
- the obstacles were triangular or rectangular of the width of s and the height of h
- the influence of non-dimensional parameter s/h and
- Reynolds number was studied

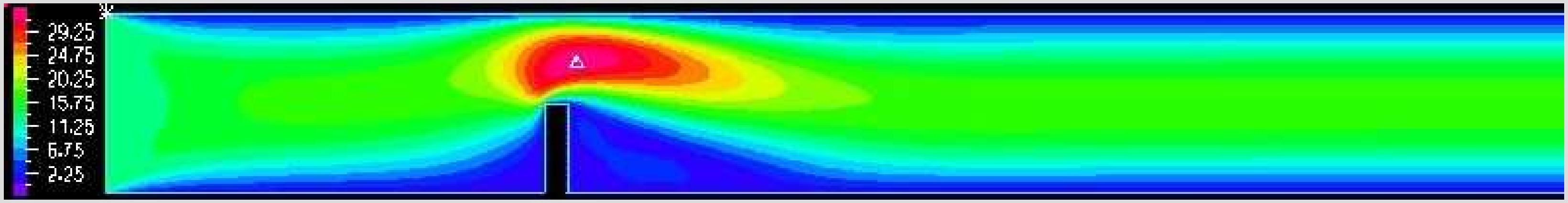


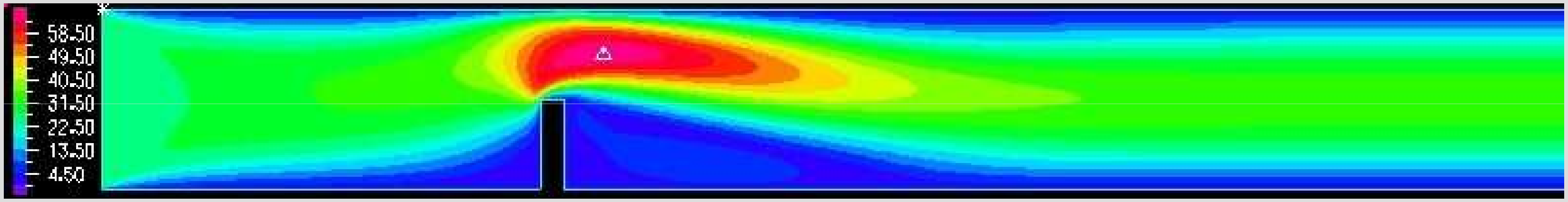
The geometry of the flow problem

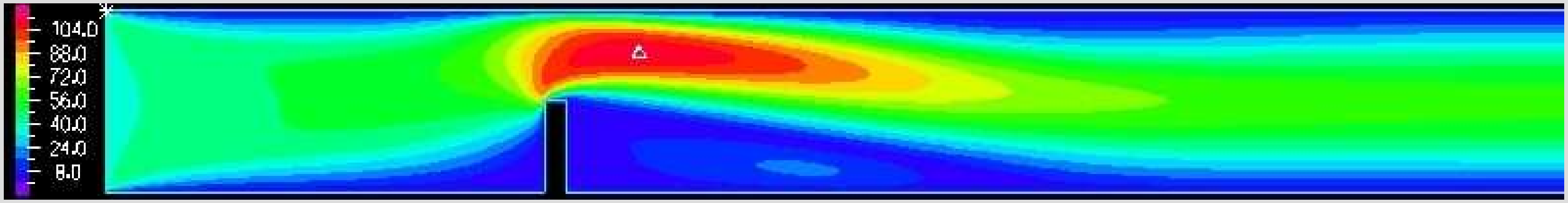


Serwer Adina –Rzeszow University of Technology
Operating System Linux
Memory 15,5 GB Ram
8 core processor AMD Opteron 8218
Timing 2.6 GHz

Results of calculations

a) 

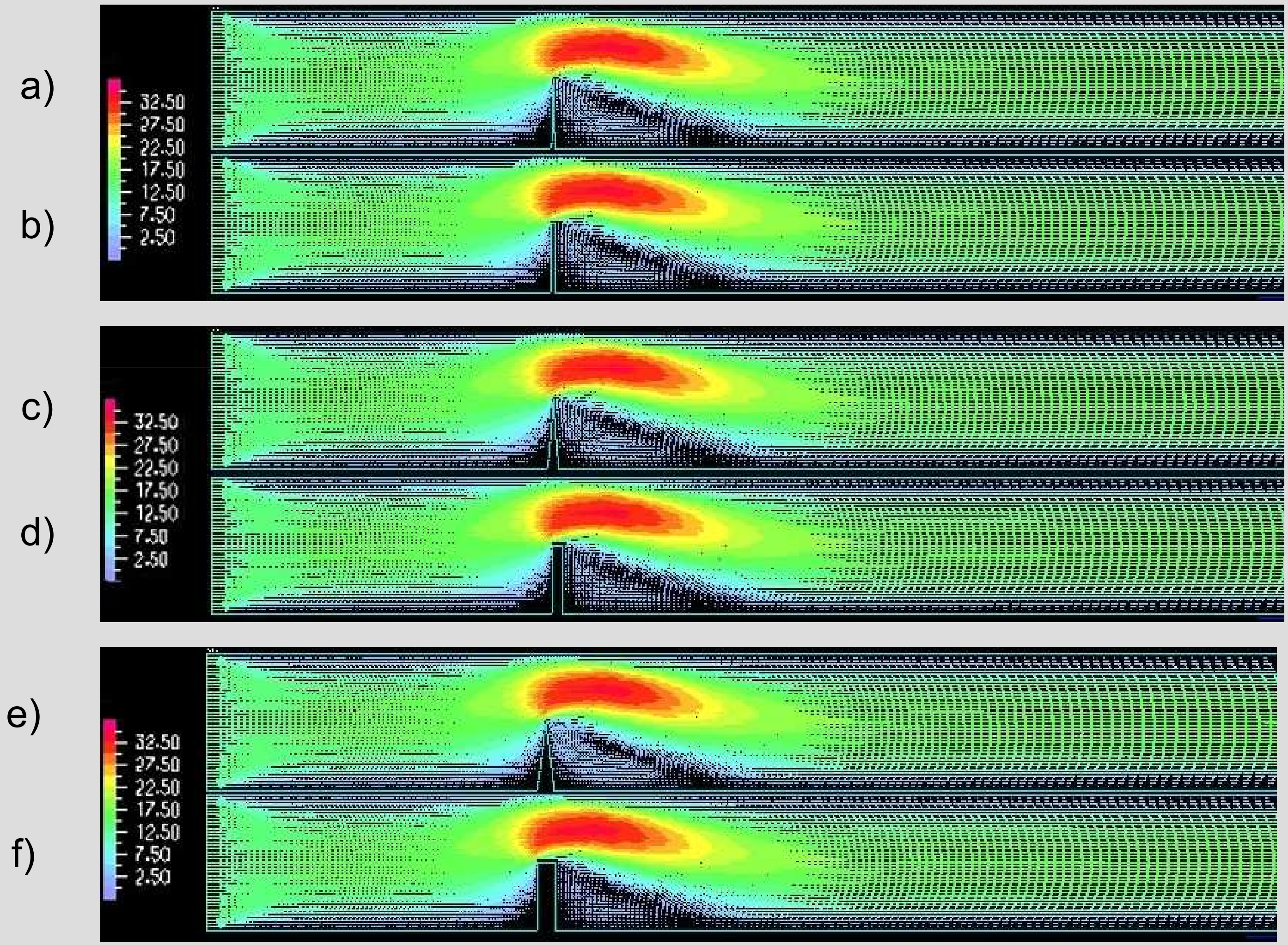
b) 

c) 

Velocity distribution in a channel with rectangular obstacle
a) Re=30; b) Re= 60; c) Re=100

M. Kmiotek 2010

Results of calculations (2)

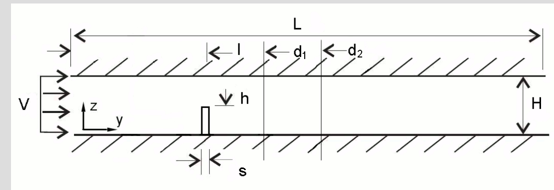


Velocity vector
for Re=30
in a channels
with triangular
and rectangular
obstacle

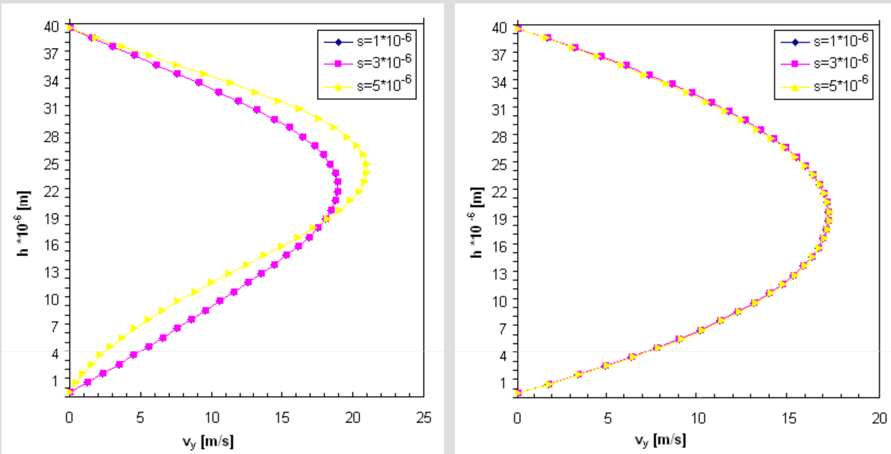
a), b) s = 1 $\cdot 10^{6}$ m
c), d) s = 3 $\cdot 10^{6}$ m
e), f) s = 5 $\cdot 10^{6}$ m

M. Kmiotek 2010

Results of calculations (3)

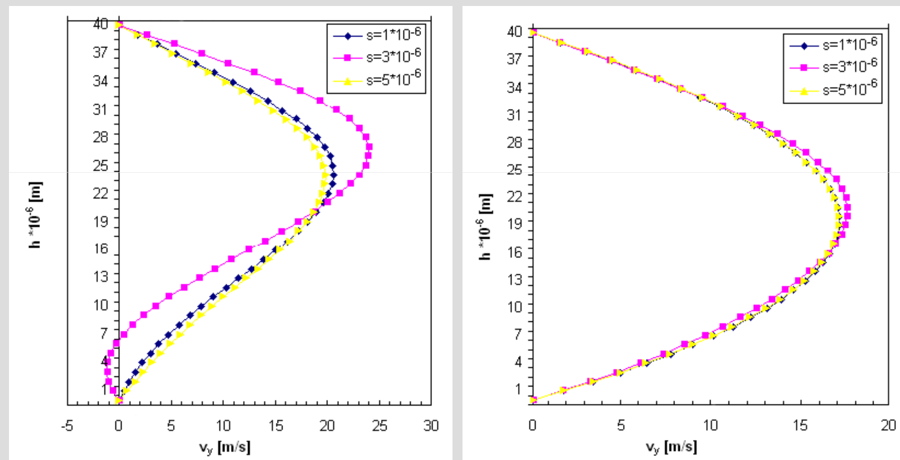


a) b)



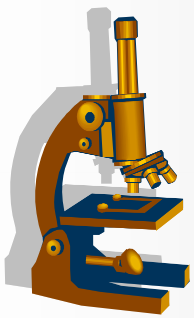
Profiles of longitudinal velocity vy
in a channel with the triangular obstacle
for re = 100 in
(a) distance d1 and
(b) d2

a) b)



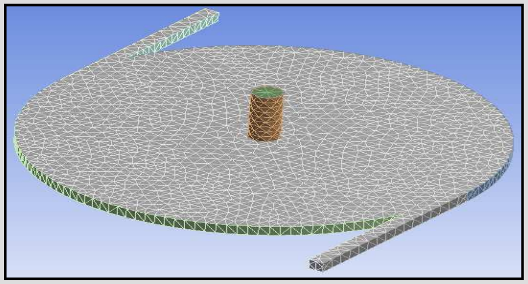
Profiles of longitudinal velocity vy
in a channel with the rectangular obstacle
for re = 100 in
(a) distance d1 and
(b) d2

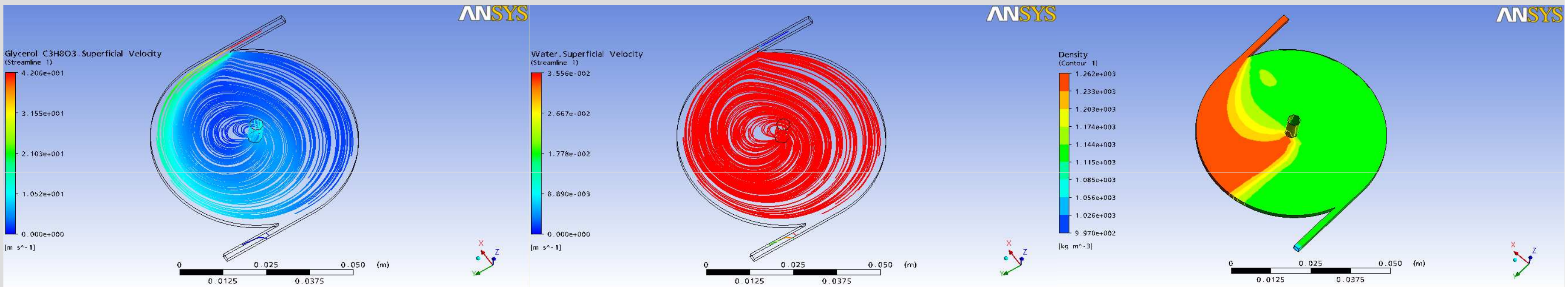
M. Kmiotek 2010

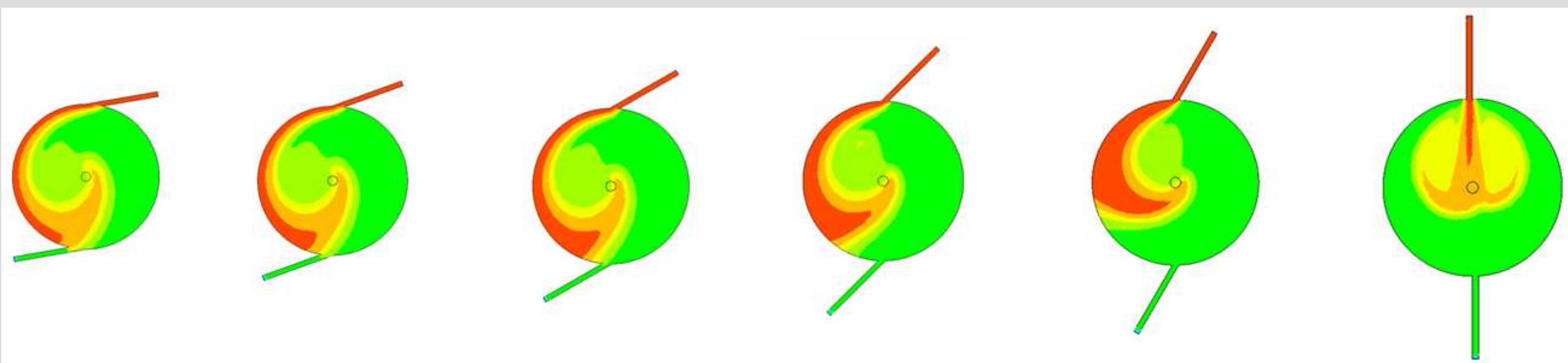


Effect of geometry on flow in micromixers

Effect of geometry on flow in micomixers







A.Mamrou 2010

Initiatives

- Microfluidics and nanofluidics Minisymposjum, GAMM 2009 Gdansk
- Polish Conference of Nano and Micromechanics (Krasiczyn 2008, 2010)
- Lectures for Phd students
- Chapter in book: Technical Mechanics Series, Biomechanics *ed. R.Bedzinski*: Micromechanics of Biological Fluid, IPPT, 2010

ISBN 978-83-89687-81-6

I Polish Conference on Nano and Micromechanics (2008)

kknm08.prz.edu.pl

- Participants: 68
- Invited Lectures 10
- Lectures and posters 58

II Polish Conference on Nano and Micromechanics (2010)

II Polish Conference on Nano and Micromechanics (2010)

kknm10.prz.edu.pl

- Participants: 98
- Invited Lectures 11
- Lectures and posters 120

Welcome to Krasiczyn (2012)

AIM^2

Advanced In-Flight Measurement Techniques 2

SEVENTH FRAMEWORK PROGRAMME

AIM²
Advanced In-flight Measurement Techniques
2010-2014
collaborative project

AIM²
Advanced In-flight Measurement Techniques
2010-2014

1. AIRBUS Operations SAS, France
2. Avia Propeller s.r.o., Czech Republic
3. Cranfield University, United Kingdom
4. <u>Deutsches Zentrum für Luft- und Raumfahrt e.V., Germany COORDINATOR</u>
5. EVEKTOR, Czech Republic
6. Moscow Power Engineering Institute (Technical University), Russian Federation
7. Stichting Nationaal Lucht- en Ruimtevaartlaboratorium, Netherlands
8. Office National d'Études et de Recherches Aérospatiales, France
9. Piaggio Aero Industries, Italy
10. Politechnika Rzeszowska im. Ignacego Lukasiewicza PRz, Poland

The aim of the project

- The development of novel non-intrusive (optical) measurement techniques: PIV, IPCT, IRT, FBG, LIDAR, BOS
- to measure the air flow and thermal parameters, as well as the aircraft surface deformation with microscale accuracy
- to develop standards for using these novel techniques for testing of the aircraft in flight on an industrial scale
- to spread up the information and knowledge during workshop which will be organised at RUT in 2013. The techniques and standards will be presented and a book on the subject will be edited
- During work on Project the methods will be developed and tested on the consortium aircrafts.
- Two of methods, IPCT, IRT will be tested on airplanes of AOC of RUT
- Moreover, numerical calculations to verify in-light test results will be caried out at RUT.

Cordially welcome to participate on AIM2 workshop in 2013 at RUT!

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Thank you for your attention