Modelling soft bodies with immersed boundaries

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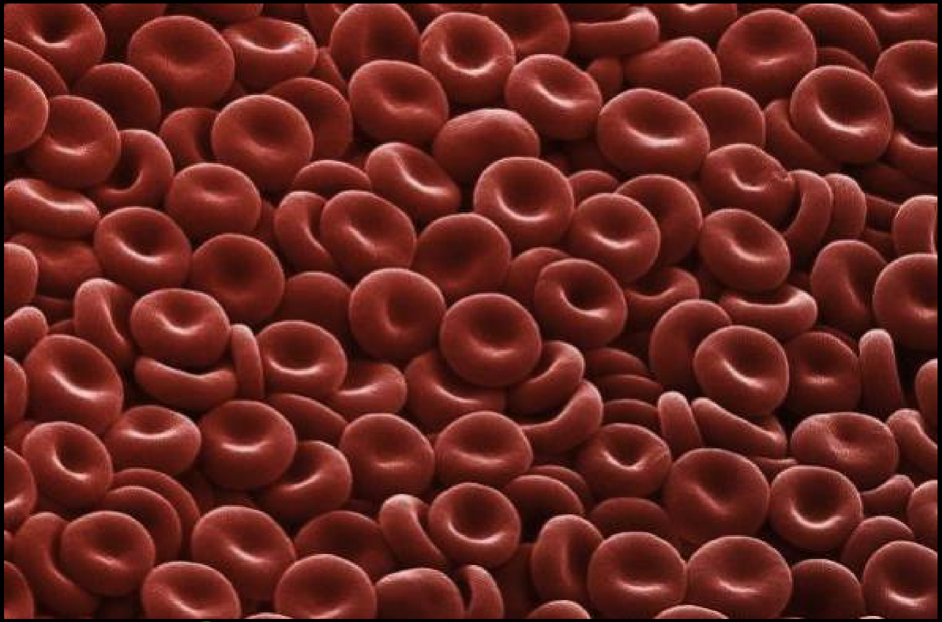
Outlook

- Why do we need immersed boundaries?
- How can we use immersed boundaries?
- Applications
- Conclusion and future prospects

Why do we need immersed boundaries?

Simulation of blood flow (on cellular level)

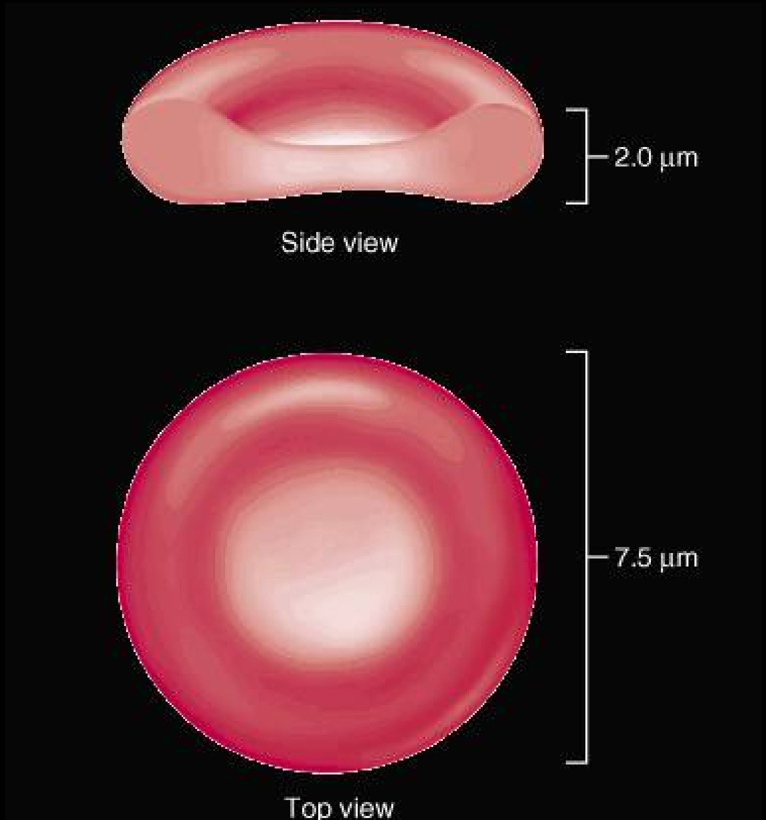
Components:



- blood plasma ✓
- blood cells ✗
- channel boundaries ✓

Red blood cell

- elastic
- preferred shape
- fixed volume
  and surface area



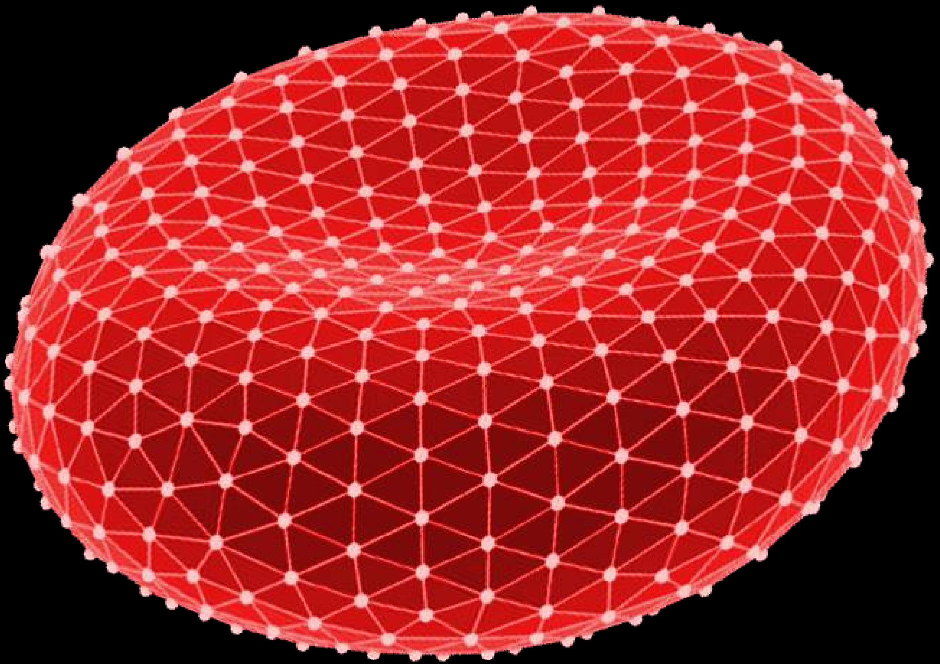
ESPResSo

- soft-matter simulations
- molecules, atoms with their own mass
- interacting with bonds and potentials
- LBM
- closed objects with their own particle management

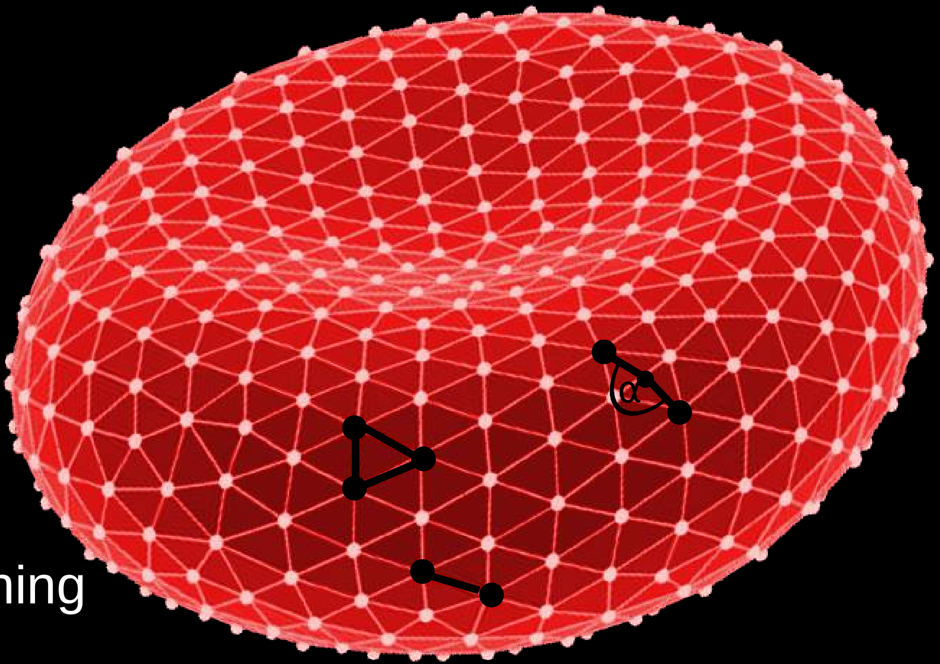
How can we use immersed boundaries?

Immersed boundary method

- discretization of object's boundary
- IB points
  - triangular mesh
  - elastic forces
  - interaction with fluid



Elastic forces*



LOCAL

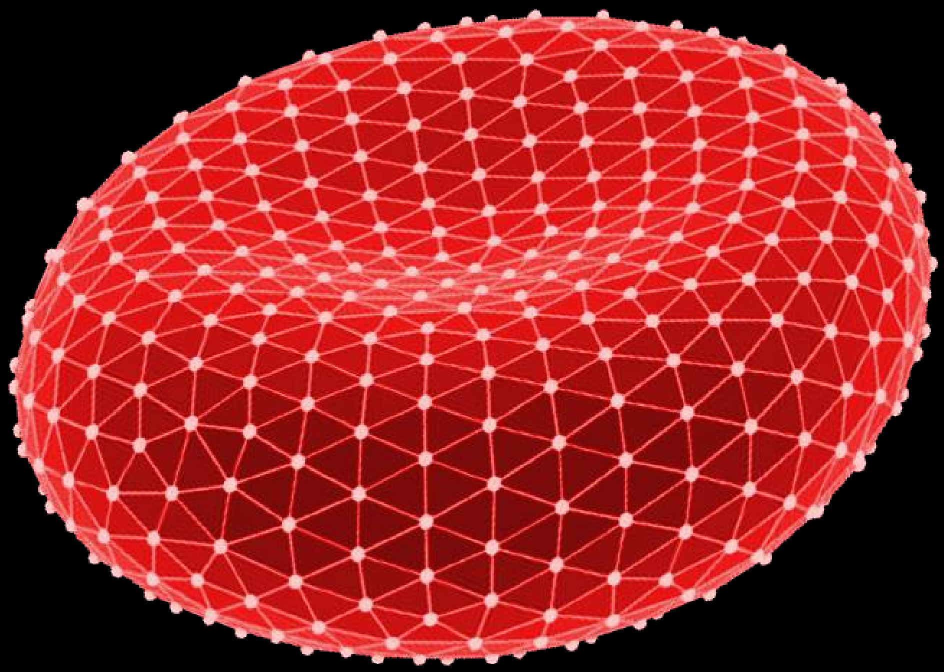
- Constant local area constraint
- Surface strain constraint – stretching
- Curvature constraint – bending

NONLOCAL

- Constant volume constraint
- Constant global area constraint

* Dupin et al., Modeling the flow of dense suspensions of deformable particles in three dimensions Physical Review E 75 (6), 066707

Interaction with the fluid



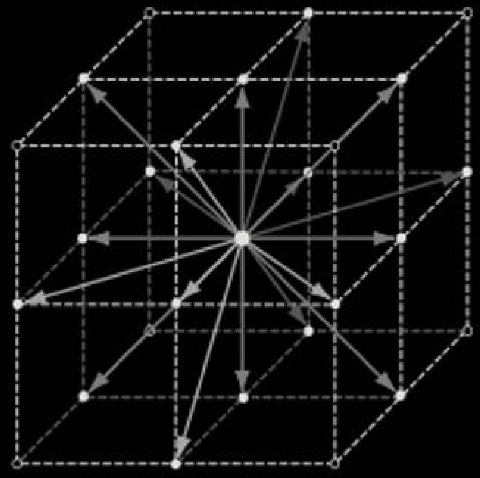
Combination of LBM and IBM

Model of blood plasma

- Fluid dynamics – lattice-Boltzmann method (LBM)

$$\underbrace{f_i(\vec{x} + \vec{e}_i\delta_t, t + \delta_t) = f_i(\vec{x}, t)}_{\text{streaming}} - \underbrace{\frac{(f_i(\vec{x}, t) - f_i^{\text{eq}}(\vec{x}, t))}{\tau}}_{\text{collision}} + \underbrace{F_i(\vec{x}, t)}_{\text{external forces}}$$

- Discrete velocities
- Fixed grid
- Parallelizable
- Explicit integration scheme:
  propagation + collision

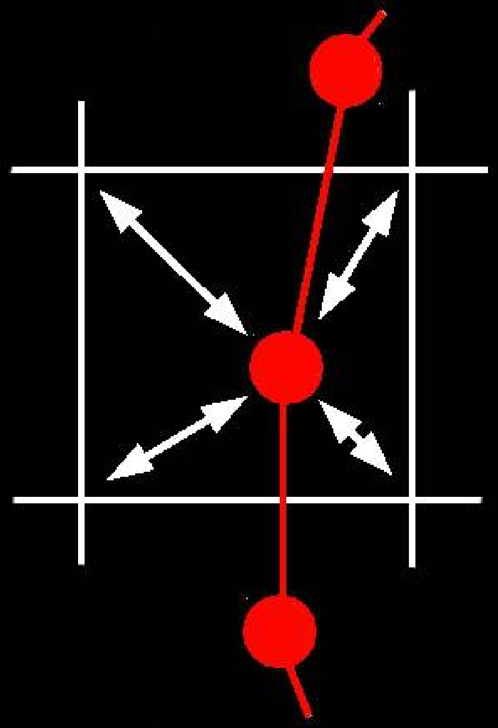


Fluid – particle interaction

<u>Immersed boundary method</u>

- Fluid:
  - – fixed grid
  - – lattice-Boltzmann equation

- Blood cell:
  - – boundary points are free in space
  - – Newton equations

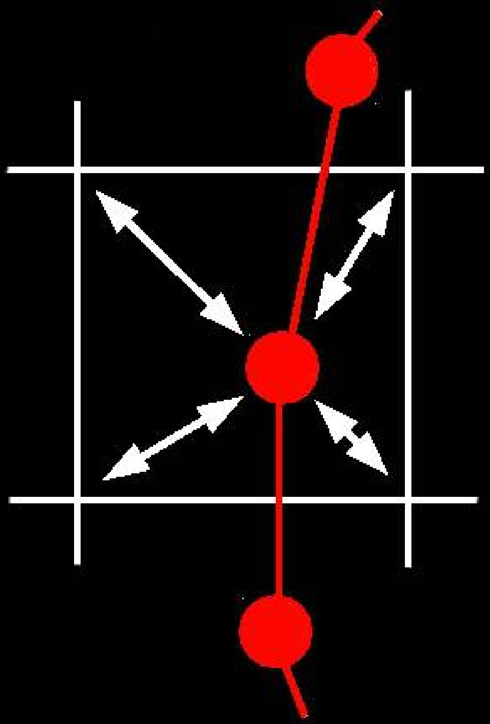


Drag force:

$F = K(u_f - u_p)$

Fluid – particle interaction

<u>Immersed boundary method</u>

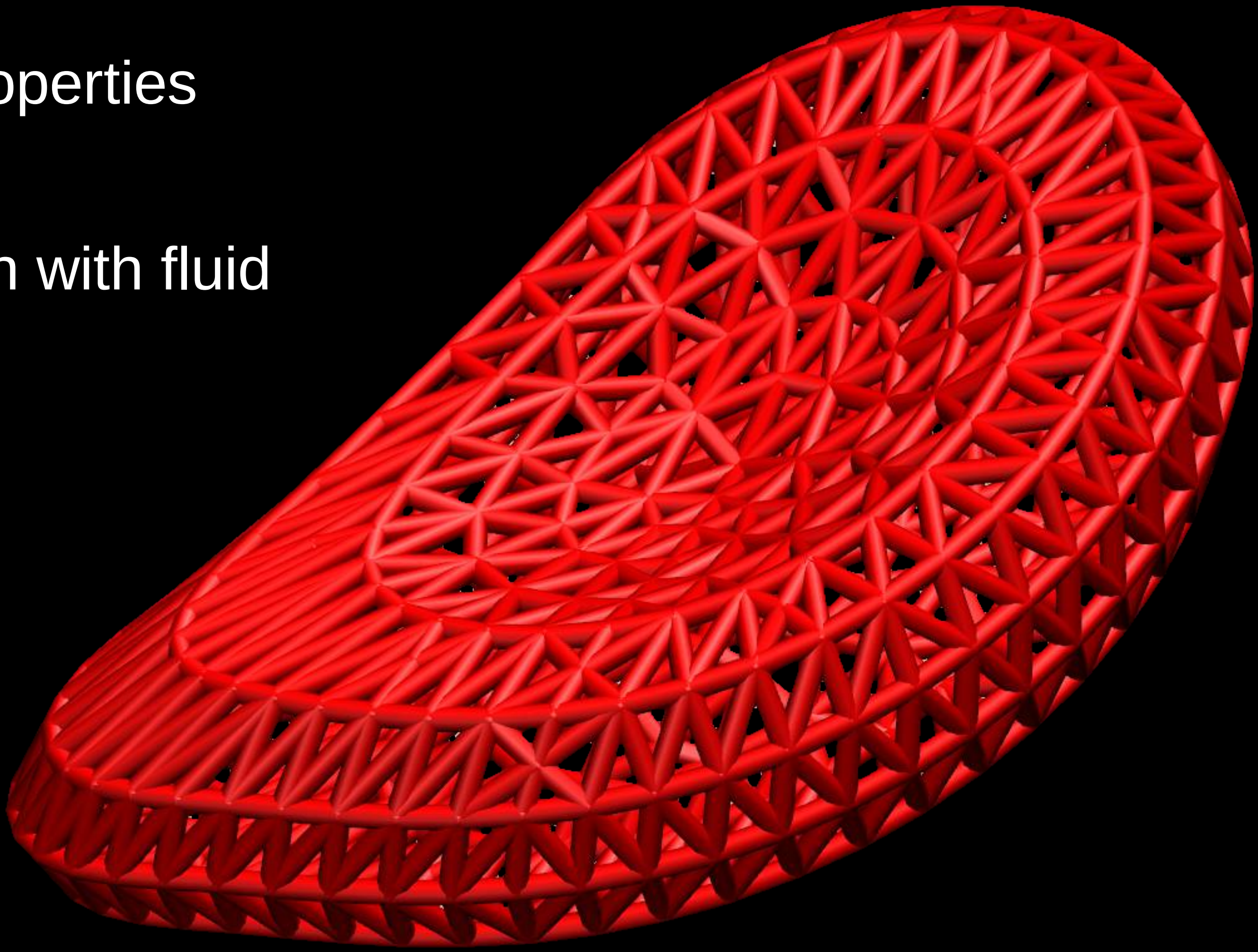


- Fluid:
  - – fixed grid
  - – lattice-Boltzmann equation
- Blood cell:
  - – boundary points are free in space
  - – Newton equations

external Force
for LBM-equation

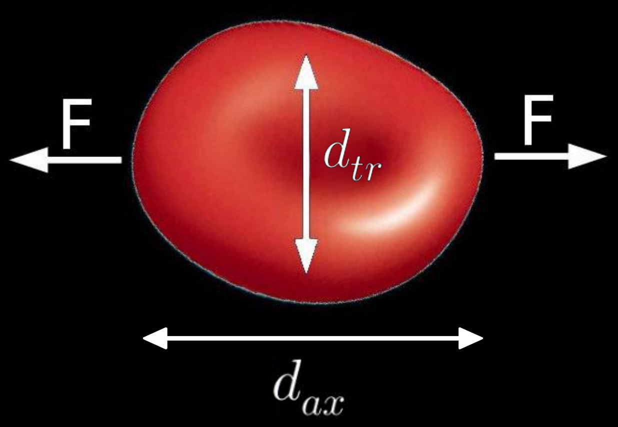
Calibration of immersed elastic objects

- elastic properties
- interaction with fluid



Calibration of elastic properties

- 5 parameters from elastic forces (stretching, bending, local area, global area, volume)



force exterted on cell	67pN	130pN	193pN
axial diameter d^0_{ax}	12.34	14.17	15.3
transverse diameter d^0_{tr}	5.05	4.53	4.29

J. P. Mills, L. Qie, M. Dao, C. T. Lim, and S. Suresh. Nonlinear elastic and viscoelastic deformation of the human red blood cell with optical tweezers. Molecular & Cellular Biomechanics, 1(3):169–180, 2004.

Calibration of elastic properties

Optimal values of elasticity parameters for a healthy RBC.

Stretching k_s	0.008
Bending k_b	0.0016
Local area k_{al}	0.01
Global area k_{ag}	1.0
Volume k_v	10.0

I. Cimrák, M. Gusenbauer, and T. Schrefl. Modelling and simulation of processes in microfluidic devices for biomedical applications. Comput. Math. Appl., 64(3):278–288, August 20127

Calibration of IB – fluid interaction

- mass of IB points
- mesh density of IB points
- friction coefficient (drag force intensity on IB point)

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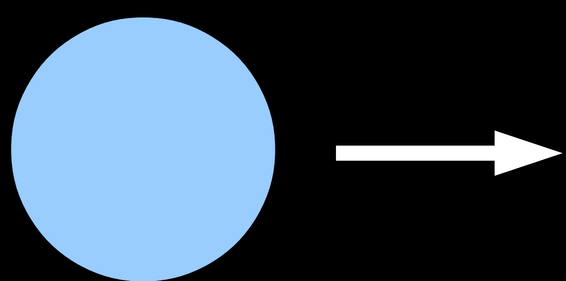

initial velocity v_0
of the sphere/ellipsoid

Calibration of IB – fluid interaction

- mass of IB points
- mesh density of IB points
- friction coefficient (drag force intensity on IB point)

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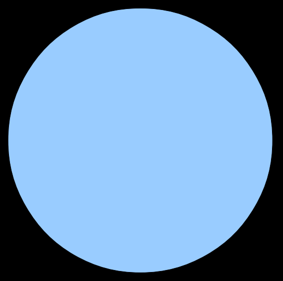
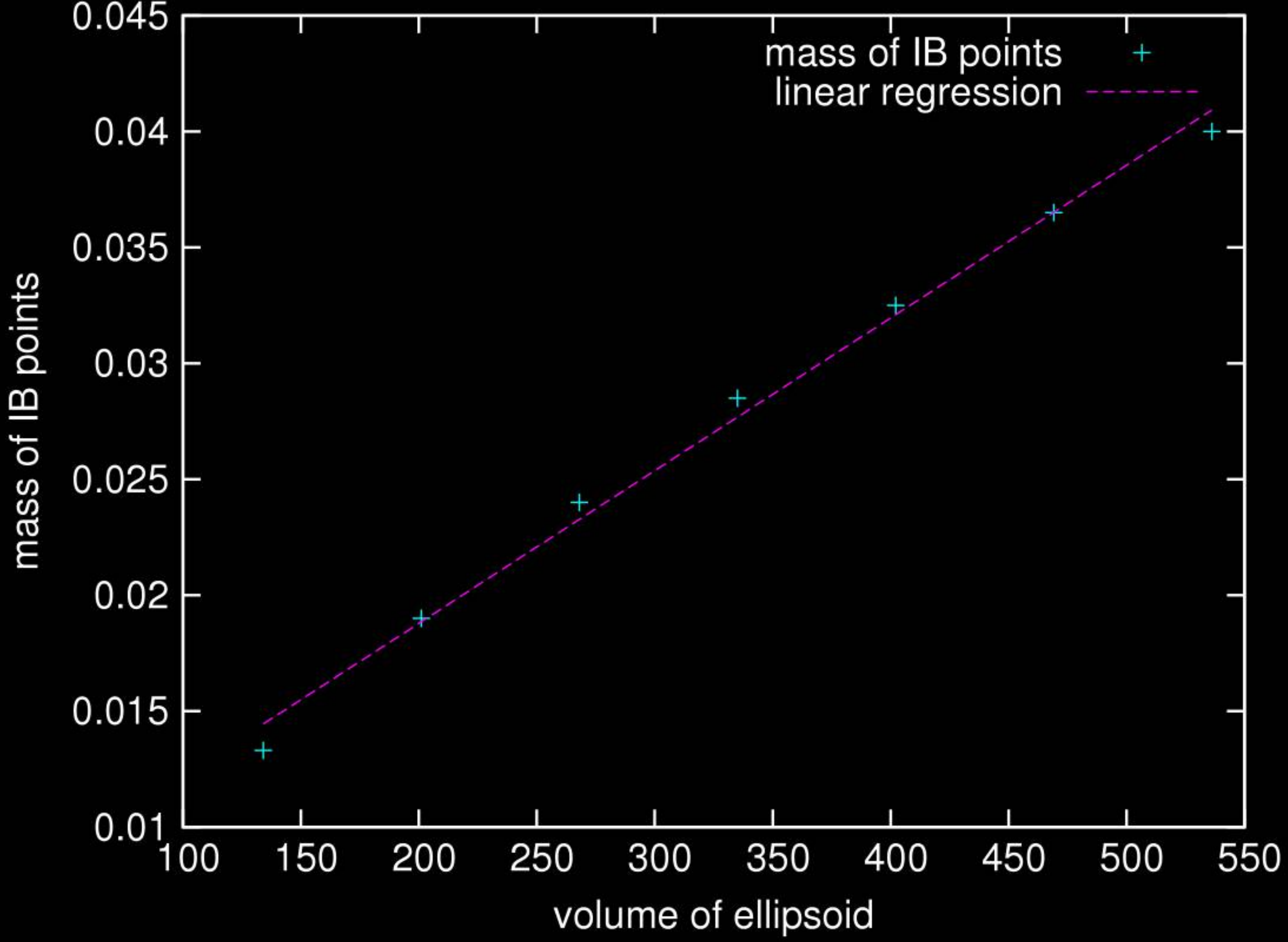


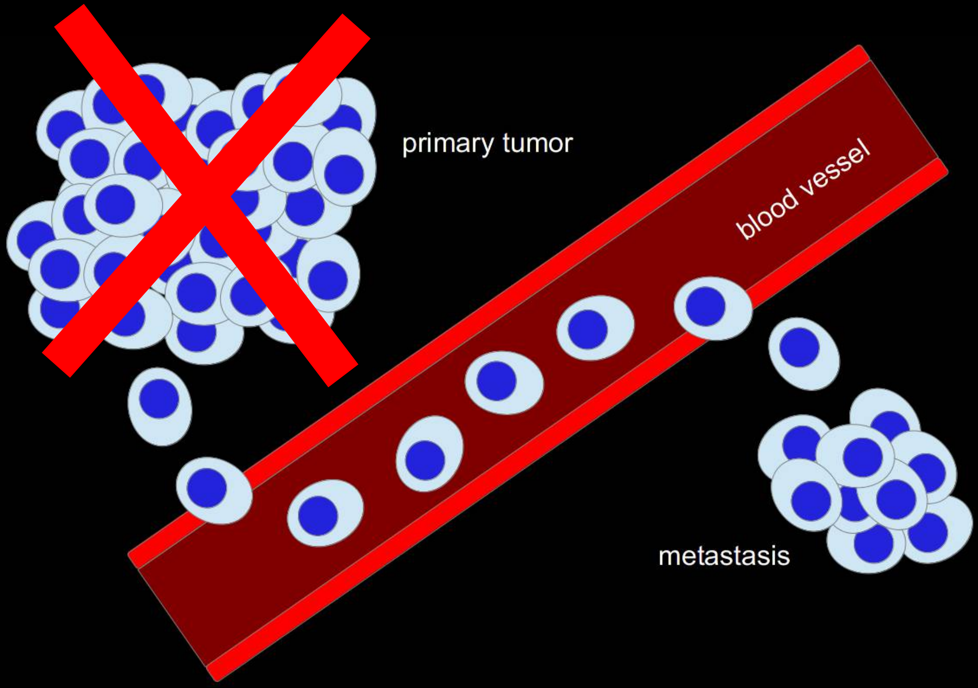
fluidic drag force slows down the sphere/ellipsoid

Calibration of IB – fluid interaction



Applications

Circulating tumor cells (CTCs)

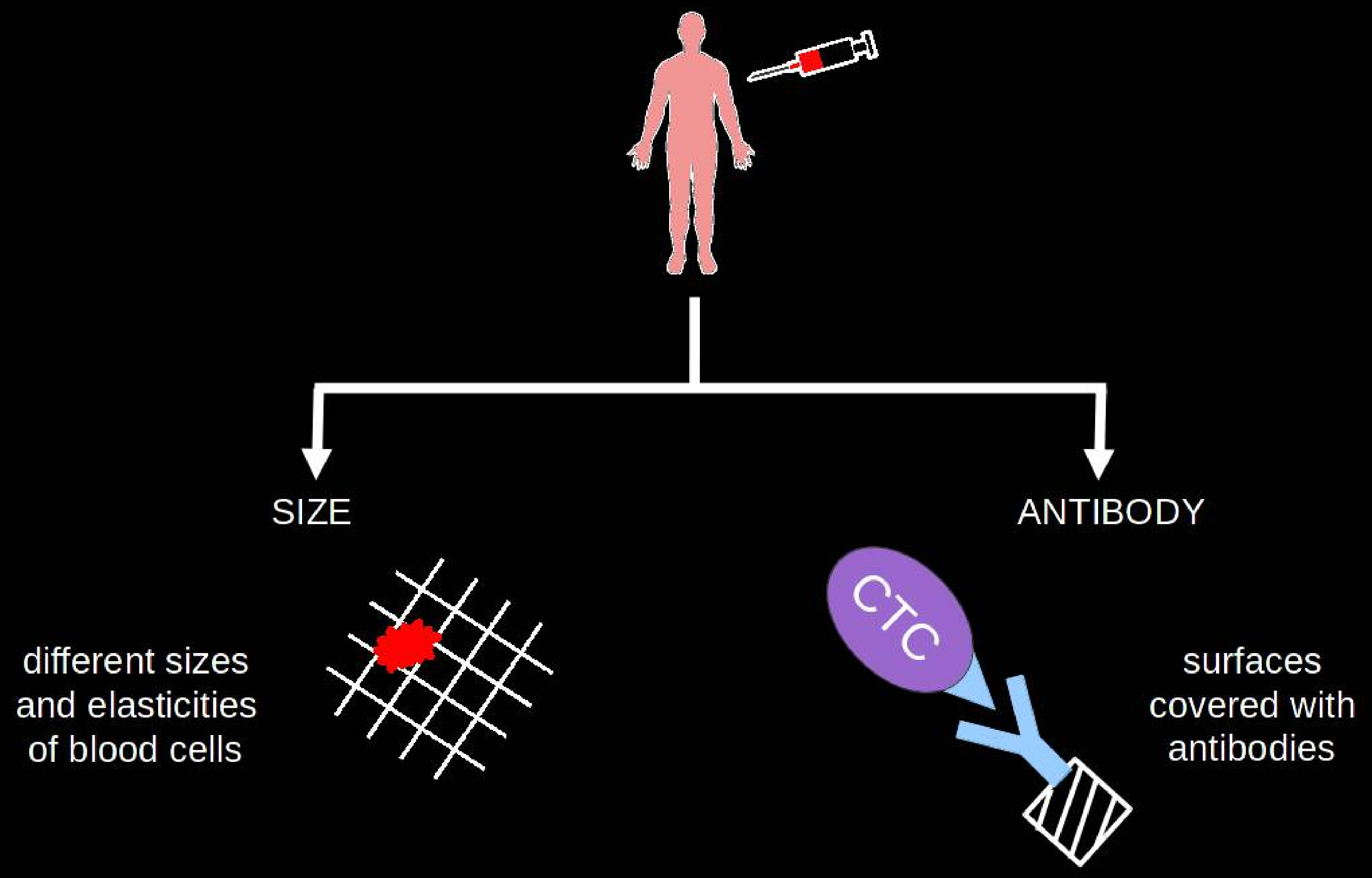


Prognostic value

- Counting of CTCs:
  - medical checkups
  - control therapies
  - recognize new tumors developing

- Genetic/molecular characterization
  - gain information about main tumor and metastasic developement
  - understanding evolution of cancer

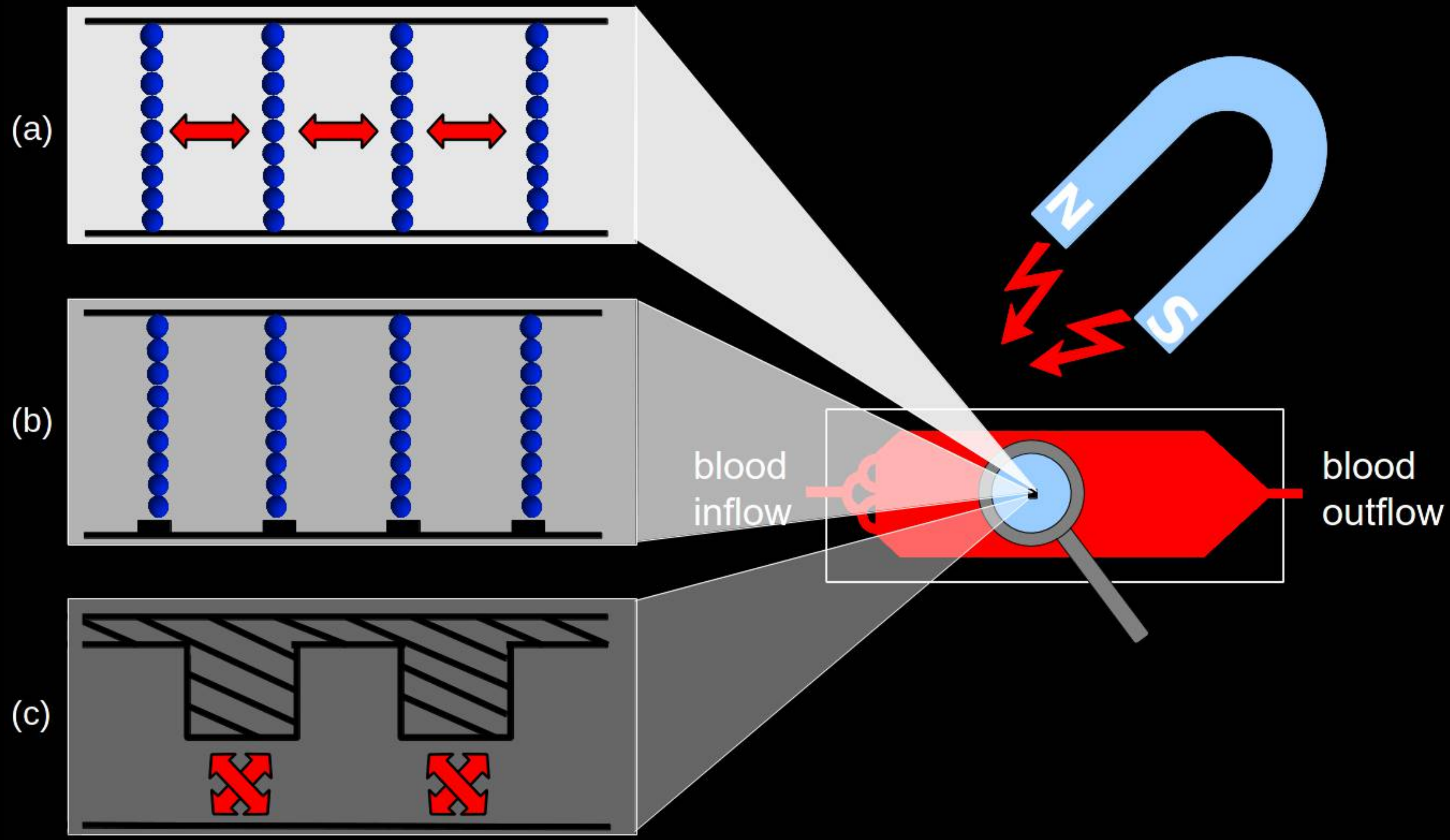
Filter methods

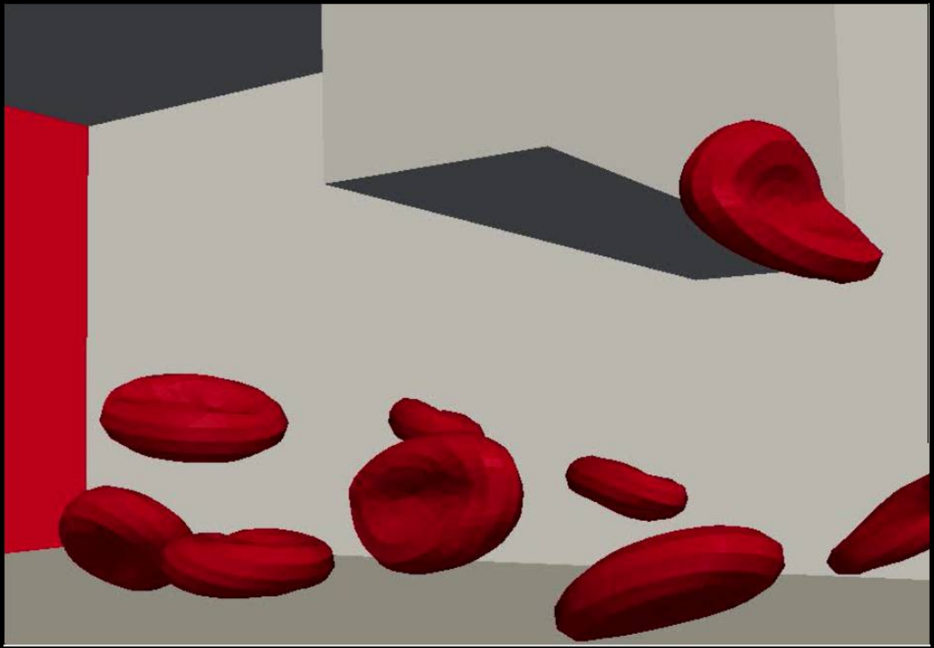


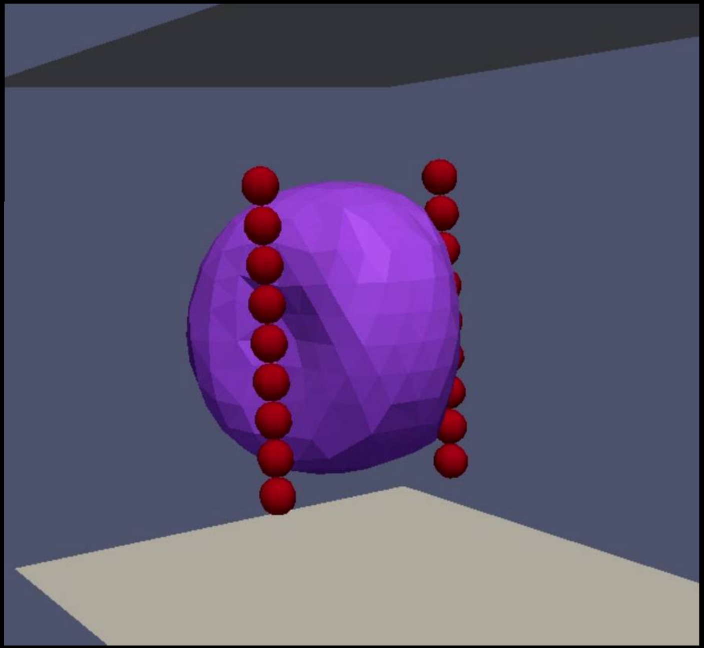
Technical challange

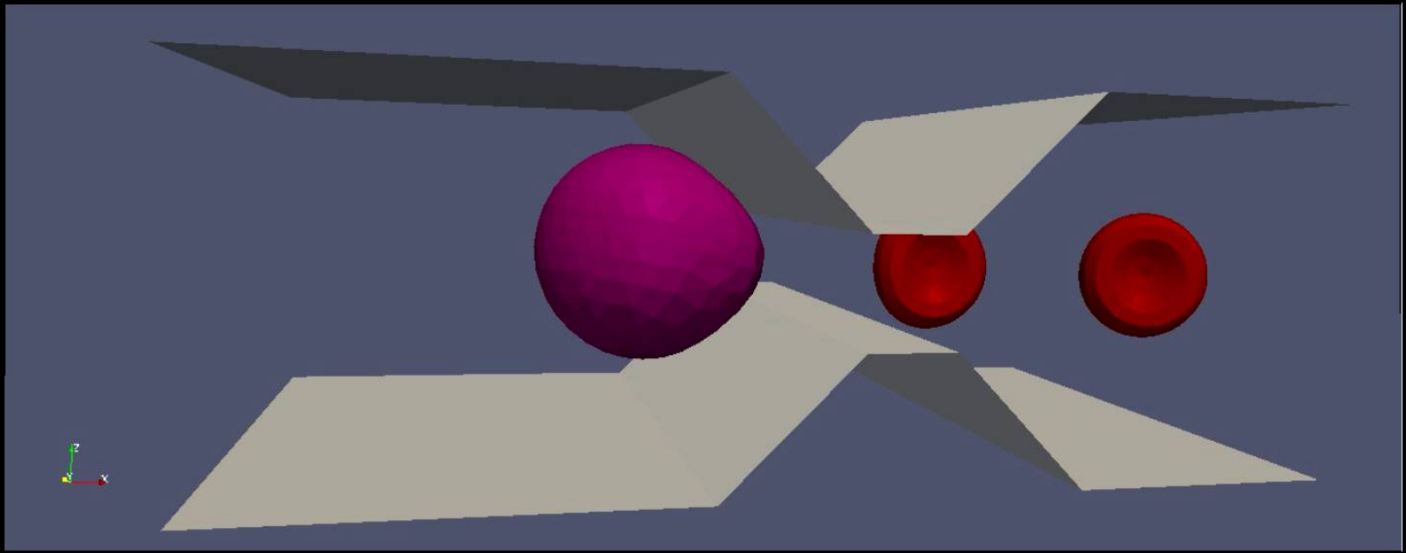
- CTCs are very rare (1-100 CTC per billions of blood cells)
- every single CTC is important
- CTCs change over time
- similar size and affinity properties to ordinary blood cells

New promising technologies









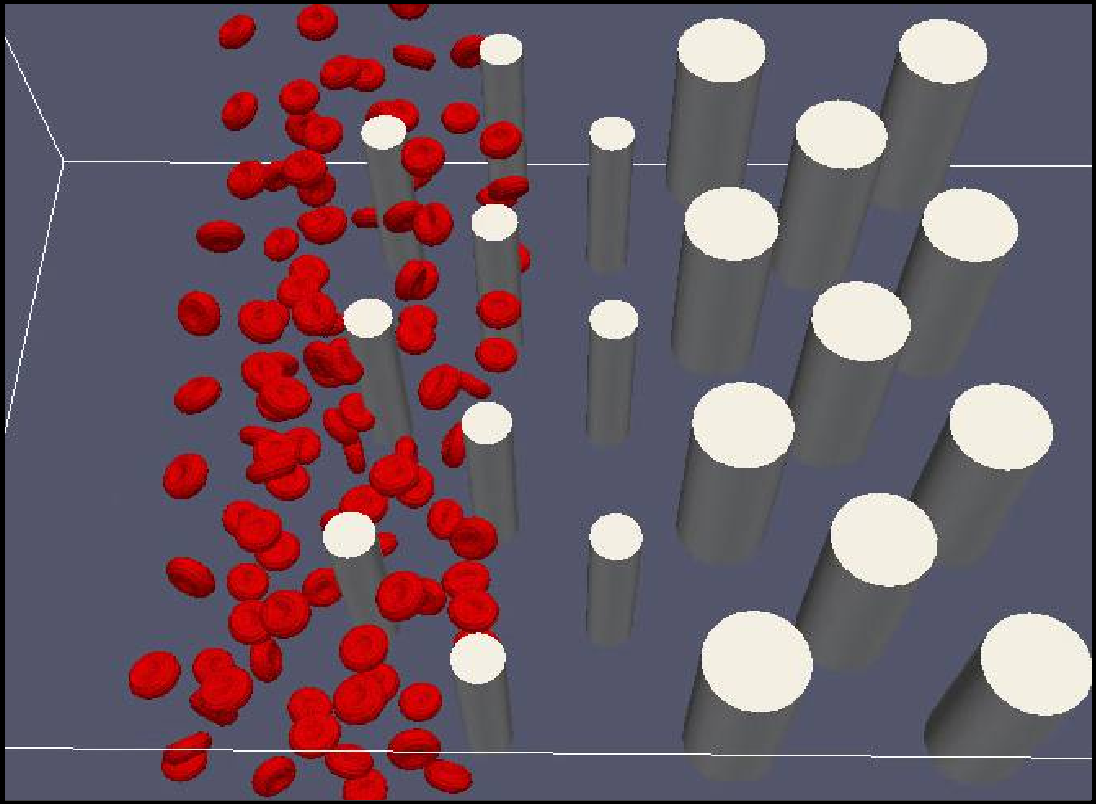
M. Gusenbauer, H. Özelt, J. Fischbacher, et al. Simulation of magnetic active polymers for versatile microfluidic devices. EPJ Web of Conferences, 40:02001, January 2013.

M. Gusenbauer, A. Kovacs, F. Reichel, et al. Self-organizing magnetic beads for biomedical applications. Journal of Magnetism and Magnetic Materials, 324(6):977–982, March 2012.

Conclusion

- Closed objects with their own particle management
- Calibration of elastic boundary and interaction with the fluid
- Applications: blood cells, bacteria, air bubbles, (magnetic) beads, dust ……...

- Speed/Performance



108 Red Blood Cells
43200 IB-points

200 x 100 x 300
6 Mio. LB cells

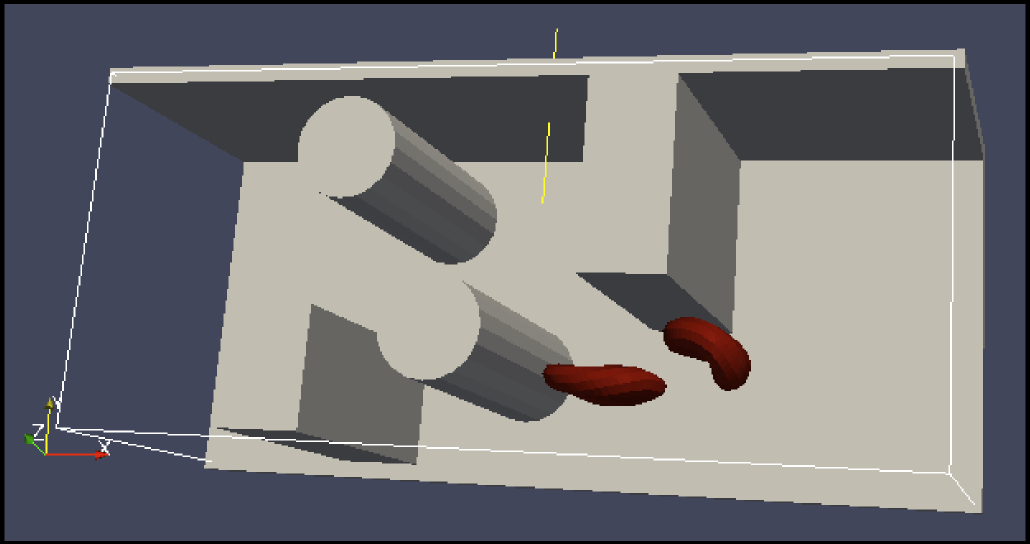
16 CPUs Intel Xeon
X5650 @ 2.67GHz

1 GPU Tesla
M2075 6 GB

500.000 timesteps
> 19 days simulation

Remember

- Today 14:00 - Hands-On:
  Immersed
  Boundary
  Conditions



- Thursday 11:00 – Lecture
  Recent and Future Developments of ESPResSo

Thank you for your attention!

http://cell-in-fluid.weebly.com/

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