Biofluid Simulation and Modeling
Lichtenberg Junior Research Group

UNIVERSITÄT BAYREUTH

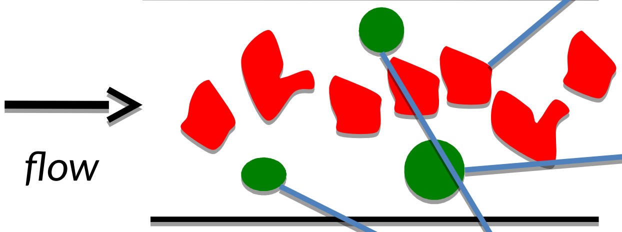
VolkswagenStiftung

KONWIHR
Kompetenznetzwerk
Wissenschaftliches Höchstleistungsrechnen

ESPResSo for blood flow

Stephan Gekle

Blood flow



Erythrocytes (red blood cells)

- highly deformable
- 15-45 volume percent (haematocrit)

Leukocytes (white blood cells)

- spherical
- stiff

Thrombocytes (blood platelets)

- elongated
- stiff

Drug delivery agents (micro-/nanoparticles)

soft → inside

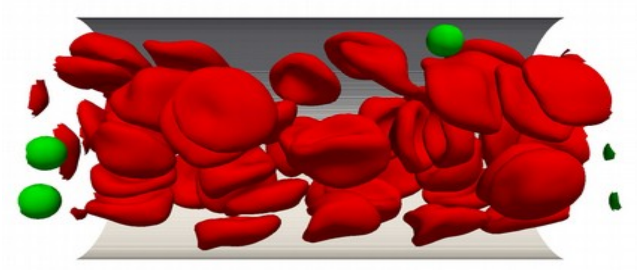
stiff → wall (margination)

I. Immersed-boundary

Motivation

Red blood cell in a microchannel

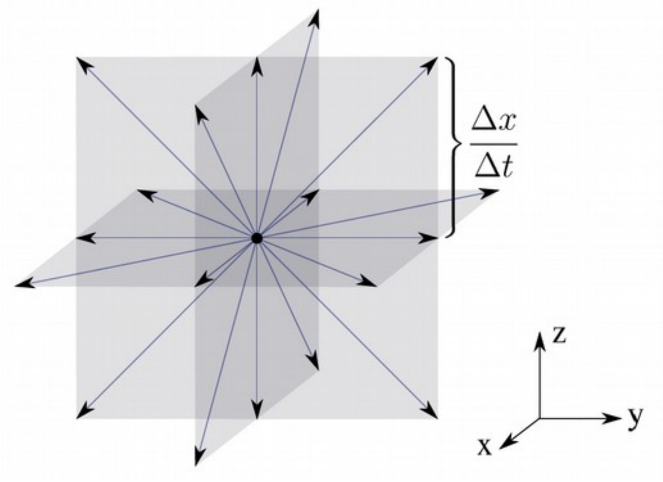
Blood flow with drug delivery agents



Immersed boundary

Lattice-Boltzmann D3Q19

- Implemented in ESPResSo

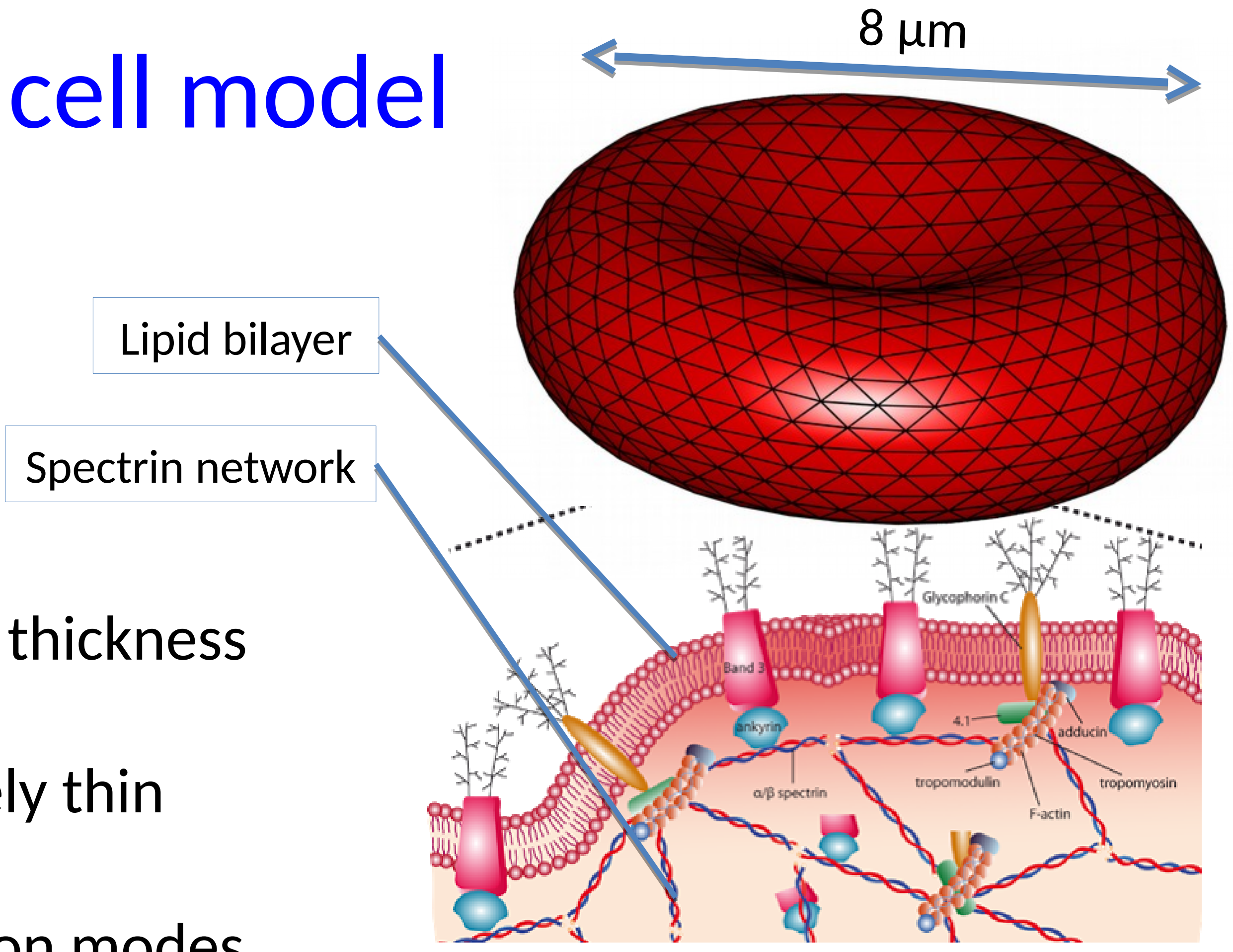


+

Immersed-Boundary for cells

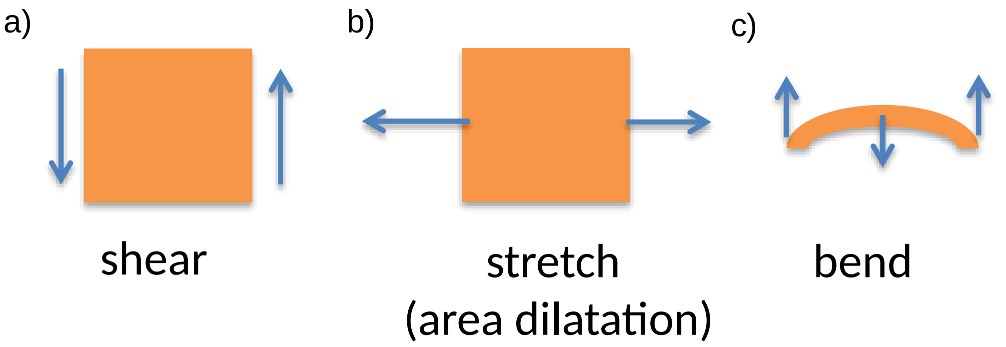
- Implemented in developer version of ESPResSo
- Python interface almost finished
- Requires
  - Computation of elastic forces
  - Two-way coupling between cell membrane and fluid

Red blood cell model



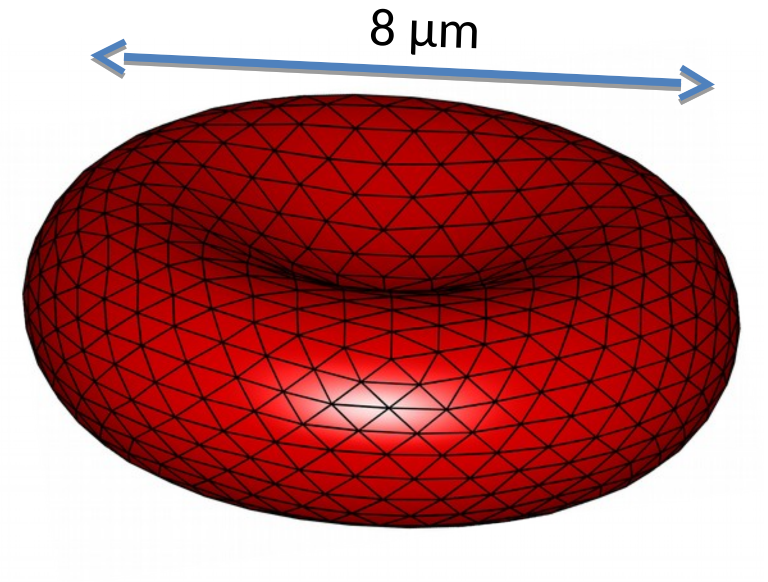
David Stokes

- Total membrane thickness ~100nm
- Model as infinitely thin elastic sheet
- Three deformation modes

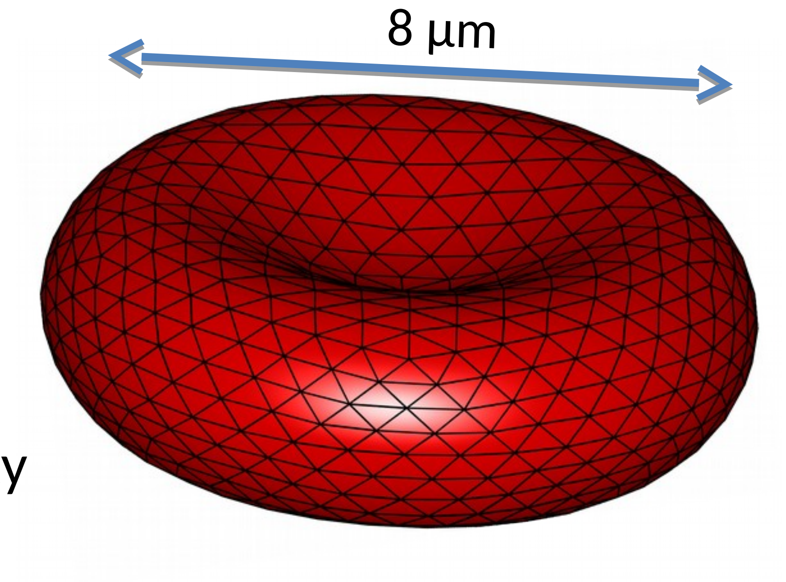


Red blood cell model

- Typical discretization
  - 1280 triangles
  - 642 nodes



Red blood cell model

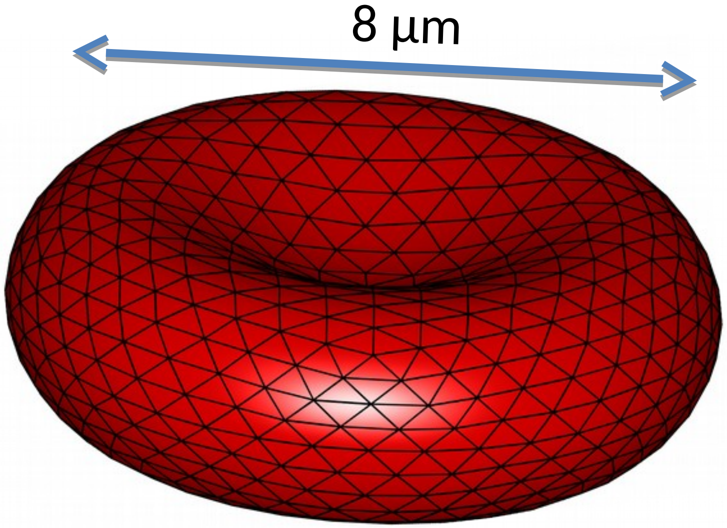


- Shear & stretch
  - Skalak model
  - phenomenological energy density

$$W = \frac{\kappa_s}{4}\left(\frac{1}{2} I_1^2 + I_1 - I_2\right) + \frac{\kappa_a}{8} I_2^2$$

  - shear modulus
  - area conservation modulus
  - parameters from experiments, e.g. optical stretching, micropipette aspiration
  - forces on nodes by taking derivatives (Hamilton formalism)

RBC model



- Bending resistance
  - Helfrich model

$$E_{\mathrm{B}} = \int_S 2\kappa_{\mathrm{B}} \left(H - H_0\right)^2 \mathrm{d}S$$

  - bending modulus κ_B
  - curvature

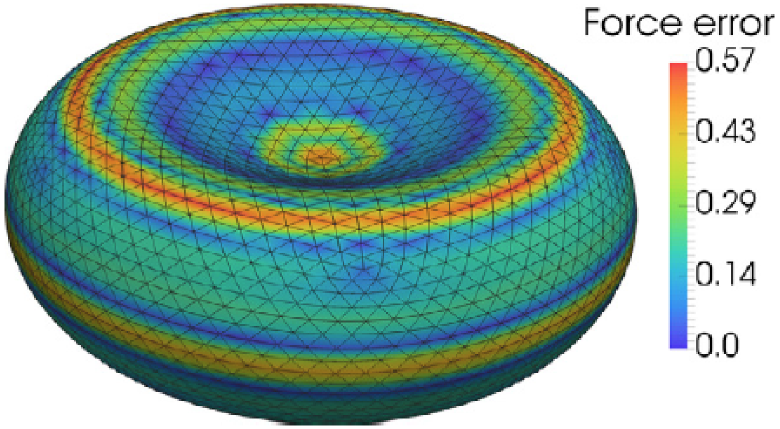
$$H(\boldsymbol{x}) = \frac{1}{2}\sum_{i=1}^{3} \left(\Delta_{\mathrm{S}} x_i\right) n_i(\boldsymbol{x})$$

  - bending force density

$$\Delta \boldsymbol{f}_{\mathrm{B}} = -2\kappa_{\mathrm{B}}\left[\Delta_{\mathrm{S}}\left(H - H_0\right) + 2\left(H - H_0\right)\left(H^2 - K + H_0 H\right)\right]\boldsymbol{n}$$

4th derivative!

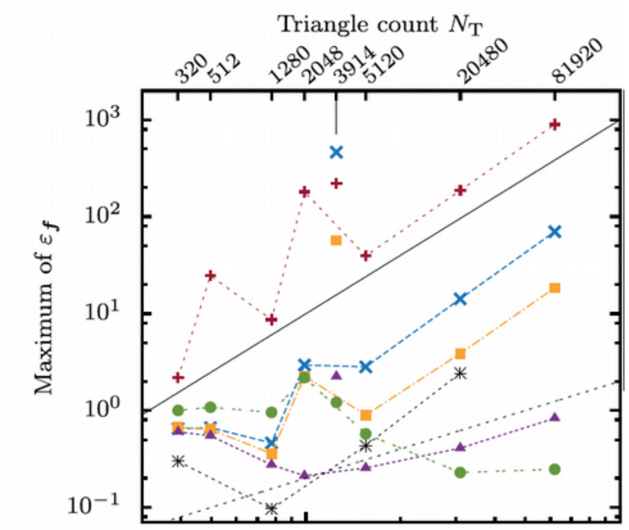
RBC model



- Bending algorithms
  - Three classes:

    weak, strong, force formulation

    Guckenberger and Gekle *J. Phys. Cond. Mat*. 2017
  - Comparison of five methods

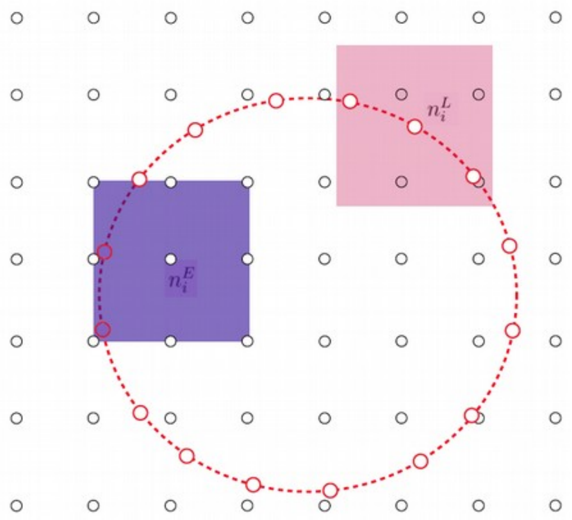


No fully converging algorithm for max. error

Guckenberger, Schraml, Chen, Leonetti and Gekle
Comput. Phys. Commun. 2016

Coupling to fluid: immersed boundary

- Membrane nodes are off-lattice
- Forces into fluid
  - force on each node acts as source term to Navier-Stokes equations
  - forces are distributed to surrounding LBM nodes
- Membrane node advection
  - interpolate velocity from surrounding LBM nodes
  - IBM nodes follow the fluid exactly
- Membrane nodes have **no** mass
  - enforces strictly no-slip
  - thermodynamically they are not independent degrees of freedom



Implementation in ESPResSo

- Membrane nodes are *virtual* particles
- They are ignored by the Verlet loop
- Skalak and Helfrich bending as new interactions
- Additional interaction for volume conservation
- Works with GPU and CPU LBM
- Current bottleneck for GPU:
  - Forces and LB fluid cannot be computed in parallel

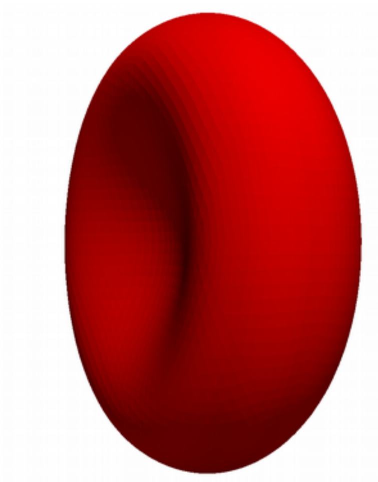
I. A single red blood cell

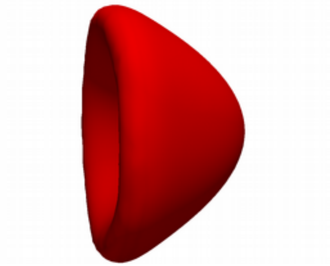
Setup

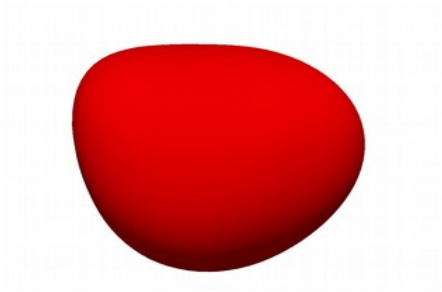
- A single red blood cell in a cylindrical microchannel
- Lattice-Boltzmann immersed boundary
- Flow driven by body force in LBM
- or by poor man‘s inflow boundary conditions

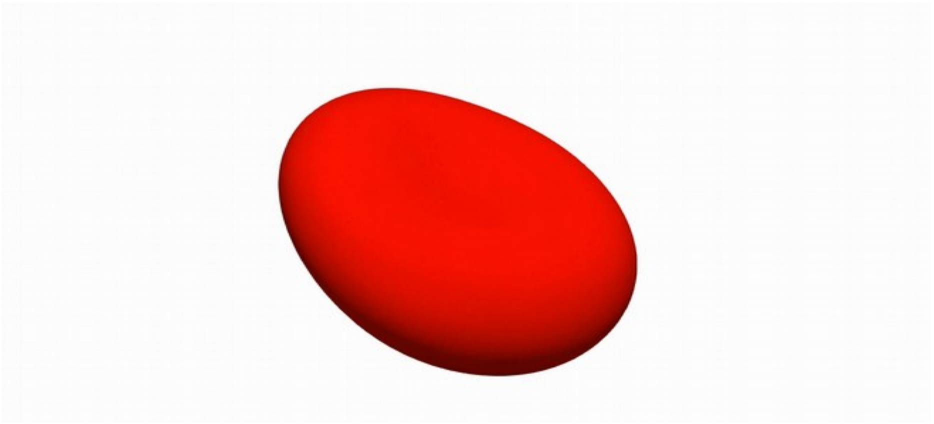
Modes of motion

- Discocyte
- Parachute
- Croissant
- Slipper
- Tumbling









Phase diagram

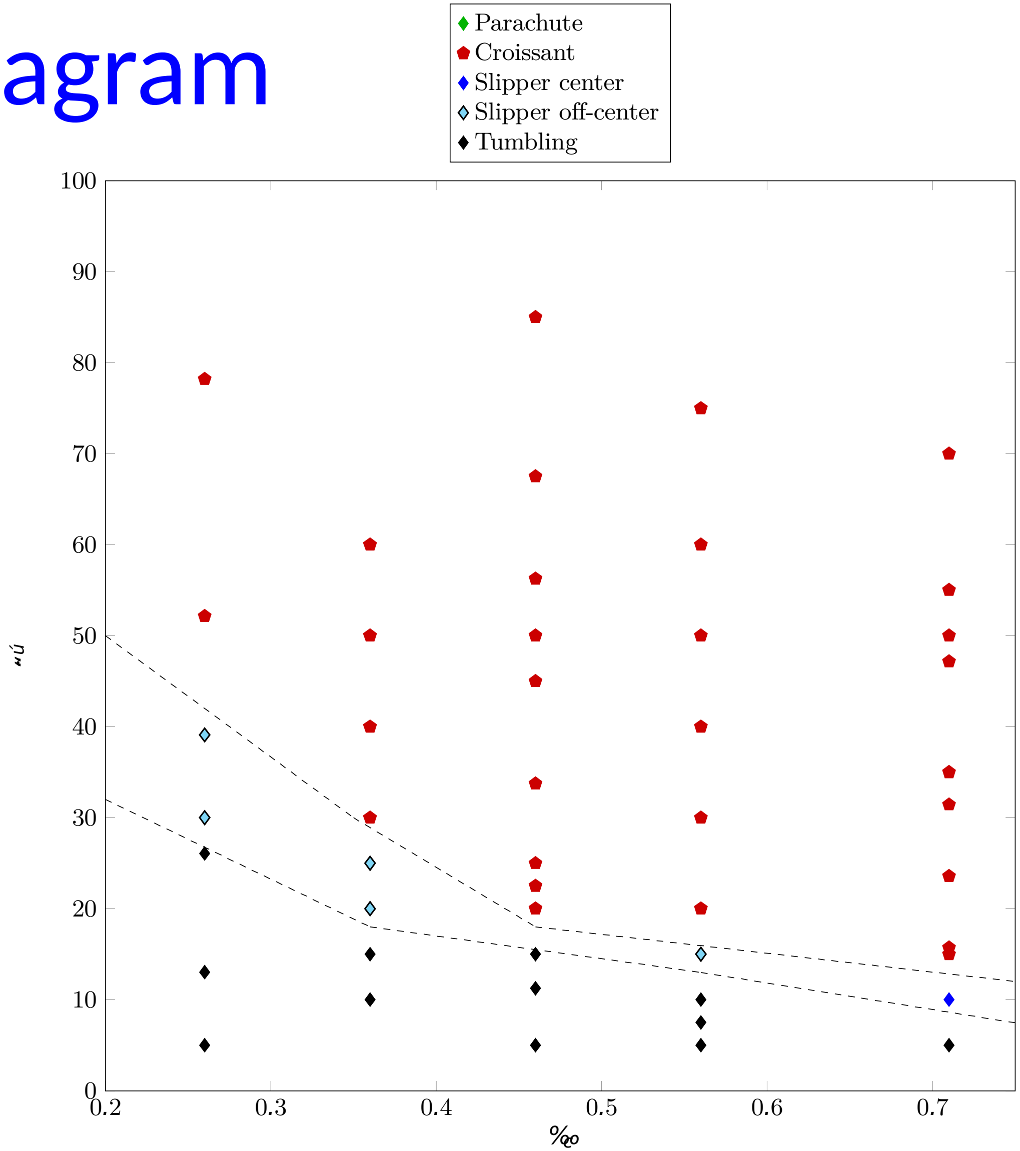
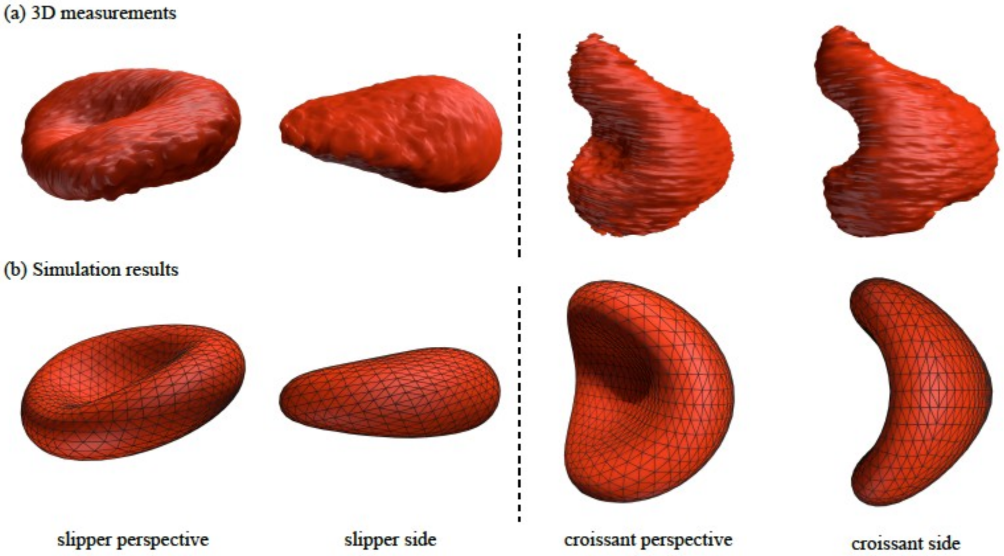


Fig. 2: Without temperature. Cells started rotated and in the center.

Model validation



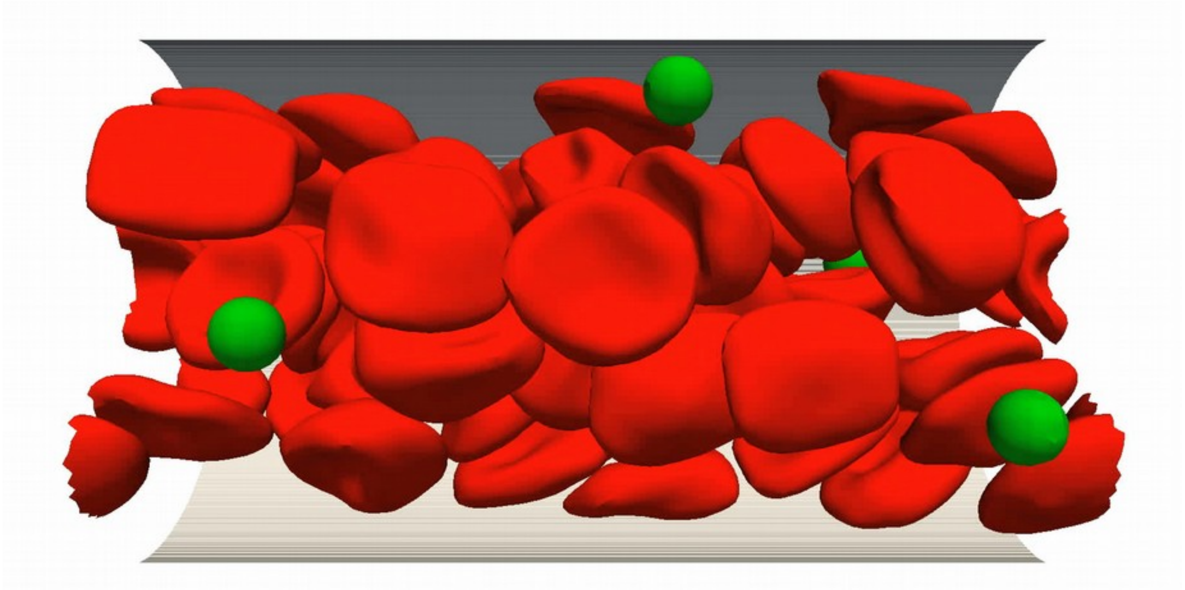
Quint, Christ, Guckenberger, Himbert, Kästner, Gekle, Wagner *Appl. Phys. Lett.* 2017
Guckenberger, Kihm, John, Wagner, Gekle *in preparation*

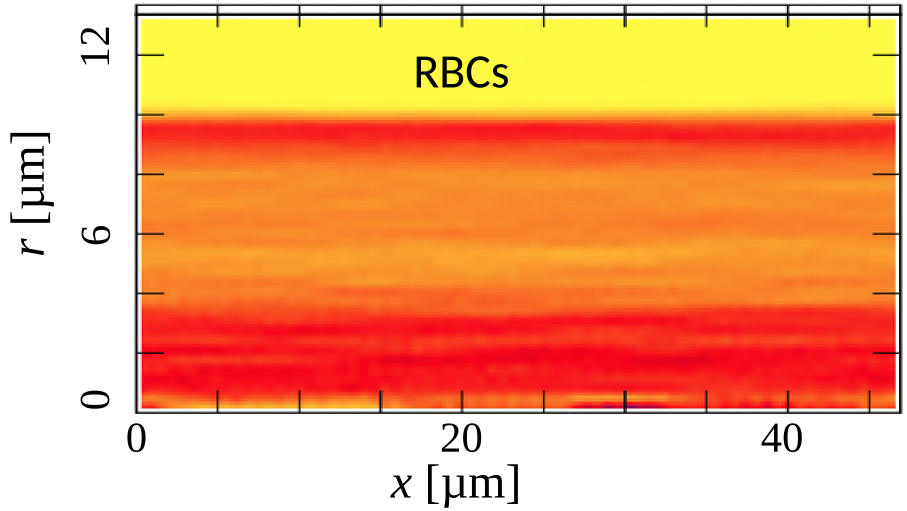
III. Margination at constrictions

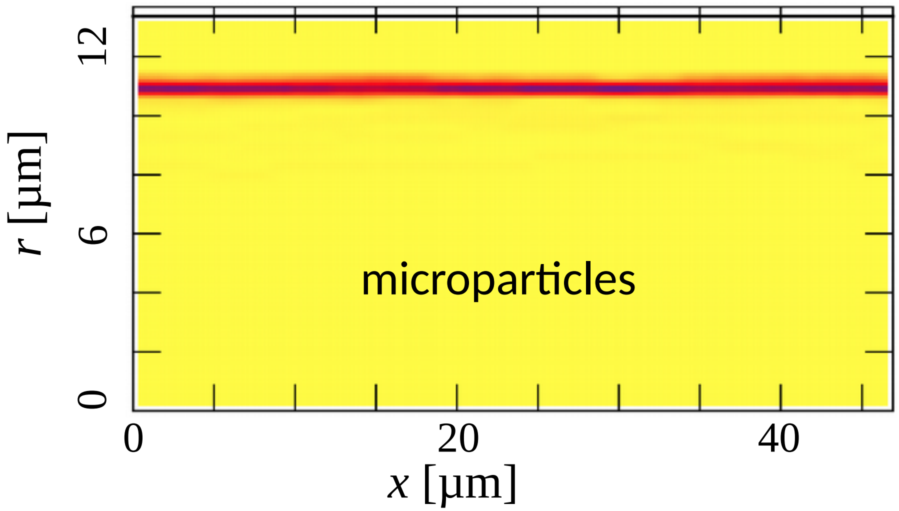
Straight channel

R_c = 13.4 µm
R_p = 1.6 µm
52 RBCs ✉ Ht = 19%
4 particles
V_{max} = 2.5mm/s

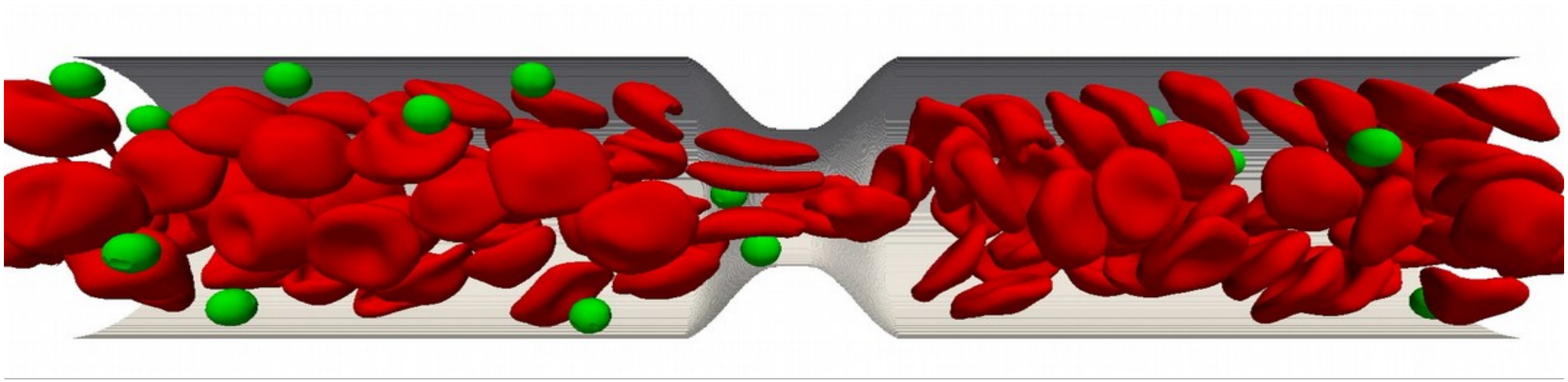
Straight channel







Constriction



R_c = 13.4 µm

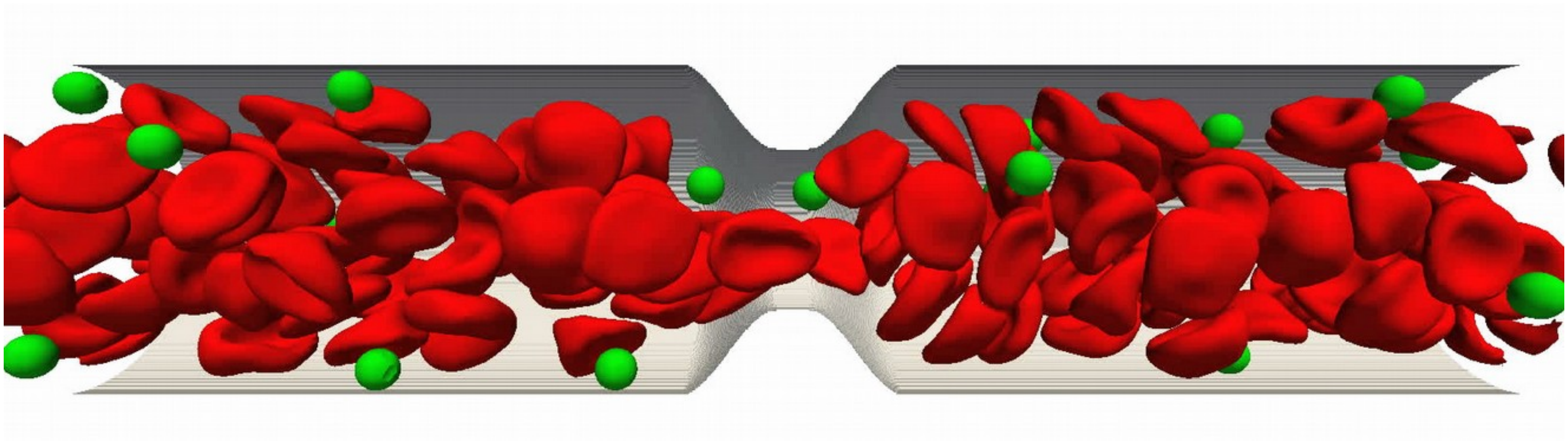
R_{constr}/R_c = 1/2

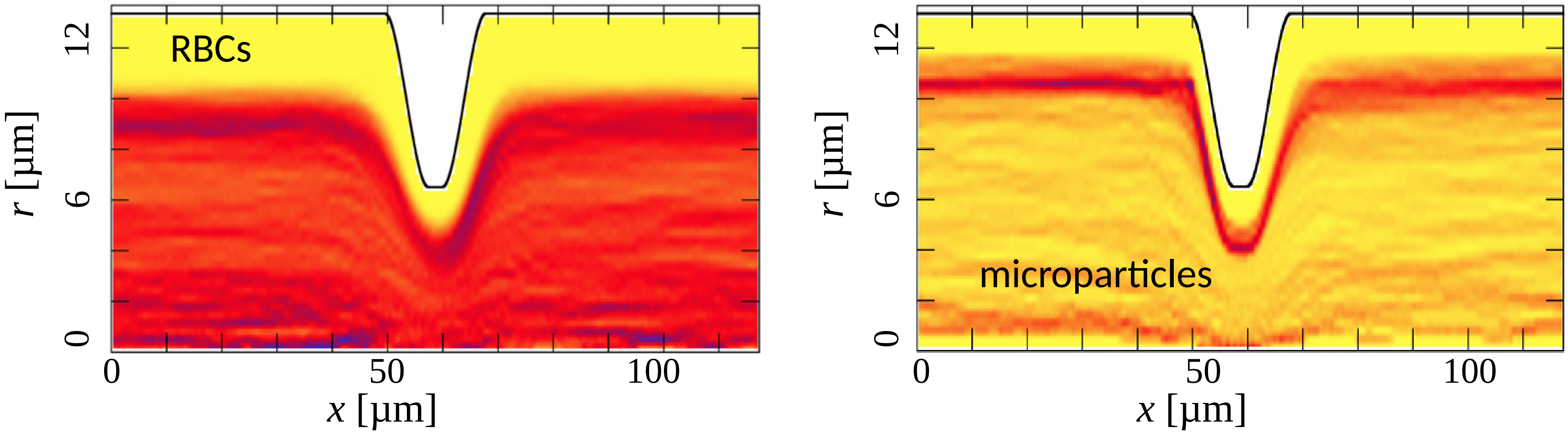
108 RBCs ✉ Ht = 16%

18 particles

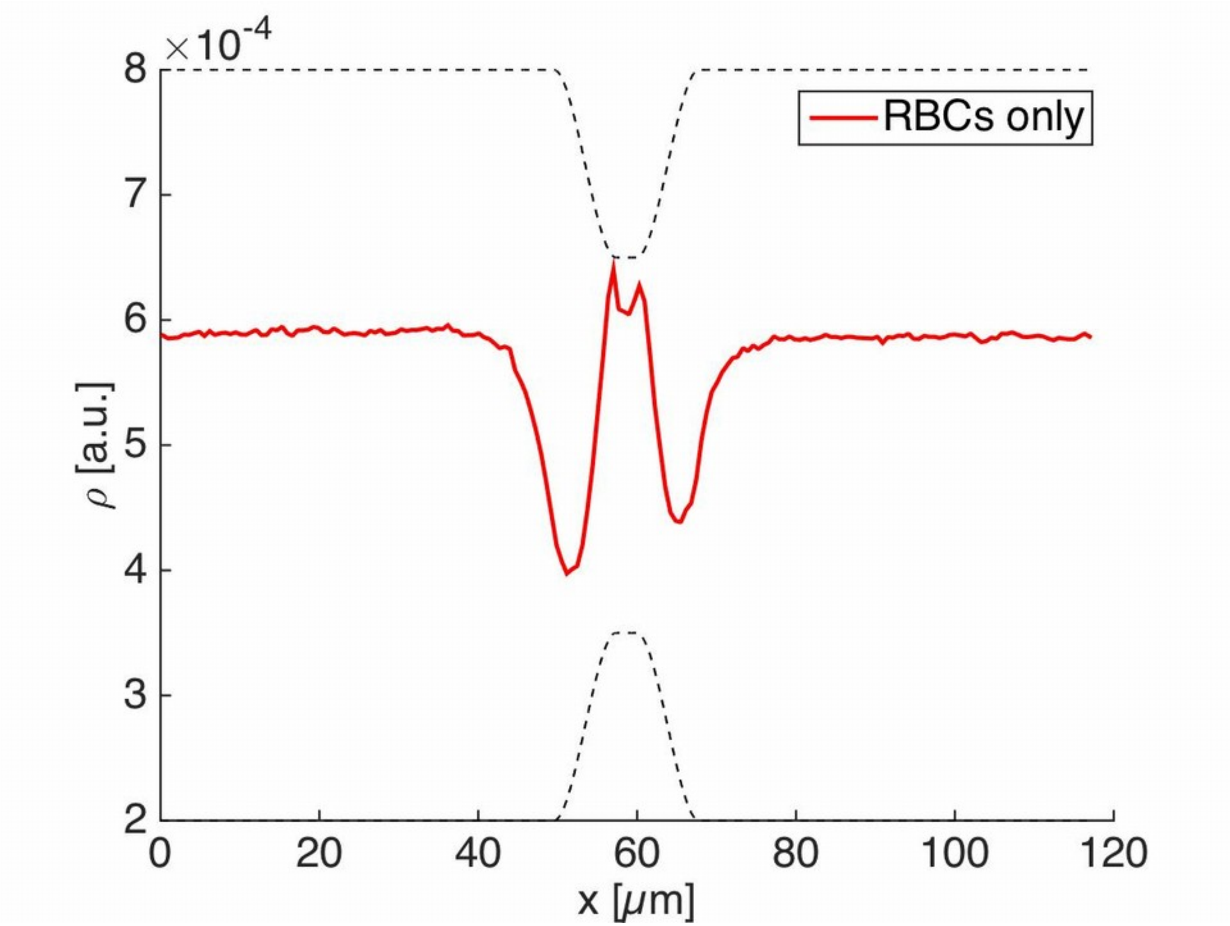
V_{max} = 1mm/s

Constriction

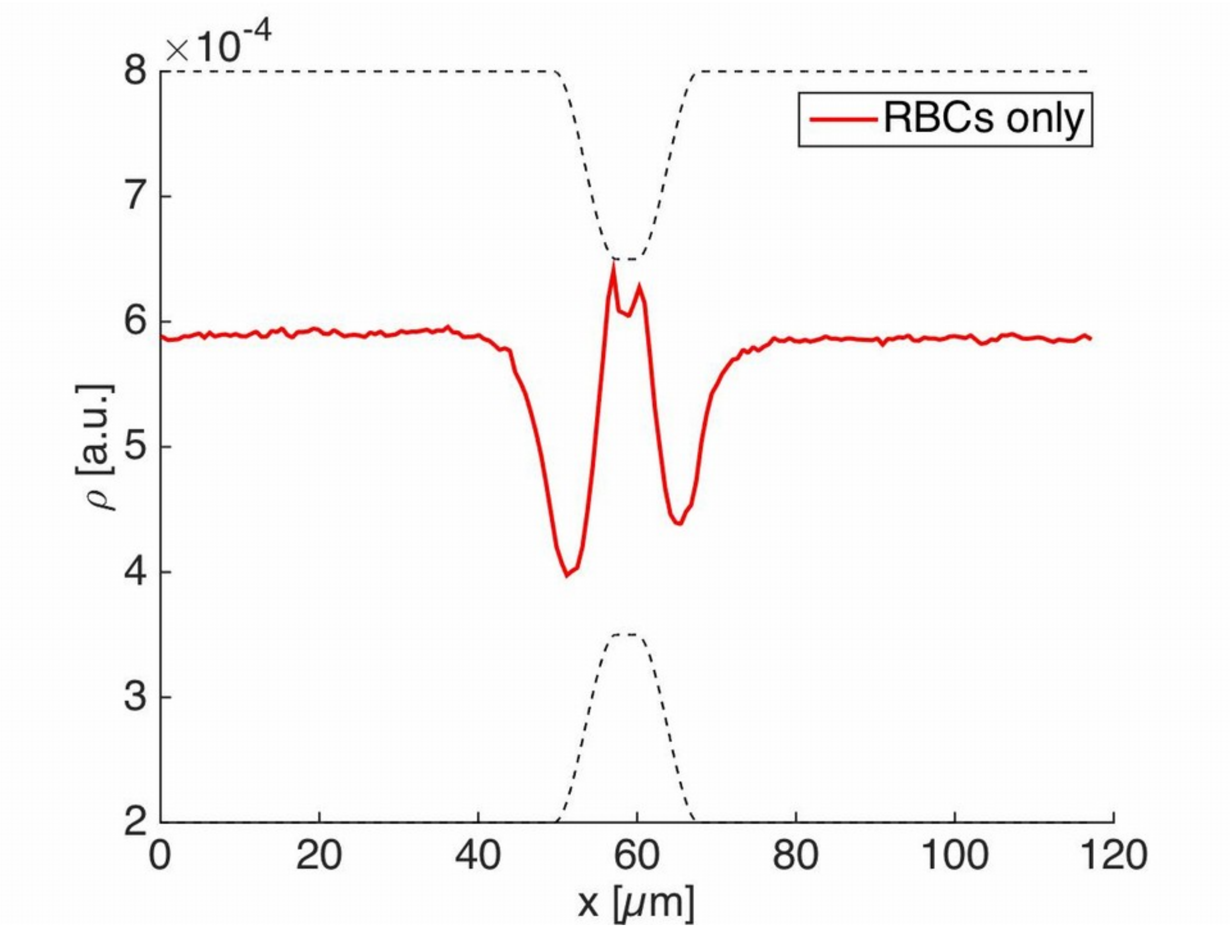




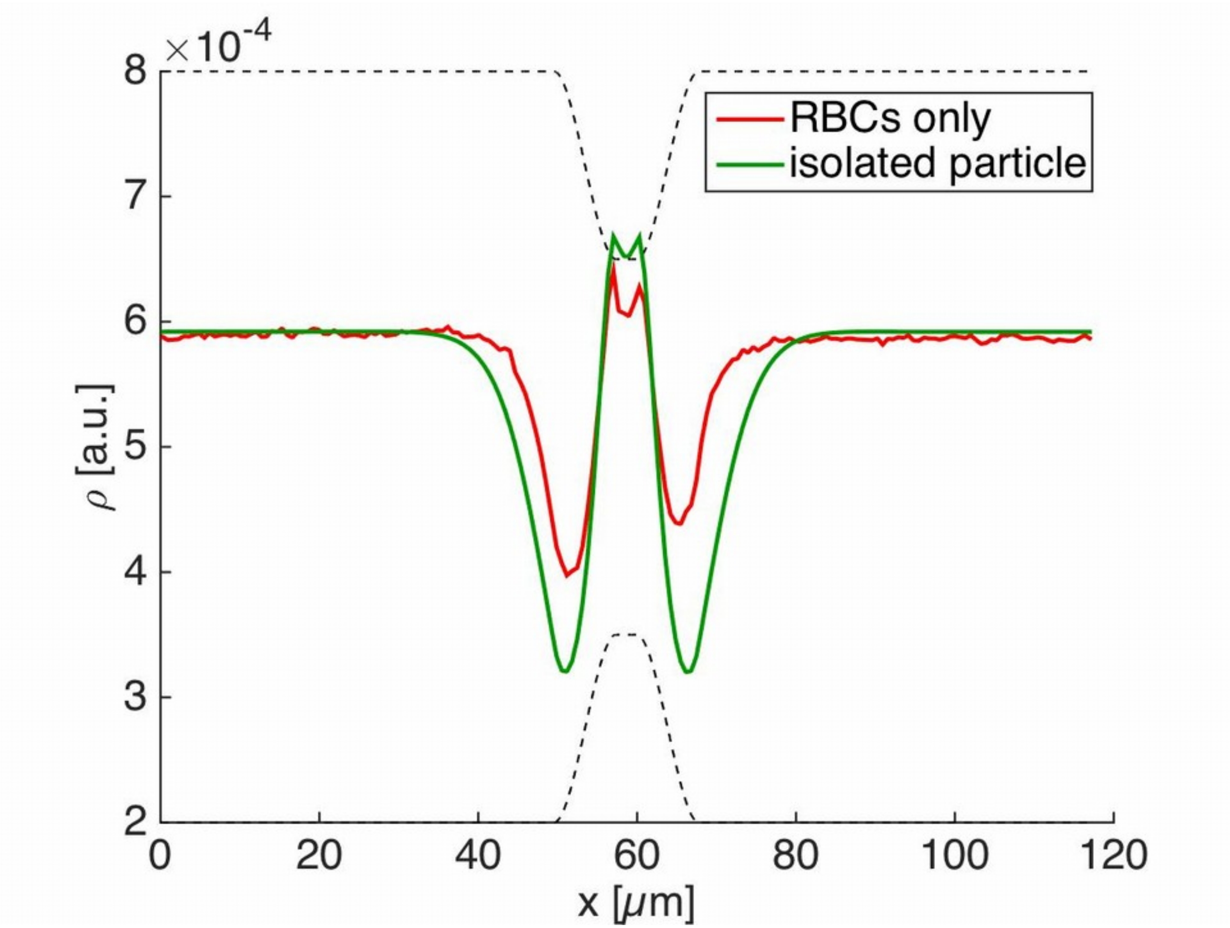
Radially averaged profile: RBCs



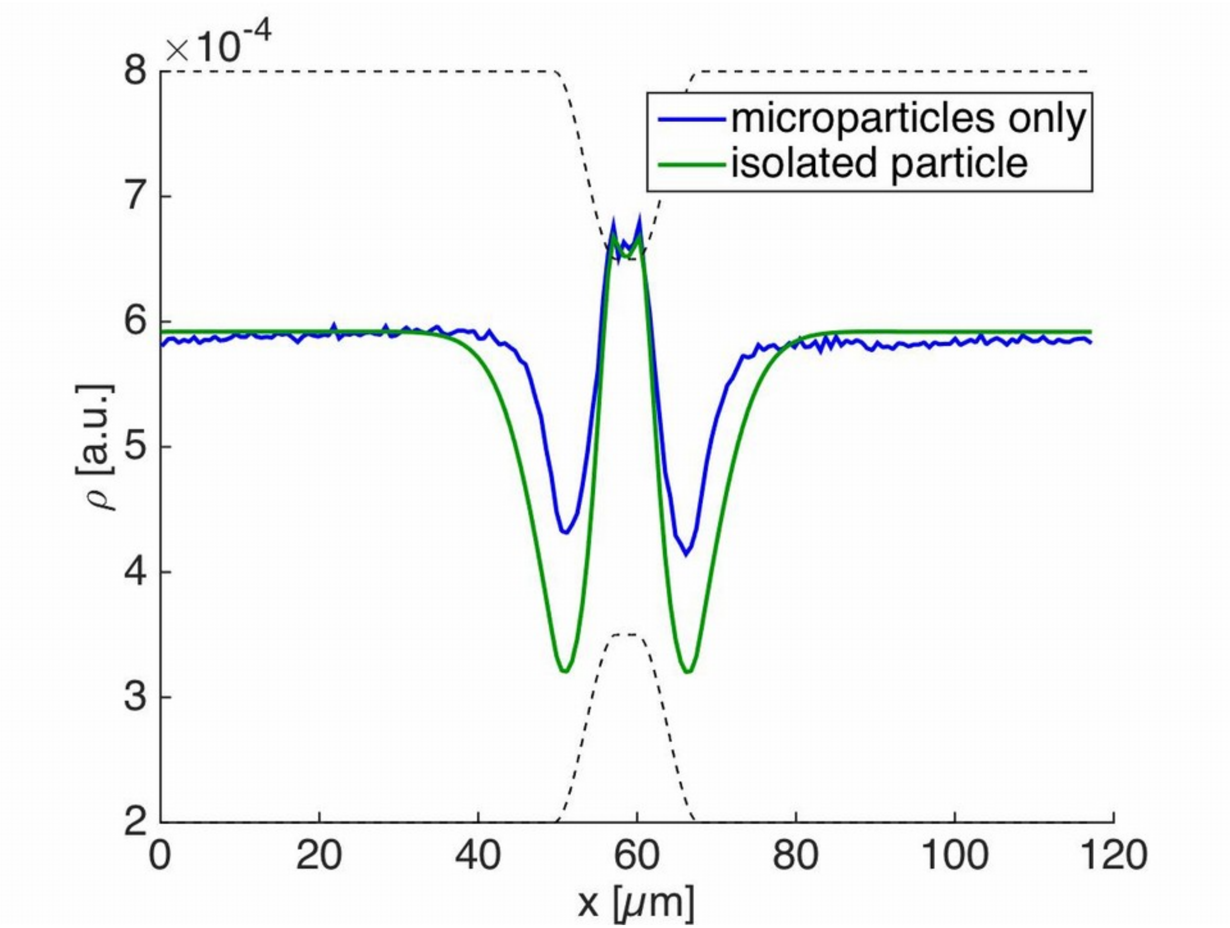
Radially averaged profile: RBCs



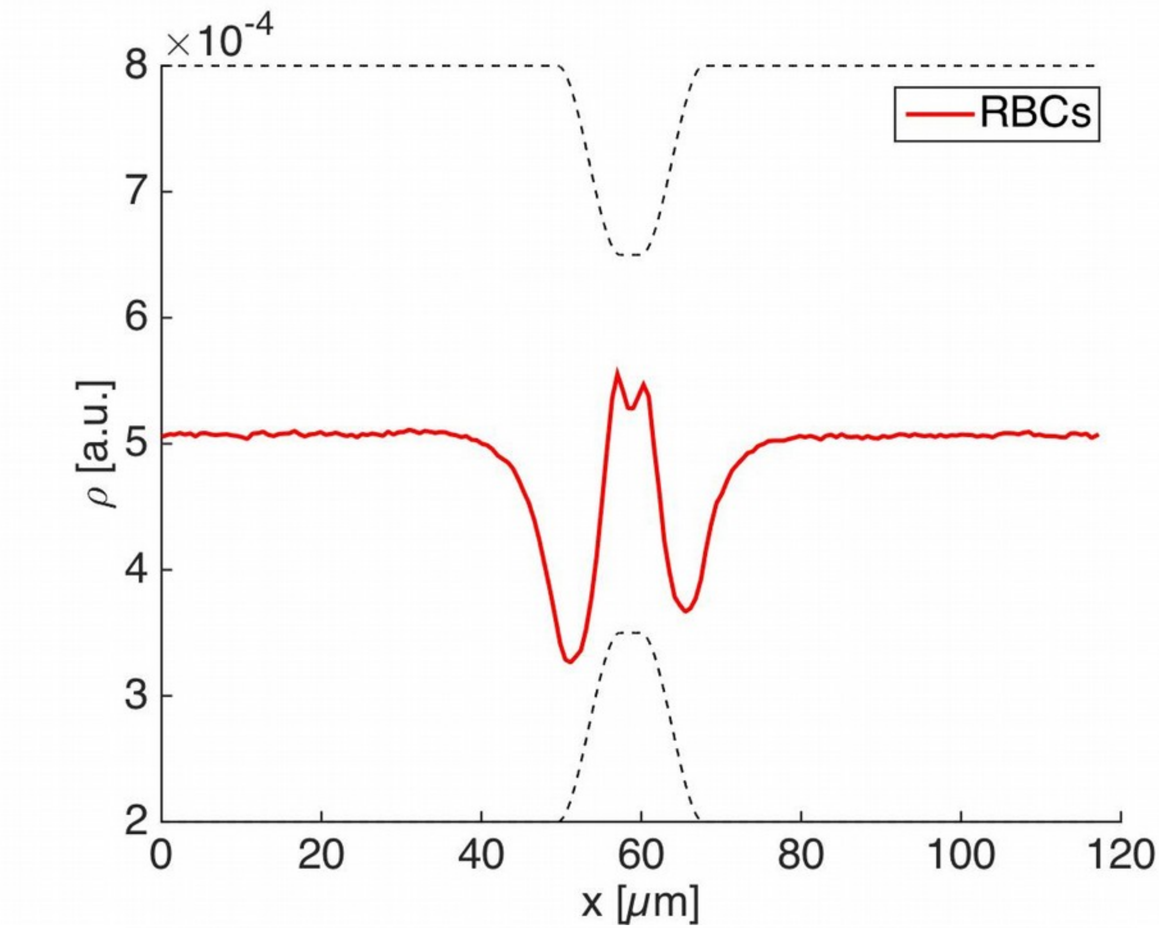
Radially averaged profile: RBCs

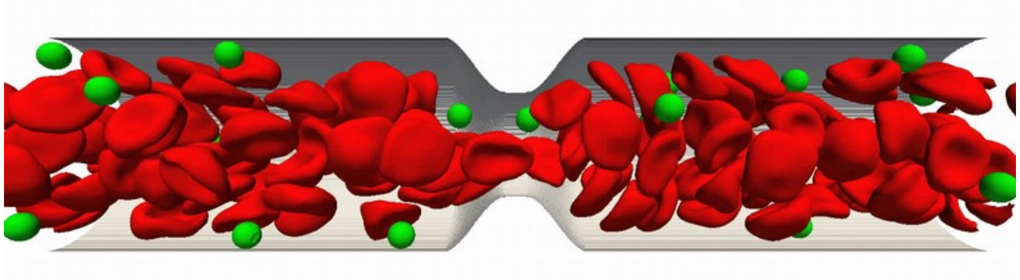


Radially averaged profile: microparticles



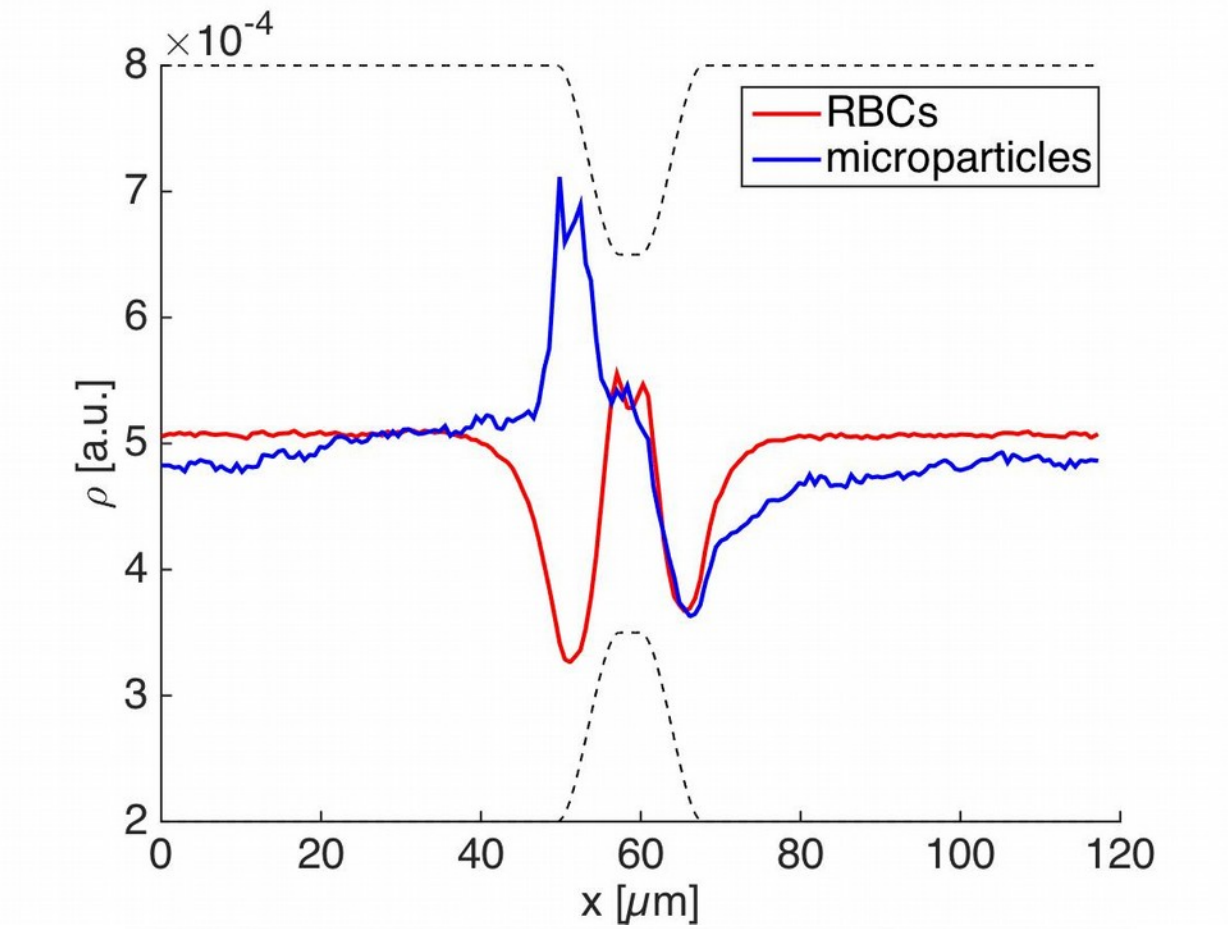
Radially averaged profile: suspension





Bächer, Schrack and Gekle
Phys. Rev. Fluids (2017)

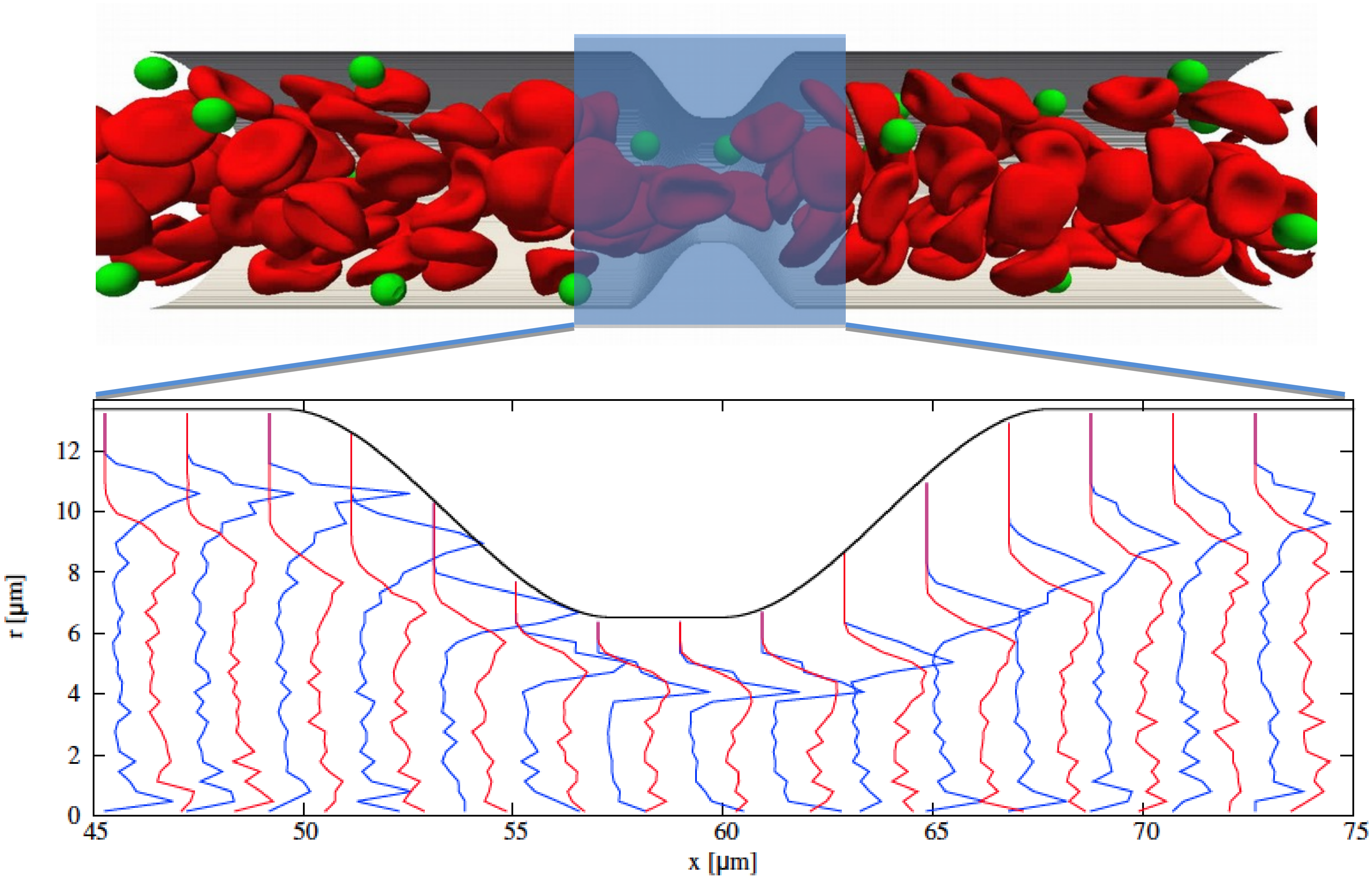
Radially averaged profile: suspension



Clustering in front of constriction for marginated particles

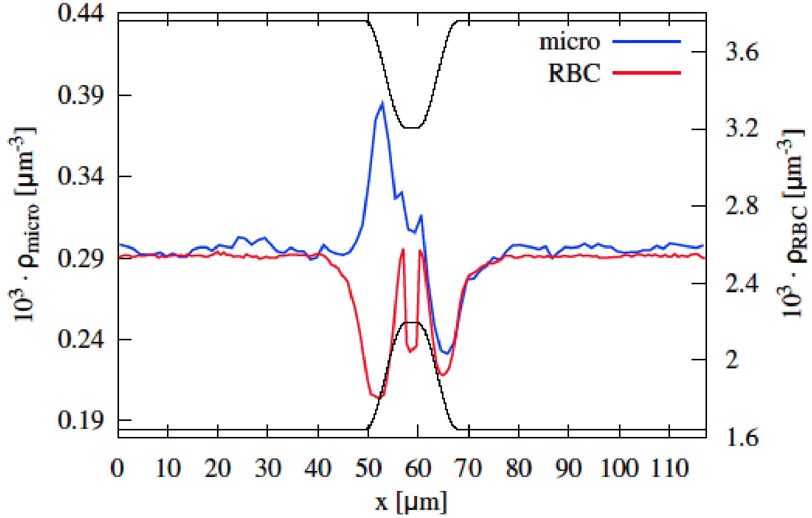
Bächer, Schrack and Gekle
Phys. Rev. Fluids (2017)

Clustering mechanism

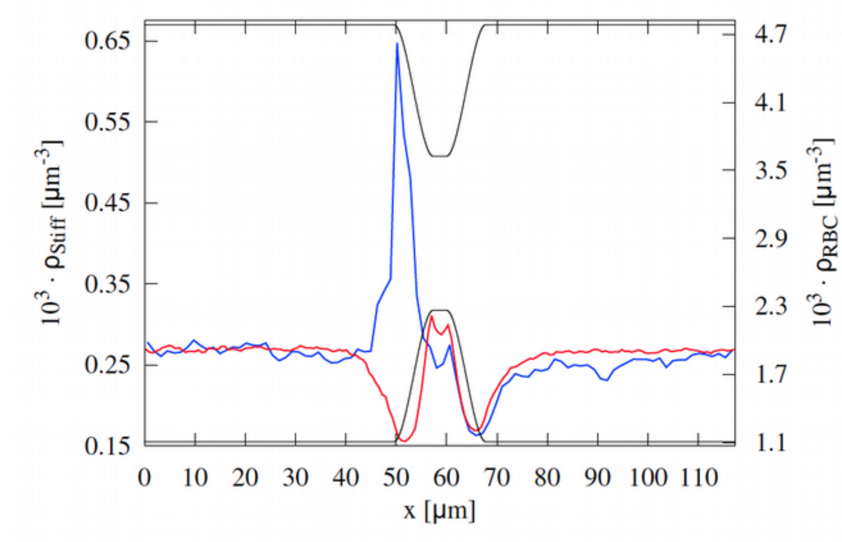


Microparticles squeeze into RBC layer

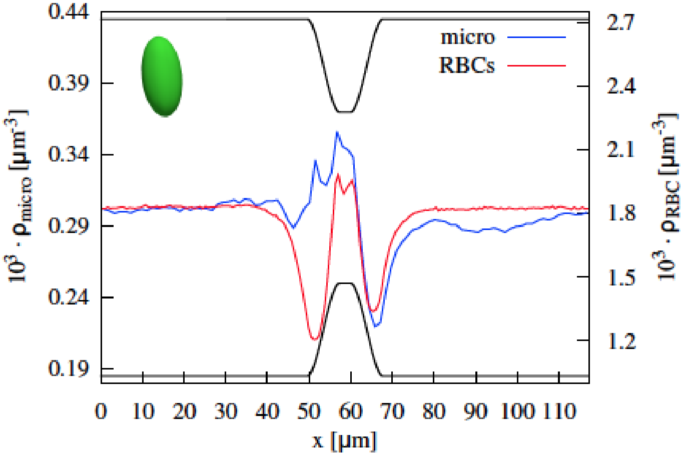
Clustering is robust



Ht=23.5%



narrow constriction



ellipsoids

→ enhanced thrombus formation?

Bächer, Schrack and Gekle
Phys. Rev. Fluids (2017)

Acknowledgements

Christian Bächer
(Constriction, bifurcation)
Achim Guckenberger
(Phase diagram)
Lukas Schrack
(Complex boundaries)
Paul Bauknecht
(Temperature)

Funding

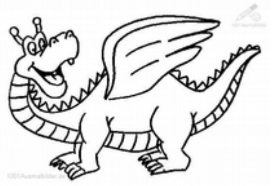
VolkswagenStiftung

KONWIHR
Kompetenznetzwerk
Wissenschaftliches Höchstleistungsrechnen

Computing power

JÜLICH
FORSCHUNGSZENTRUM

lrz



SMAUG