Presented at the COMSOL Conference 2008 Hannover

Bielefeld University
Department of Physics

A. Weddemann, A. Auge,
F. Wittbracht, S. Herth, A. Hütten

Interactions of magnetic particles in a rotational magnetic field

D2 PHYSICS

Bielefeld University

Outline

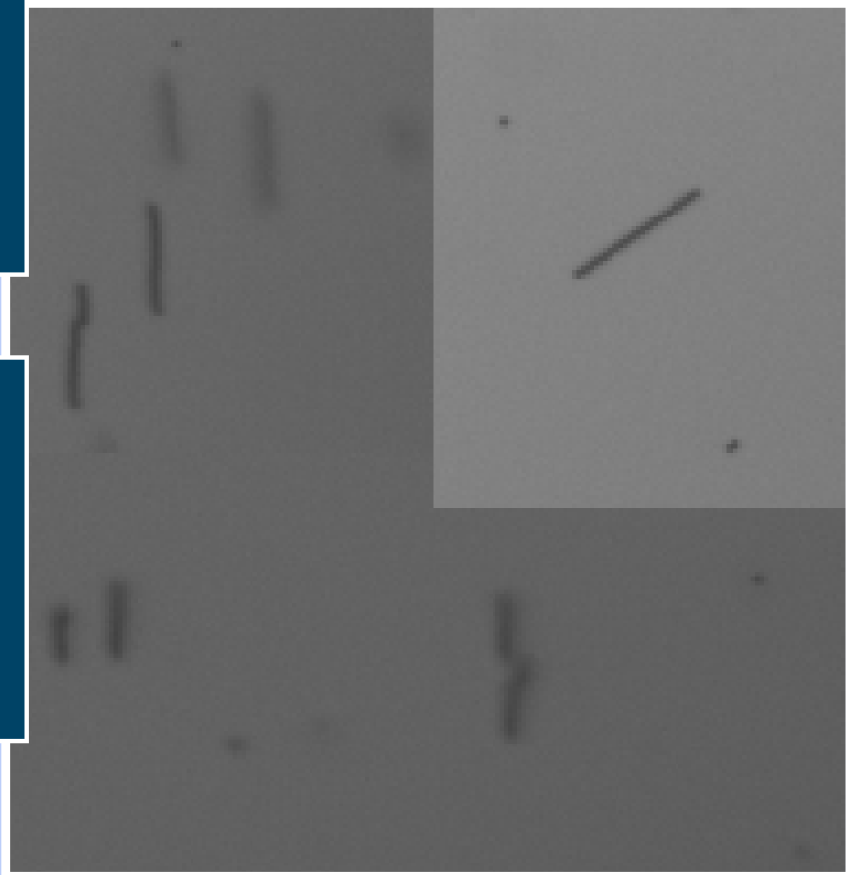
A. Weddemann, A. Auge,
F. Wittbracht, S. Herth, A. Hütten
06.11.2008

1. Motivation
2. Governing equation
   1. Particle motion
   2. Technical realization – ALE-approach
      1. Second domain triangulation
3. Interactions of beads in fluids
   1. Simple system
   2. Comparison between magnetic and hydrodynamic forces
4. Conclusions and Outlook

Motivation

Magnetic micro- or nanoparticles can interact very strongly:

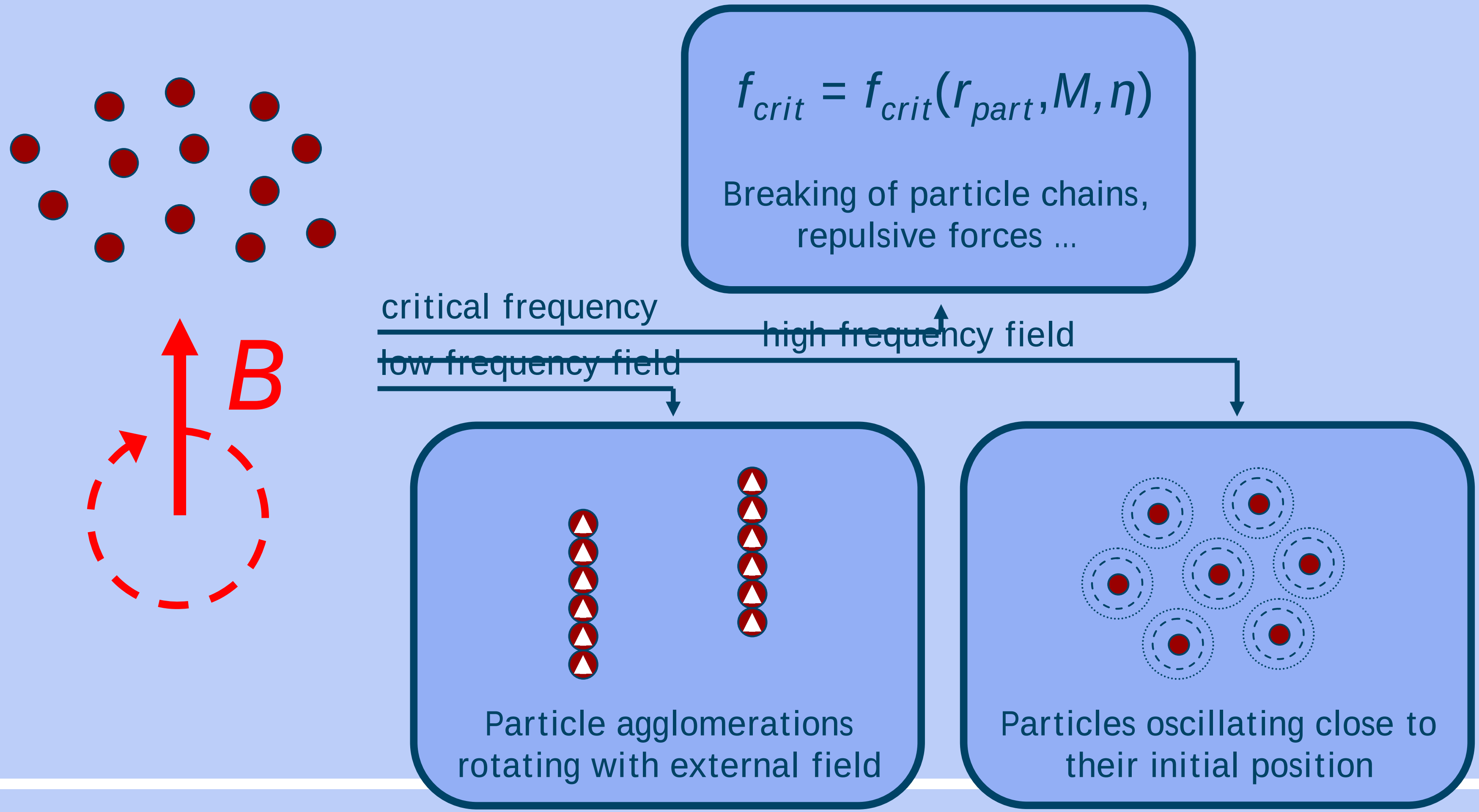
Under the influence of an external homogenous magnetic field particle create chains



Question: Can magnetic interactions be neglected when modeling particles in microfluidic systems?

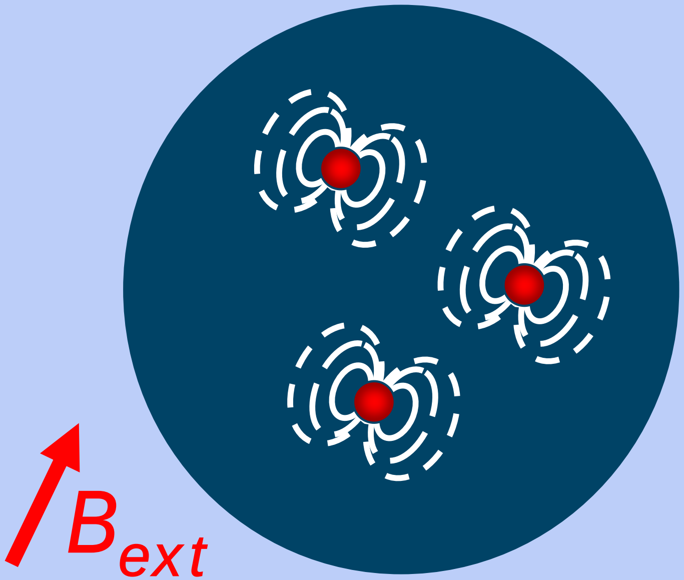
Motivation

Expect ferro- or superparamagnetic particles in a solution, being manipulated by an external magnetic field.



Particle motion

Governing equations:



Particle motion:

$$M\frac{d}{dt}U(t) = F_{mag} + F_{visc} + F_{pen}$$

$$F_{mag} = \int_{particle} f\,dx = -\int_{particle} \mathrm{grad}\langle M, B\rangle\,dx$$

F_{visc} □ viscous force term

F_{pen} □ force term preventing particles from overlapping

$U(t) = (v_x^{part_1}, v_y^{part_1}, v_x^{part_2}, \ldots)^T$ □ velocity vector

$M □ B_{ext}$ $\quad |M| = M_s$

$$\int_{\Omega_t} \langle \mathrm{grad}\,\psi_{A_z}, \mathrm{grad}\,A_z\rangle dx - \mu_0 \int_{\Omega_t} \left(M_y \frac{\partial \psi_{A_z}}{\partial x} - M_x \frac{\partial \psi_{A_z}}{\partial y} \right) dx = 0$$

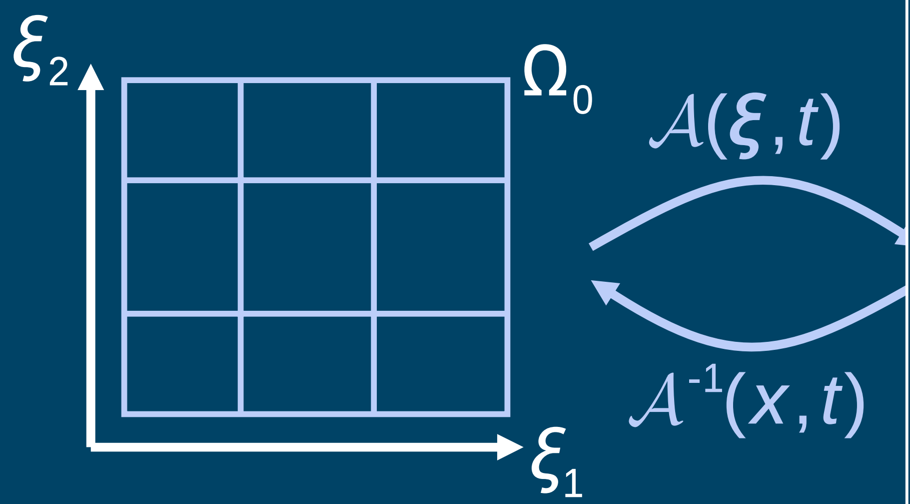
$$M\frac{d}{dt}U(t) = F_{mag} + F_{visc} + F_{pen}$$

Particle movement requires mesh displacement

→ ALE-formalism

ALE-formulation

The basic idea of ALE-methods is to use different coordinate systems, a reference and a spatial system.



Calculation transformed to reference system

Example:

$$\frac{\partial u}{\partial t}(x,t)+\mathcal{L}[u](x,t)=0$$

weak formulation

$$\int_{\Omega_t}\psi(x,t)\cdot\frac{\partial u}{\partial t}(x,t)dx+\int_{\Omega_t}\psi(x,t)\cdot\mathcal{L}[u](x,t)dx=0$$

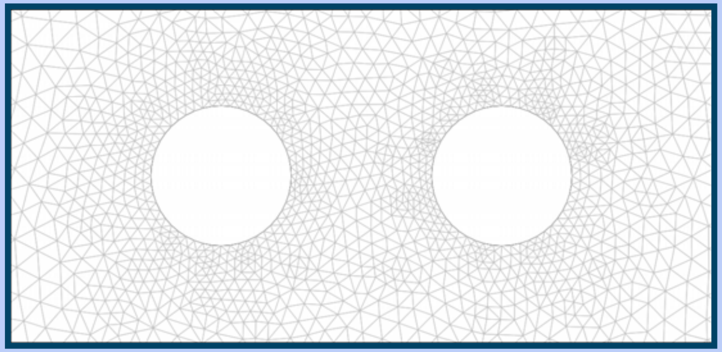
domain transformation

$$\int_{\Omega_0}\psi(\mathcal{A}(\xi,t))\cdot\frac{\partial u}{\partial t}(\mathcal{A}(\xi,t),t)\cdot\det J_{\mathcal{A}_t}(\xi,t)\,d\xi$$
$$+\int_{\Omega_0}\psi(\mathcal{A}(\xi,t))\cdot\mathcal{L}[u](\mathcal{A}(\xi,t),t)\cdot\det J_{\mathcal{A}_t}(\xi,t)\,d\xi=0$$

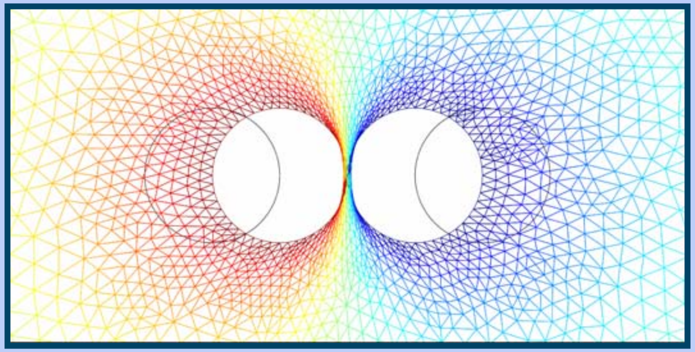
ALE-formulation

Limitations of ALE-methods:

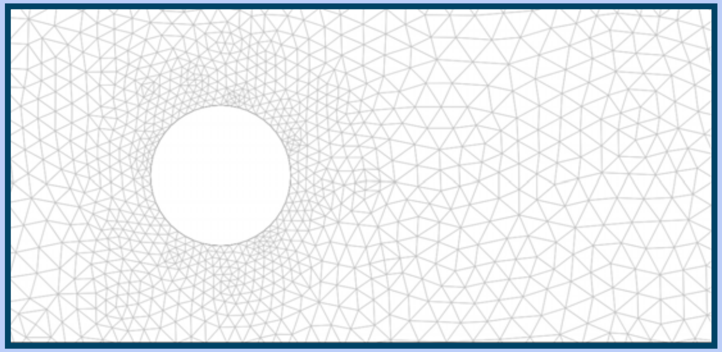
- Topological changes:



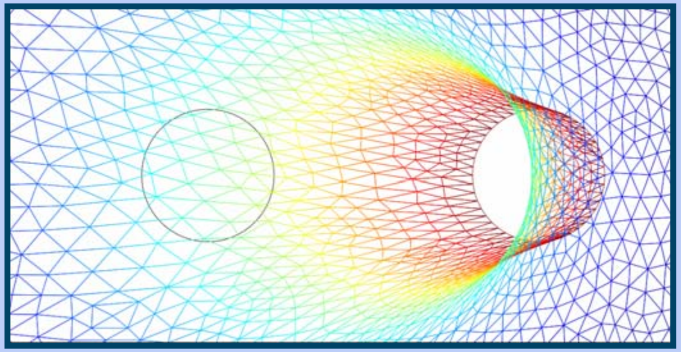
particles moving towards each other →



- Very strong displacements:

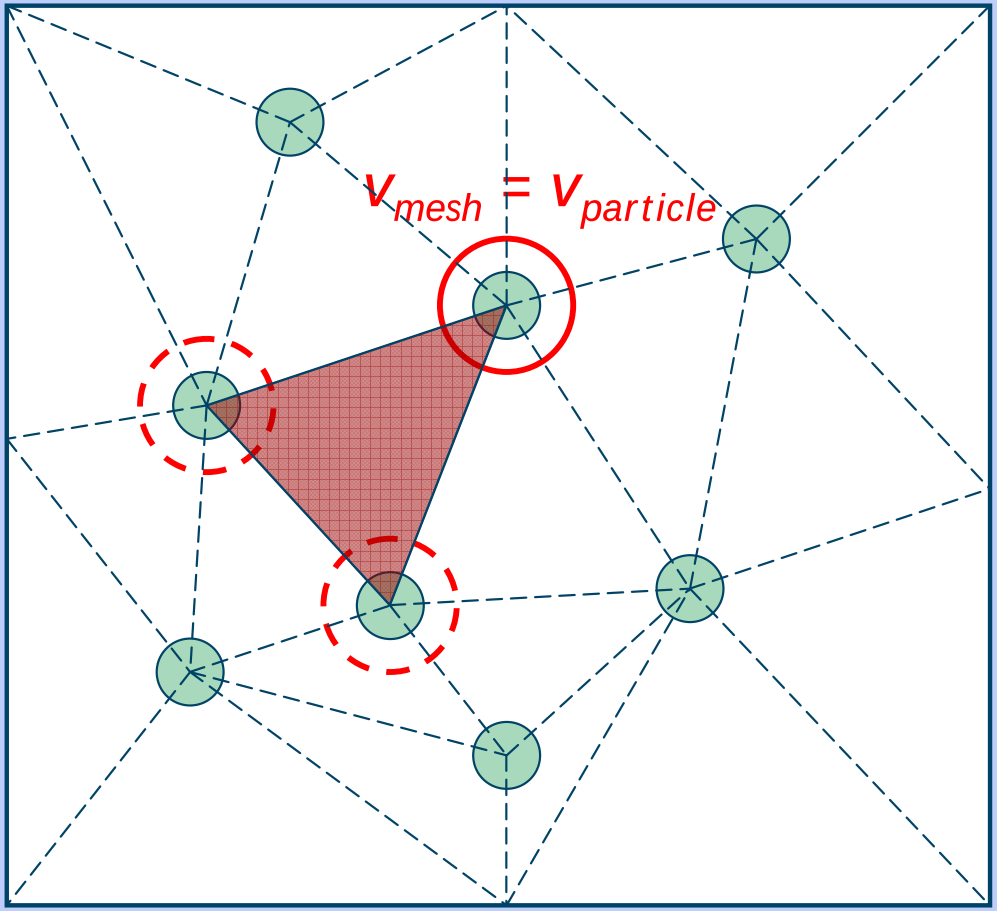


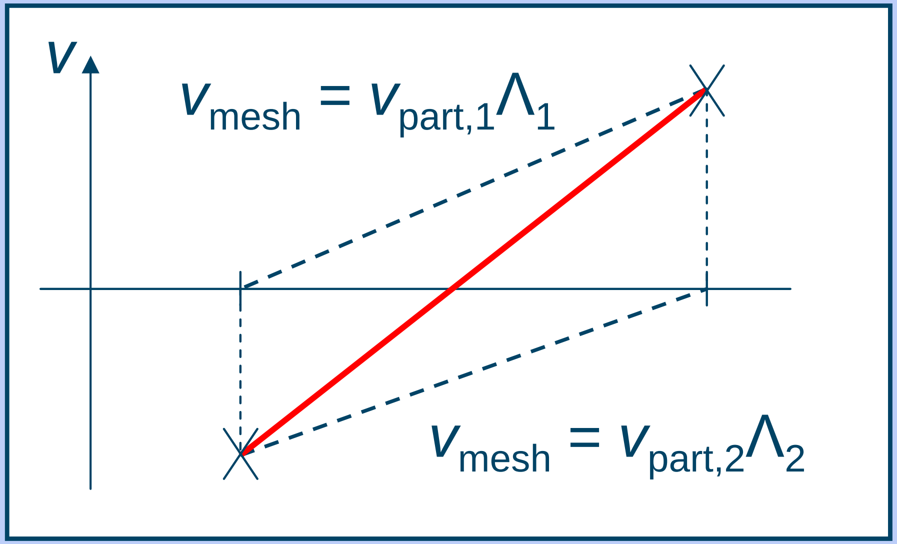
particle moving too far in one direction →



ALE-formulation

Calculation of ALE-mesh-displacement:



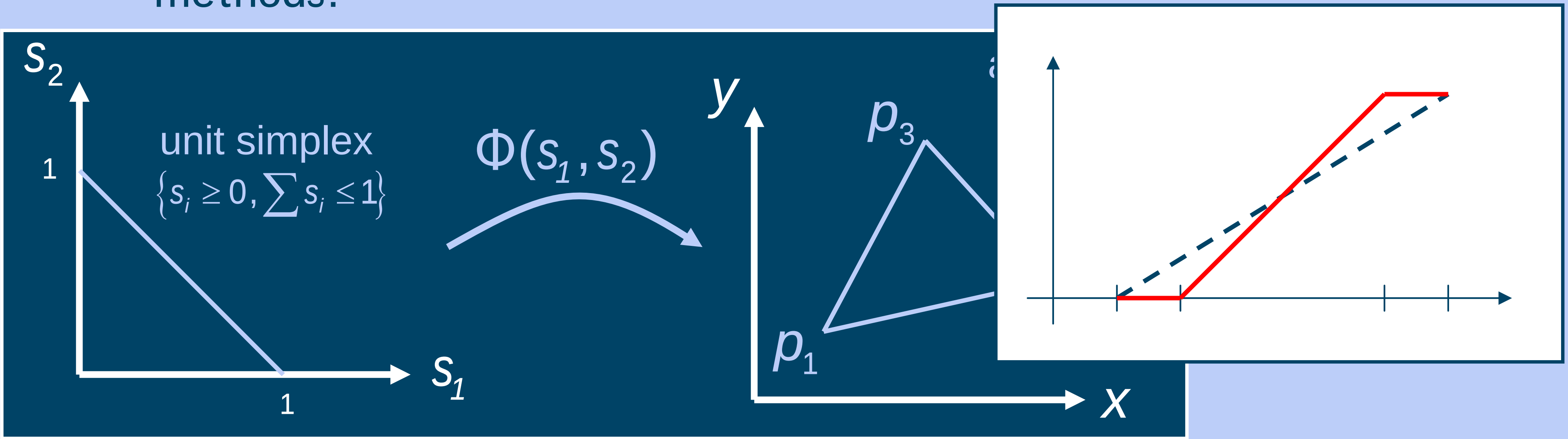


$$v_{\text{mesh}} = \sum_{\text{nodes}} v_{\text{part},i}\Lambda_i$$

second FEM-triangulation
with linear basis set Λ

Second domain triangulation

The parameter functions Λ can be calculated by standard FEM-methods:



with affine linear mapping

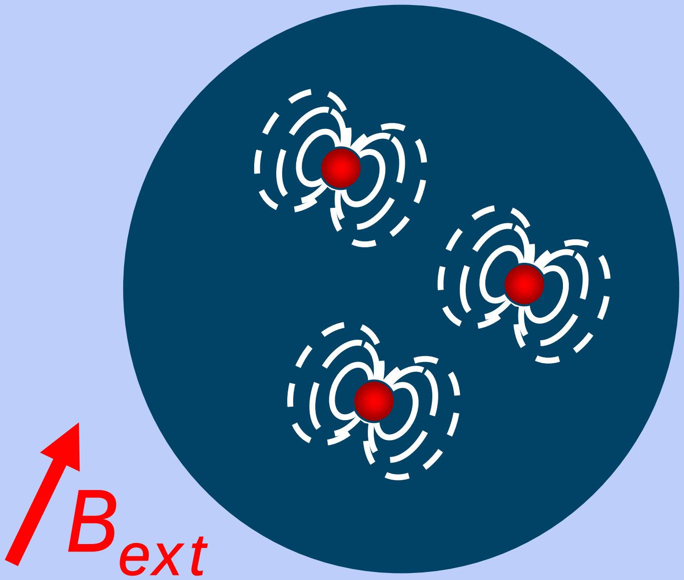
$$\Phi_{x_1x_2x_3}(s_1,s_2)=\begin{pmatrix}x_1\\y_1\end{pmatrix}+s_1\begin{pmatrix}x_2-x_1\\y_2-y_1\end{pmatrix}+s_2\begin{pmatrix}x_3-x_1\\y_3-y_1\end{pmatrix}$$

$$\Lambda(x)=\Lambda\left(\Phi^{-1}_{x_1x_2x_3}(x)\right)=\frac{(x_3-x)(y_3-y_2)-(x_3-x_2)(y_3-y)}{(x_2-x_1)(y_3-y_1)-(x_3-x_1)(y_2-y_1)}$$

$$f(\Lambda,\theta_1,\theta_2)=\frac{\Lambda-\theta_1}{1-(\theta_1+\theta_2)}\cdot\Theta(\Lambda-\theta_1)\cdot\Theta(1-\Lambda-\theta_2)+\Theta(\Lambda-(1-\theta_2))$$

Particle motion

Governing equations:



Particles induce fluid flow:

$$\rho \frac{\partial u}{\partial t} + \rho (u \nabla) u = -\operatorname{grad} p + \eta \Delta u + \rho f$$

$$\operatorname{div} u = 0$$

Total mesh displacement:

$$\Delta r = \sum_i (r_i - \xi_i) \cdot f(\Lambda_i(r), \theta_1, \theta_2)$$

Additional remeshing condition:

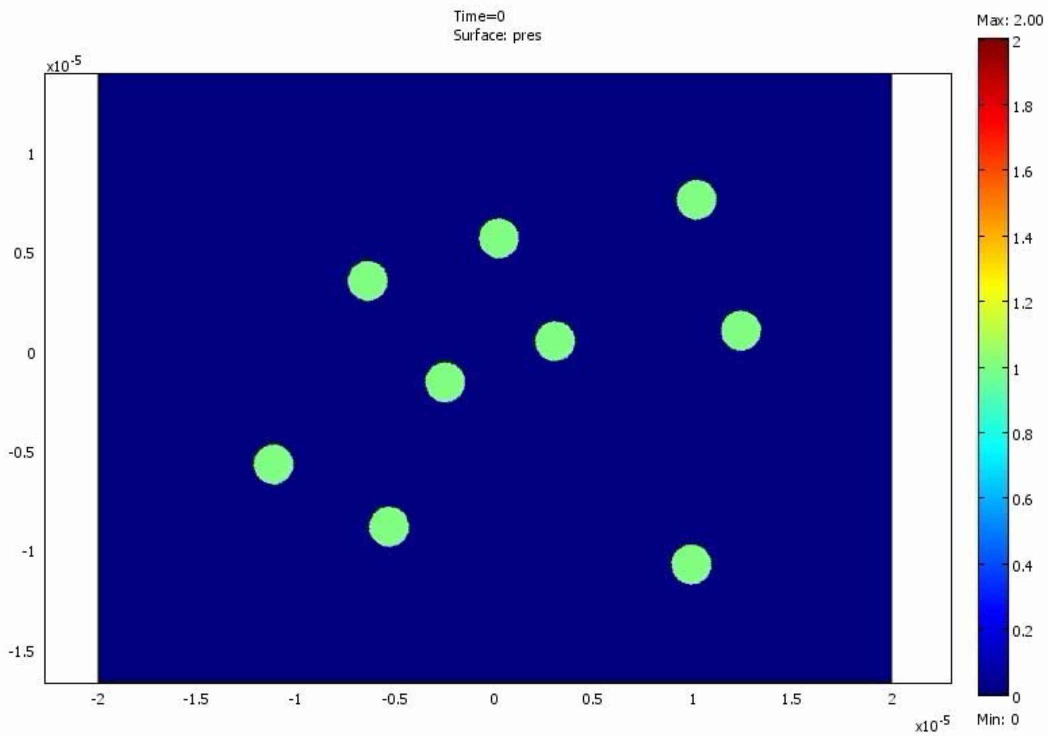
$$\min_{T \in \mathcal{T}} \operatorname{qual} T < \sigma$$

$$M \parallel B_{ext} \qquad |M| = M_s$$

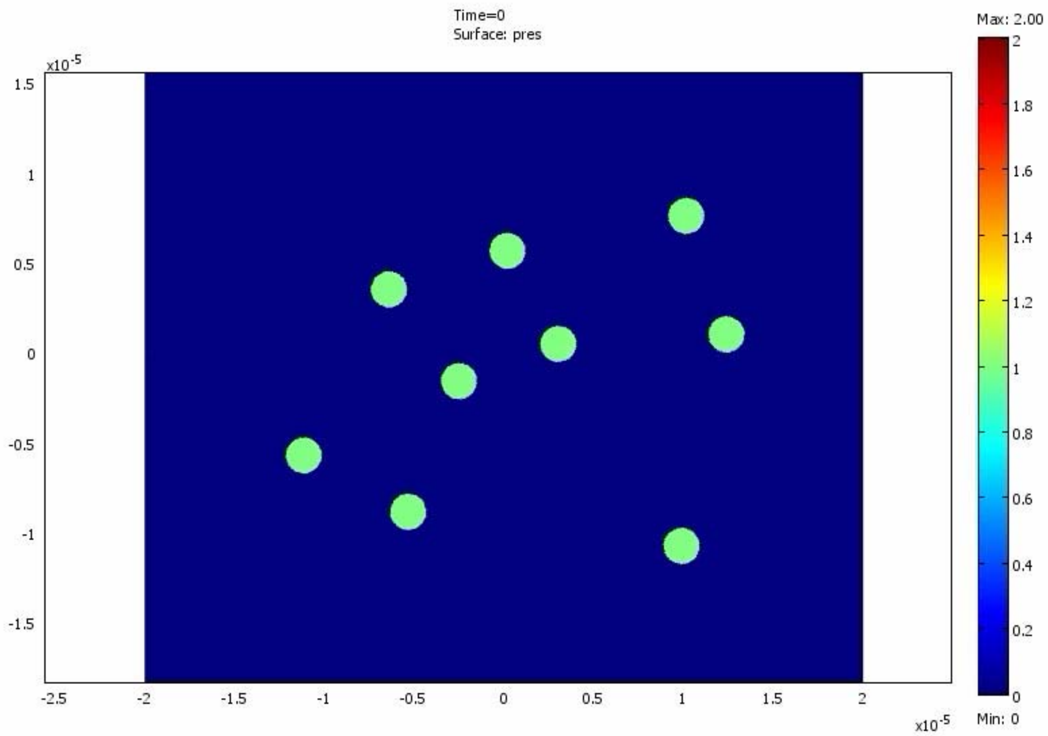
$$\int_{\Omega_t} \langle \operatorname{grad} \psi_{A_z}, \operatorname{grad} A_z \rangle dx - \mu_0 \int_{\Omega_t} \left(M_y \frac{\partial \psi_{A_z}}{\partial x} - M_x \frac{\partial \psi_{A_z}}{\partial y} \right) dx = 0$$

$$M \frac{d}{dt} U(t) = F_{mag} + F_{visc} + F_{pen}$$

Interactions of beads in fluids



$f = f_0$



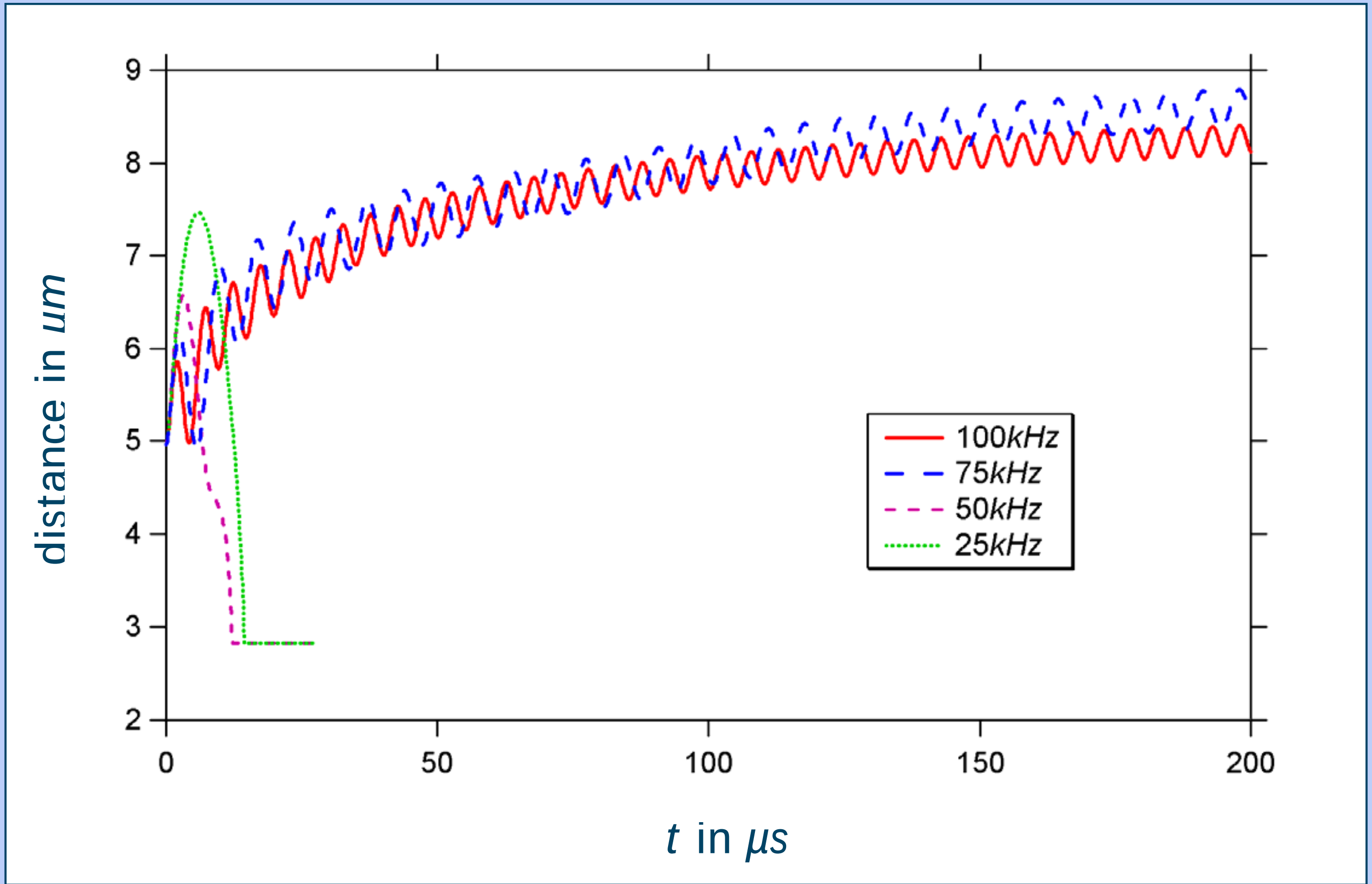
$f = 1.5f_0$

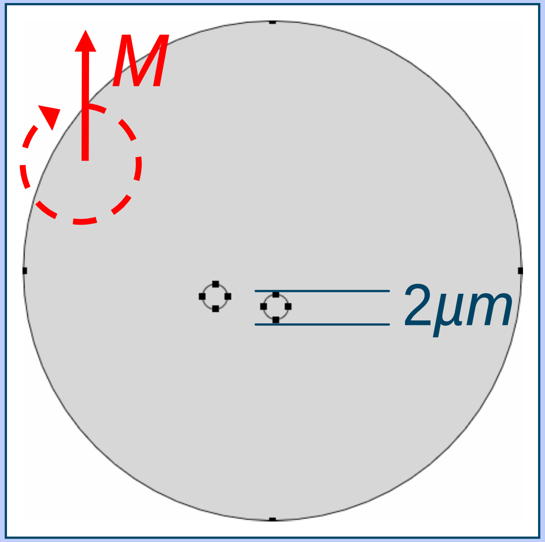
Different phenomena:

- chain creation
- particles oscillating against each other

Interactions of beads in fluids

Frequency dependence for different initial conditions:



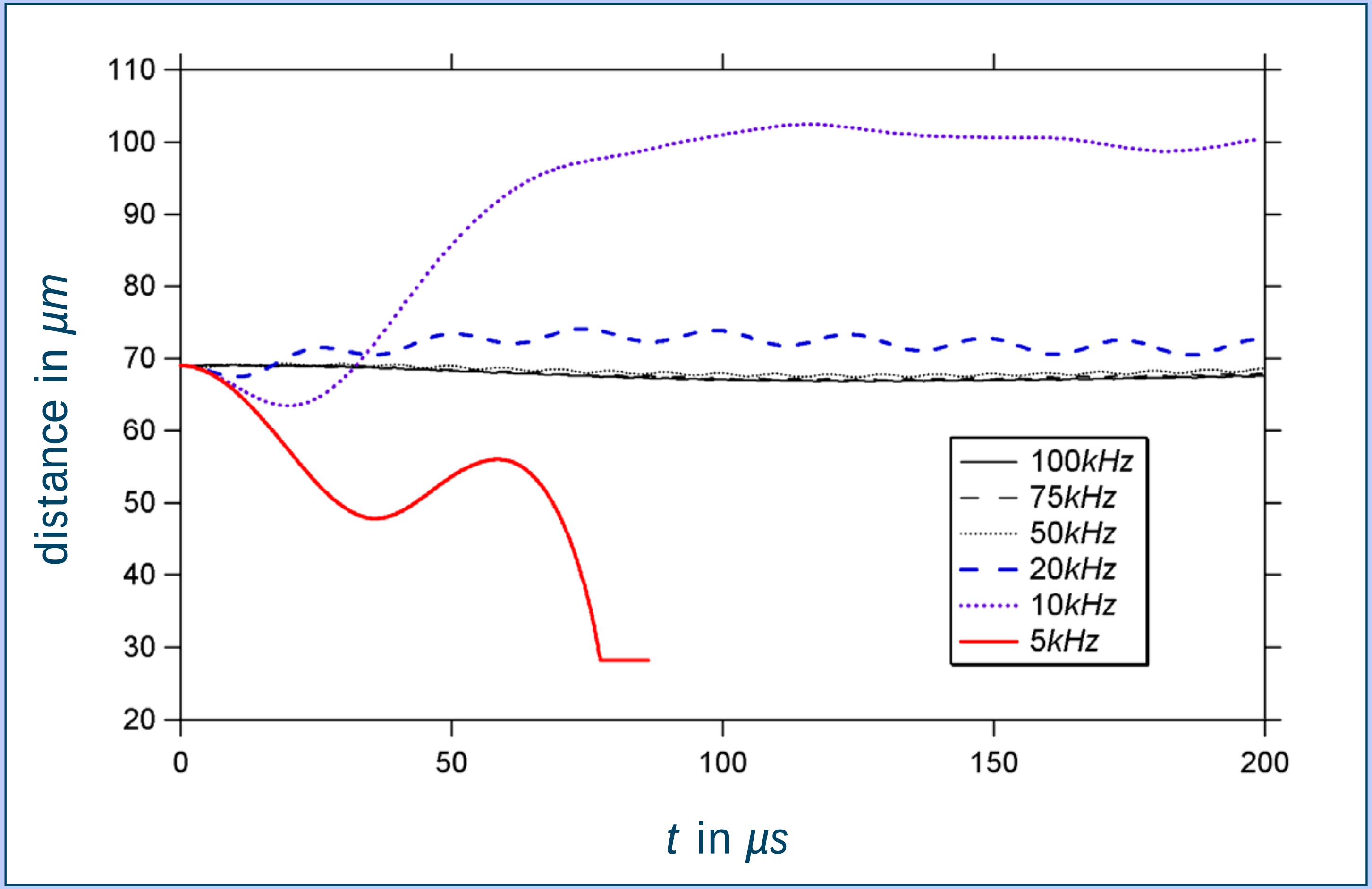


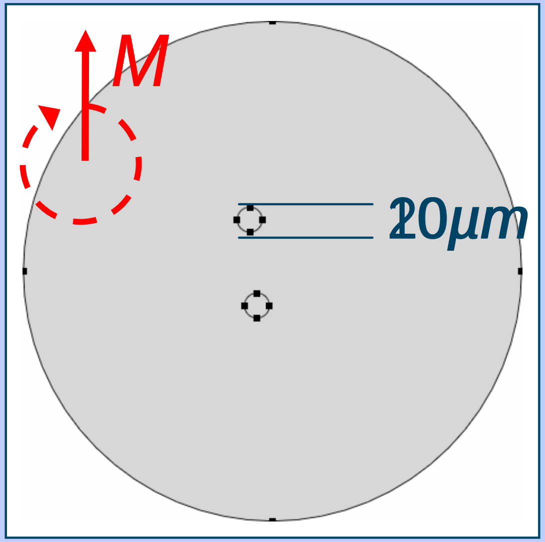
$M_s = 1000 kAm^{-1}$

$r = 1 \mu m$

Interactions of beads in fluids

Frequency dependence for different particle diameters:



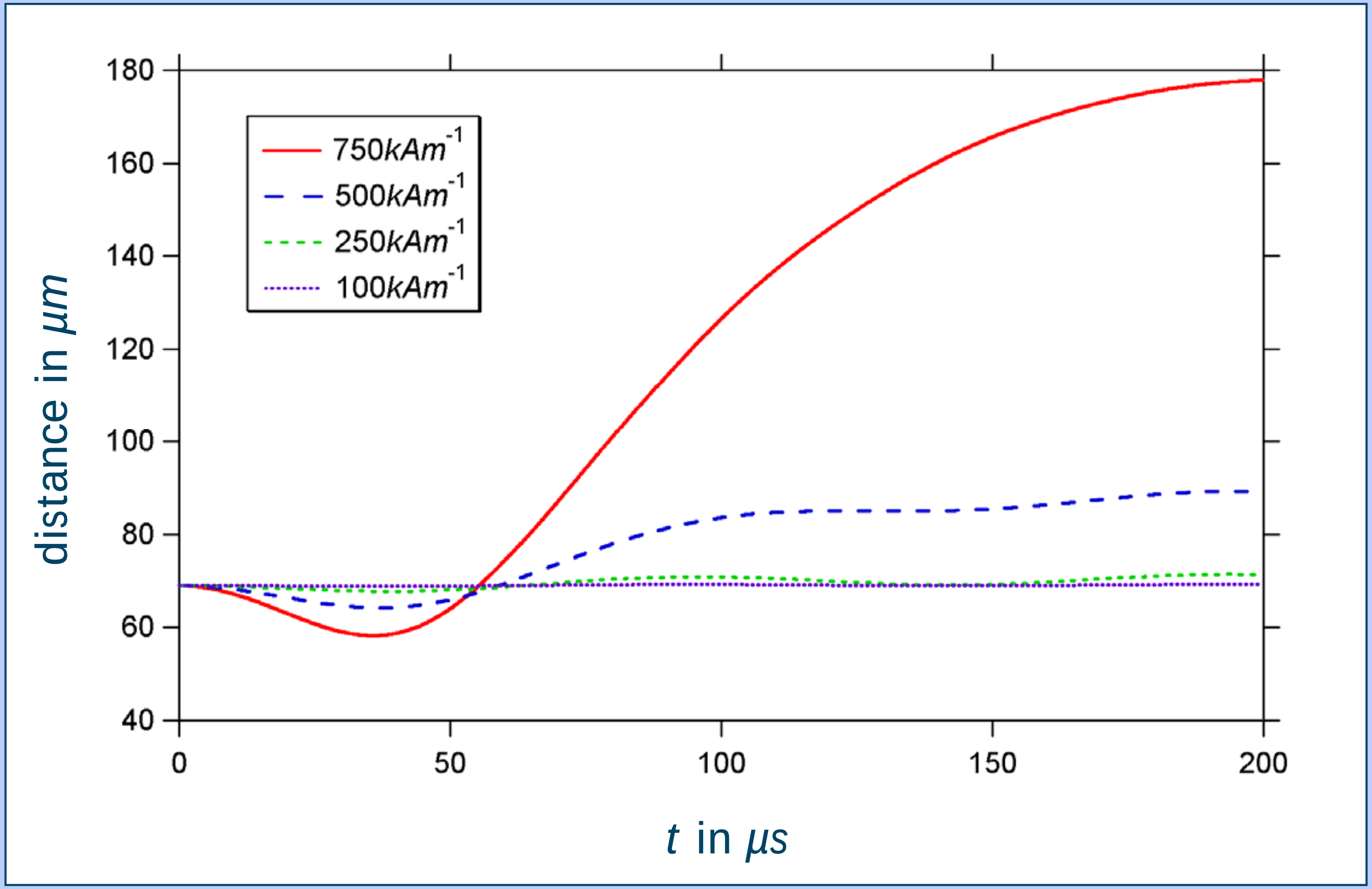


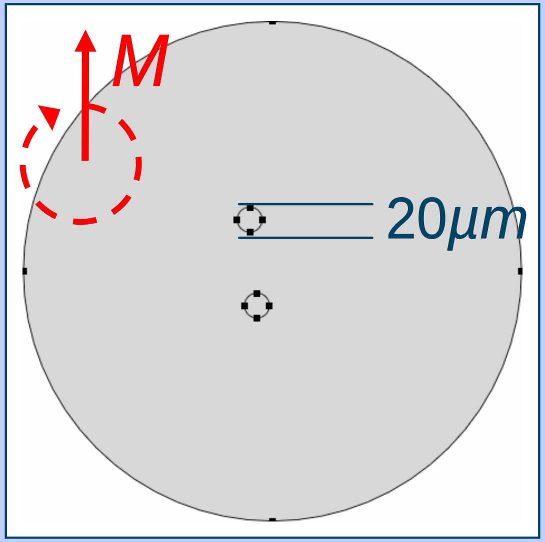
$M_s = 1000 kAm^{-1}$

$r = 20 \mu m$

Interactions of beads in fluids

Frequency dependence for different particle magnetizations:



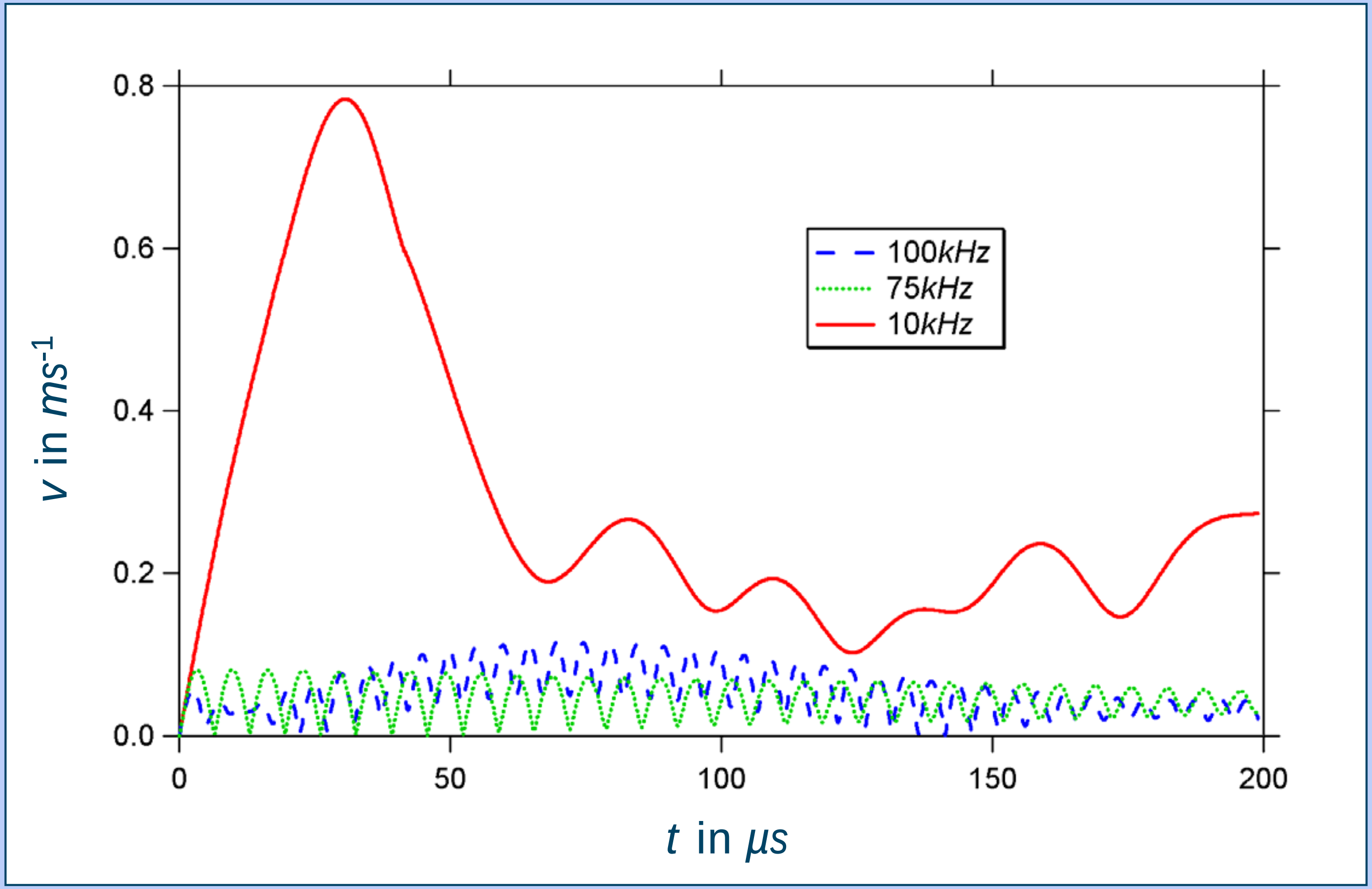


$f = 20kHz$

$r = 20\mu m$

Interactions of beads in fluids

Observation:



$M_s = 1000 kAm^{-1}$

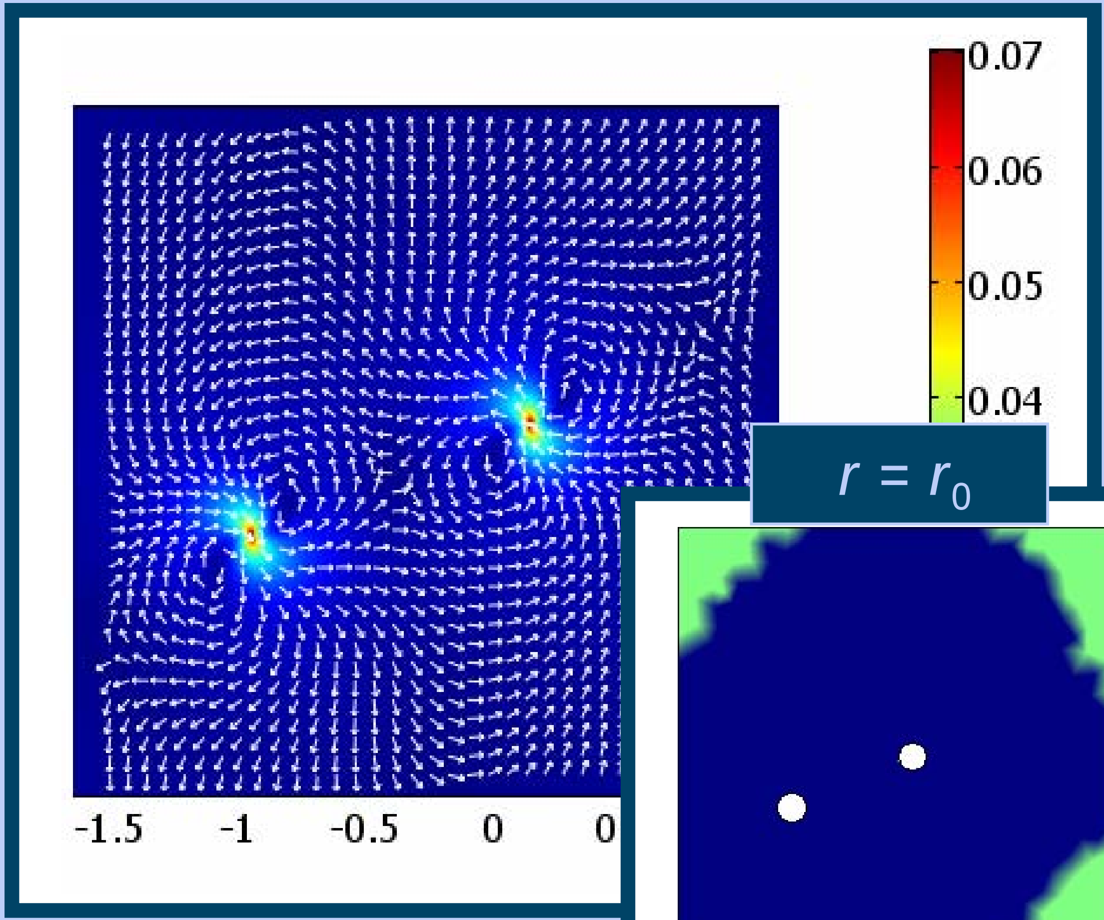
$r = 10 \mu m$

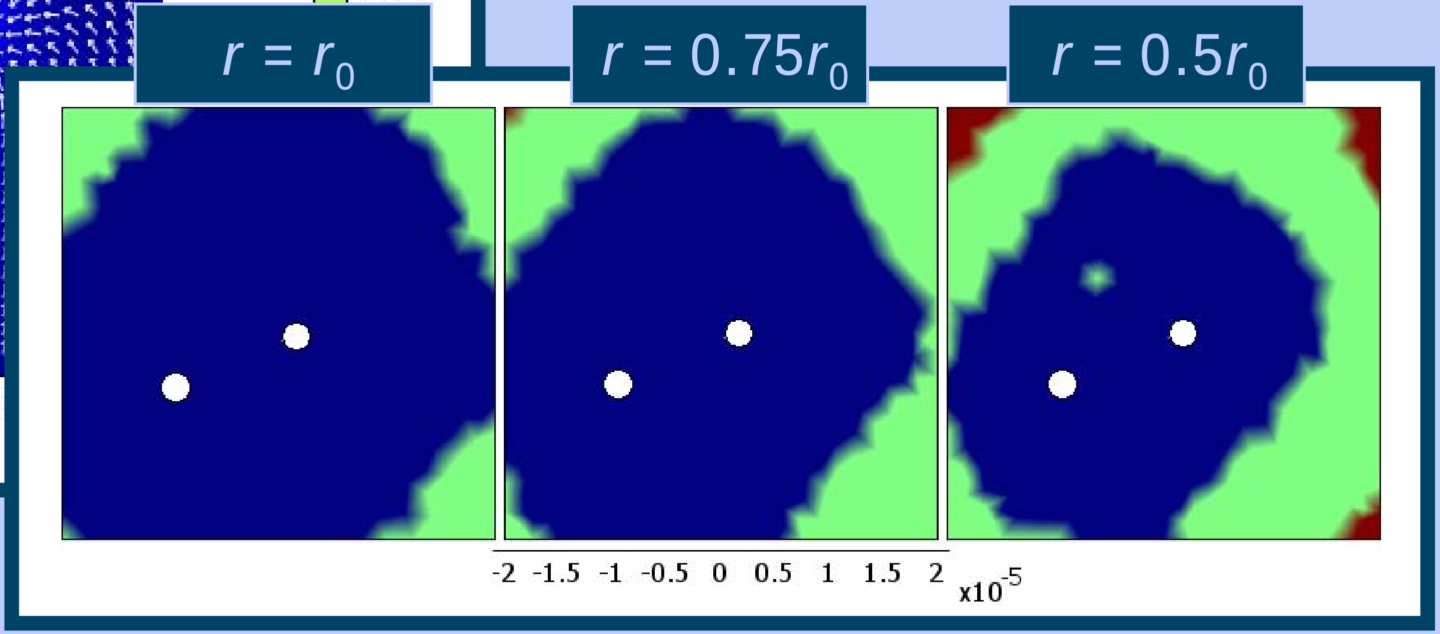
high velocities might lead to non-laminar fluid behaviour on microscale!!

Comparison between forces

r_0 = 1μm

M_s = 1000kAm^{-1}





Conclusion & Outlook

Conclusion

- We have developed a model to describe the dynamic behaviour of magnetic beads
- We have simulated experimentally known effects (chain creation)
- We have shown that the magnetic interaction of particles can induce strong fluidic particle interactions that gain importance when dealing with different particle sizes

Outlook

- Finding proper clearcuts for different force regimes
- Implementing ferromagnetic particles