

# A Phase-field for Fluid-Structure Interaction with Application to Cell Biology

Sebastian Aland<sup>1,2</sup>, Helmut Abels<sup>3</sup>, Dominic Mokbel<sup>2</sup>

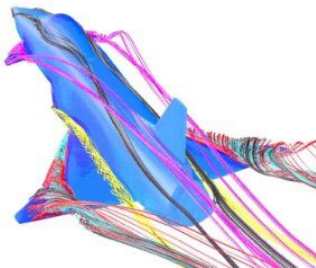
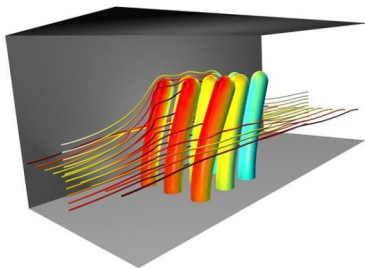
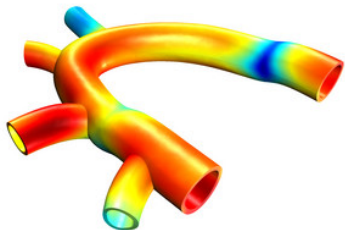
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<sup>2</sup>TU Dresden, Germany

<sup>3</sup>Universität Regensburg

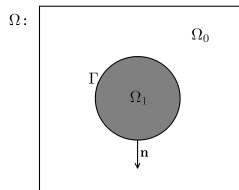
SIAM Life Science, Minneapolis, 2018

# Fluid-Structure Interaction



# Classical two-phase setting

- ▶  $\Omega_0$  ... incompressible fluid
- ▶  $\Omega_1$  ... incompressible elastic solid



## Classical two-phase model

Balance of momentum and mass

$$\begin{aligned}\rho_i \partial_t^\bullet \mathbf{v} - \nabla \cdot \mathbb{S}_i + \nabla p_i &= 0 \\ \nabla \cdot \mathbf{v} &= 0\end{aligned}$$

$$\text{in } \Omega_i(t), i = 0, 1$$

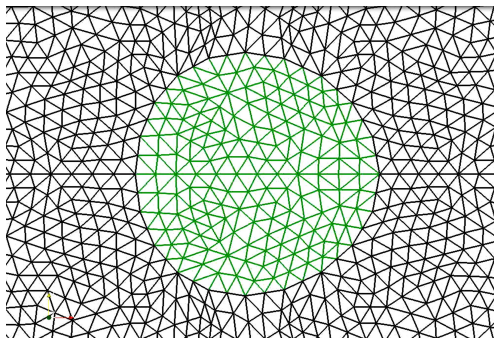
$$\text{in } \Omega_i(t), i = 0, 1$$

Force balance at the interface  $\Gamma$

$$\mathbf{n} \cdot [\mathbb{S}_i - p_i \mathbb{I}]_0^1 = 0$$

$$\text{on } \Gamma(t)$$

# The standard method: ALE



- ▶ Solid grid points (green) move with the velocity field  $\mathbf{v}_1$
- ▶ Fluid grid points (black) move with auxiliary velocity  $\tilde{\mathbf{v}}$  resulting from following Laplace problem

$$\begin{aligned}\Delta \tilde{\mathbf{v}} &= 0 && \text{in } \Omega_0, \\ \tilde{\mathbf{v}} &= 0 && \text{on } \delta\Omega_0 \setminus \Gamma, \\ \tilde{\mathbf{v}} &= \mathbf{v}_1 && \text{on } \Gamma,\end{aligned}$$

to harmonically extend the interface movement into  $\Omega_0$

- ▶ Problem: this fails for larger deformations/translations/rotations (re-triangulation necessary)

# Challenges

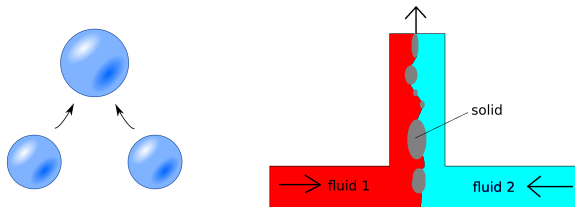
- ▶ complex deformations that cannot be tackled by simple grid movement



- ▶ interactions of fluid, elastic and viscoelastic phases



- ▶ topological changes, solidification, fluidization



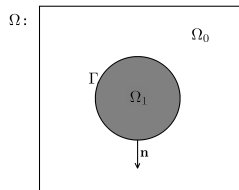
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# Distribution form

momentum equation:

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Weak form

$$\int_{\Omega_0} \rho_0 \partial_t^\bullet \mathbf{v} \xi + \mathbb{S}_0 : \nabla \xi - p_0 \nabla \cdot \xi + \int_{\Omega_1} \rho_1 \partial_t^\bullet \mathbf{v} \xi + \mathbb{S}_1 : \nabla \xi - p_1 \nabla \cdot \xi = 0$$

Use characteristic functions  $\chi_i$  for  $\Omega_i$ , resp., such that:  $\int_{\Omega_i} \psi = \int_{\Omega} \chi_i \psi$

$$\int_{\Omega} (\rho_0 \chi_0 + \rho_1 \chi_1) \partial_t^\bullet \mathbf{v} \xi + (\chi_0 \mathbb{S}_0 + \chi_1 \mathbb{S}_1) : \nabla \xi - (\chi_0 p_0 + \chi_1 p_1) \nabla \cdot \xi = 0$$

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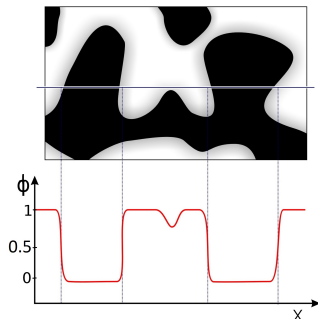
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## strong form

$$\begin{aligned}(\rho_0 \chi_0 + \rho_1 \chi_1) \partial_t^\bullet \mathbf{v} - \nabla \cdot (\mathbb{S}_0 \chi_0 + \mathbb{S}_1 \chi_1) + \nabla p &= 0 && \text{in } \Omega \\ \text{where } p &= \chi_0 p_0 + \chi_1 p_1\end{aligned}$$

# Phase field model

- ▶ Introduce a phase field  $\phi$  to represent the different domains ( $\phi = 1$ ,  $\phi = 0$ )
- ▶ Interface given by  $\Gamma = \{x | \phi(x) = 0.5\}$
- ▶ Allow for a partial mixing:  
 $\phi = \frac{m_1}{m_0 + m_1}$  mass ratio
- ▶ Smooth transition at the interface of thickness  $\epsilon$



## Useful properties:

- ▶ interface normal

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$$

- ▶ phase field approximates characteristic functions

$$\chi_1 \approx \phi$$

$$\chi_0 \approx 1 - \phi$$

$$\delta_\Gamma \approx |\nabla\phi|$$

# Coupled model for viscous/elastic phases

We obtain the general phase field approximation

## Multiphase balance equations

$$\begin{aligned}\rho(\phi)\partial_t^\bullet \mathbf{v} - \nabla \cdot (\phi \mathbb{S}_0 + (1 - \phi)\mathbb{S}_1) + \nabla p &= 0 && \text{in } \Omega \\ \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega\end{aligned}$$

where

$$\rho(\phi) = \phi\rho_1 + (1 - \phi)\rho_0$$

- ▶ can in principle be used for any material stress
- ▶ grid movement replaced by transport of phase field
- ▶ no re-triangulation necessary!
- ▶ converges to the sharp interface equation for  $\epsilon \rightarrow 0$

**Open question:** How to define the stress  $\mathbb{S}$  for an elastic material

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# The left Cauchy-Green strain tensor

- ▶ left Cauchy-Green strain tensor

$$\mathbb{B} = \frac{\partial X}{\partial \bar{X}} \frac{\partial X^T}{\partial \bar{X}}$$

where  $\bar{X}, X(\bar{X}, t)$  are material point positions in initial and current configuration, resp.

- ▶ stress free (initial) configuration:  $\mathbb{B} = \mathbb{I}$
- ▶ stress in single (neo-Hookean) elastic material

$$\mathbb{S} = \mu(\mathbb{B} - \mathbb{I})$$

where  $\mu$  is the materials shear modulus

- ▶ define upper-convected time derivative: stretches and rotates  $\mathbb{B}$  with the flow

$$\overset{\nabla}{\mathbb{B}} := \partial_t^\bullet \mathbb{B} - \nabla \mathbf{v}^T \cdot \mathbb{B} - \mathbb{B} \cdot \nabla \mathbf{v}$$

- ▶ for a purely elastic material

$$\overset{\nabla}{\mathbb{B}} = 0 \quad \text{where initially } \mathbb{B} = \mathbb{I}$$

# Combined strain model

Elastic strains in the two materials

$$\begin{aligned} \mathbb{B} &= 0 && \text{in } \Omega_1 \\ \mathbb{B} &= \mathbb{I} && \text{in } \Omega_0 \end{aligned}$$

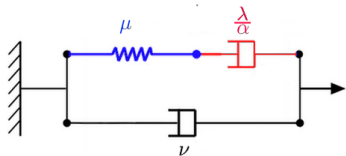
can be combined to

## Combined strain model

$$\lambda(\phi) \mathbb{B} + \alpha(\phi)(\mathbb{B} - \mathbb{I}) = 0 \quad (\text{strain})$$

$$\mathbb{S}(\phi) = \nu(\phi)(\nabla \mathbf{v} + \nabla \mathbf{v}^T) + \mu(\phi)(\mathbb{B} - \mathbb{I}) \quad (\text{stress})$$

where the only free parameter is the relaxation time  $\lambda/\alpha$



viscosity	shear modulus			material
$\nu(\phi)$	$\mu(\phi)$	$\lambda(\phi)$	$\alpha(\phi)$	
*	0	0	1	viscous fluid
0	*	$T$	0	elastic solid
*	*	$T$	0	Kelvin-Voigt
0	*	*	1	Maxwell



# Energy dissipation

Define the total energy

$$E = \int_{\Omega} \underbrace{\frac{\rho(\phi)}{2} |\mathbf{v}|^2}_{\text{kinetic energy}} + \underbrace{\frac{\mu(\phi)}{2} \text{tr}(\mathbb{B} - \ln \mathbb{B} - \mathbb{I})}_{\text{elastic energy}} + \underbrace{\tilde{\gamma} \left( \frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{\epsilon} W(\phi) \right)}_{\text{surface energy}} dx$$

Insert the balance laws

## Phase field Oldroyd-B model (unspecified)

$$\begin{aligned} \rho(\phi) \partial_t^\bullet \mathbf{v} &= -\nabla p + \nabla \cdot \left( \nu(\phi) (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \right) + \nabla \cdot (\mu(\phi) (\mathbb{B} - \mathbb{I})) + \mathbf{F} && \text{in } \Omega \\ \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega \\ \partial_t^\bullet \phi &= -\nabla \cdot \mathbf{J} && \text{in } \Omega \\ \lambda(\phi) \overset{\nabla}{\mathbb{B}} &= -\alpha(\phi) (\mathbb{B} - \mathbb{I}) && \text{in } \Omega \end{aligned}$$

# Energy dissipation II

Obtain non-increasing energy,

$$\begin{aligned} d_t E &= - \int_{\Omega} \frac{\nu}{2} |\nabla \mathbf{v} + \nabla \mathbf{v}^T| + \frac{1}{m(\phi)} |\mathbf{J}|^2 \, dx - \int_{\Omega \setminus \{\lambda=0\}} \frac{\mu\alpha}{2\lambda} \operatorname{tr}(\mathbb{B} + \mathbb{B}^{-1} - 2\mathbb{I}) \, dx \\ &\leq 0. \end{aligned}$$

for the choice

$$\begin{aligned} \mathbf{F} &= -\nabla \cdot (\rho'(\phi) \mathbf{v} \otimes \mathbf{J}) - \epsilon \tilde{\gamma} \nabla \cdot (\nabla \phi \otimes \nabla \phi), \\ \mathbf{J} &= -m(\phi) \nabla \left[ \frac{\mu'(\phi)}{2} \operatorname{tr}(\mathbb{B} - \ln \mathbb{B} - \mathbb{I}) + \tilde{\gamma} \left( \frac{1}{\epsilon} W'(\phi) - \epsilon \Delta \phi \right) \right] \end{aligned}$$

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[Mokbel, Abels, Aland; 'A phase-field model for fluid-structure interaction'; J. Comp. Phys. (2018)]

# Governing equations

## Phase field Oldroyd-B model

$$\begin{aligned}\rho(\phi)\partial_t^\bullet \mathbf{v} &= -\nabla p + \nabla \cdot \left( \nu(\phi)(\nabla \mathbf{v} + \nabla \mathbf{v}^T) \right) + \nabla \cdot (\mu(\phi)(\mathbb{B} - \mathbb{I})) \\ &\quad - \nabla \cdot (\rho'(\phi)\mathbf{v} \otimes \mathbf{J}) - \epsilon \tilde{\gamma} \nabla \cdot (\nabla \phi \otimes \nabla \phi) && \text{in } \Omega \\ \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega \\ \partial_t^\bullet \phi &= -\nabla \cdot \left( -m(\phi)\nabla \left[ \frac{\mu'(\phi)}{2} \text{tr}(\mathbb{B} - \ln \mathbb{B} - \mathbb{I}) + \tilde{\gamma} \left( \frac{1}{\epsilon} W'(\phi) - \epsilon \Delta \phi \right) \right] \right) && \text{in } \Omega \\ \lambda(\phi)\overset{\nabla}{\mathbb{B}} &= -\alpha(\phi)(\mathbb{B} - \mathbb{I}) && \text{in } \Omega\end{aligned}$$

- ▶ thermodynamically consistent (energy decreasing) model
- ▶ stability problems due to strain contribution in phase field flux
- ▶ **red term** can be omitted, resulting error in thermodynamical consistency is higher order

# Asymptotic analysis

Outer expansion at leading order

$$\begin{aligned}\partial_t^\bullet (\rho_i \mathbf{v}_0) - \nabla \cdot \left( \nu_i \left( \nabla \mathbf{v}_0 + \nabla \mathbf{v}_0^T \right) + \mu_i (\mathbb{B}_0 - \mathbb{I}) \right) + \nabla p_0 &= 0 && \text{in } \Omega_i, \\ \nabla \cdot \mathbf{v}_0 &= 0 && \text{in } \Omega_i, \\ \mathbb{B}_0 &= \mathbb{I} && \text{in } \Omega_0, \\ \nabla \mathbb{B}_0 &= 0 && \text{in } \Omega_1,\end{aligned}$$

Inner expansion at leading order

$$\begin{aligned}[\mathbf{v}_0]_0^1 &= 0 \\ -2[\nu D\mathbf{v}_0]_0^1 \mathbf{n} + [p_0]_0^1 \mathbf{n} - [\mu(\phi_0)(\mathbb{B}_0 - \mathbb{I})]_0^1 \mathbf{n} &= \tilde{\gamma} \kappa \mathbf{n}.\end{aligned}$$

Hence, convergence to sharp interface limit for  $\epsilon \rightarrow 0$  **with and without** the 'red' term

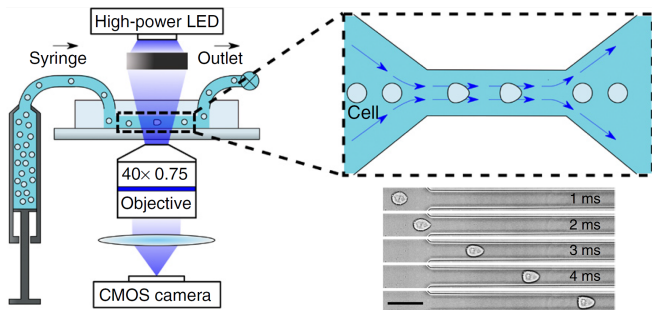
Phase field modeling

Benchmark for cells in flow

Summary

# Test case: biological cells in flow channel

- ▶ Biological cells behave similar to elastic solids (Young's modulus  $\approx 1\text{kPa}$ )
- ▶ Elastic properties change with cell phenotype and morbidity
- ▶ Elasticity measurements used to identify cells and their medical condition
- ▶ A flow scenario to measure cell elasticity proposed <sup>5</sup>:

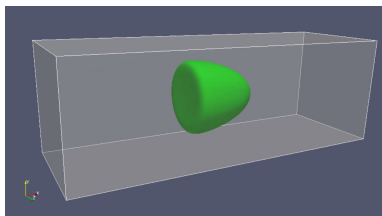


- ▶ cell deformation measured by camera image analysis
- ▶ offers extremely fast cell screening (1000 cells per second)
- ▶ comparison to simulations needed to determine elastic modulus

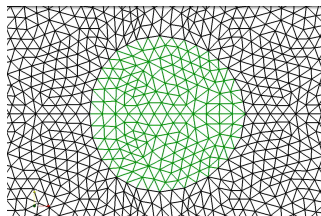
<sup>5</sup>Otto et al. Nature Methods (2015)

# Simulation of a single elastic cell

- ▶ can be simulated with our phase field approach (cell moving, periodic boundaries) and ALE method (cell centered)



Phase-field simulation (cell moving)

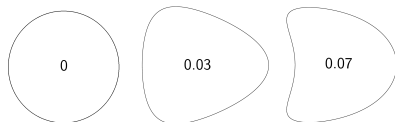


ALE simulation (cell centered)

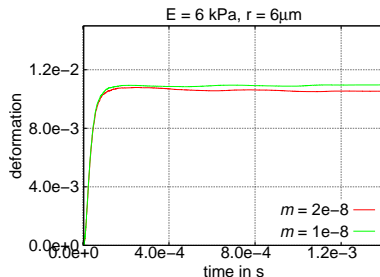
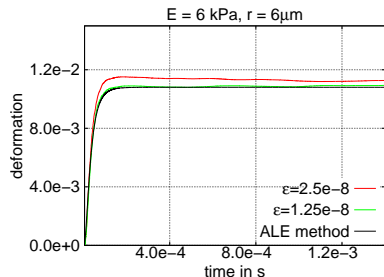
- ▶ introduce measure for deformation

$$\text{deformation} = 1 - \text{circularity} = 1 - \frac{2\sqrt{\pi A}}{P}$$

- ▶ example shapes



# Influence of interface thickness and mobility

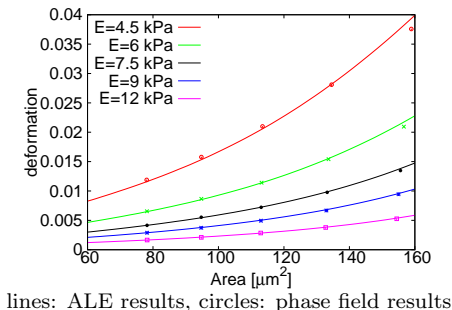


- ▶ convergence to reference solution for interface thickness  $\epsilon \rightarrow 0$
- ▶ almost no influence of mobility



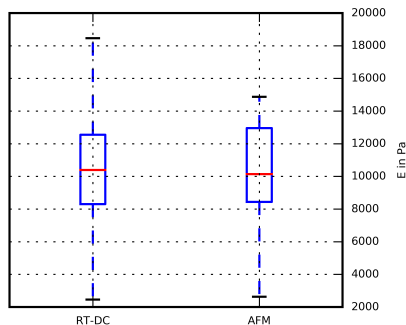
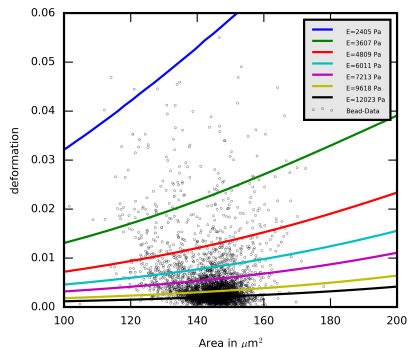
# Validation with ALE model

- ▶ compare (almost) stationary shapes



- ▶ very good agreement over a range of cell areas and E-moduli

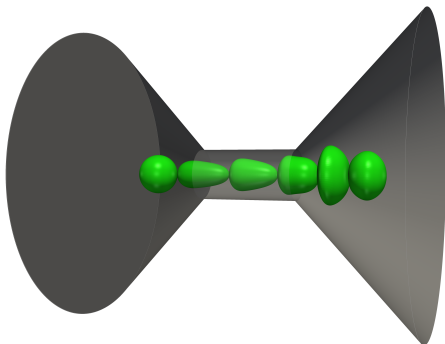
# Validation with elastic beads



- ▶ measured elasticity from simulations (RT-DC) matches perfectly with reference values (AFM) <sup>1</sup>
- ▶ highly promising method for cell diagnostics
- ▶ Phase field approach can be used to extract additional cell parameters by simulating inflow/outflow, membrane tension, bending stiffness, ...

<sup>1</sup>Mokbel, Mietke, Otto, Guck, Aland; ACS Biomat. Sci. Eng. (2017)

# Beyond AFM simulations: large translations

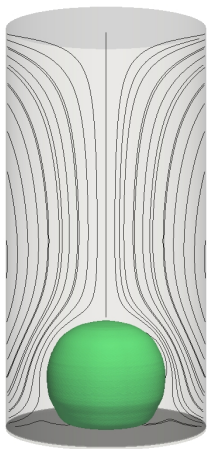


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[Mokbel, Abels, Aland; 'A phase-field model for fluid-structure interaction'; *J. Comp. Phys.* (2018)]



# Simulation of a bouncing ball



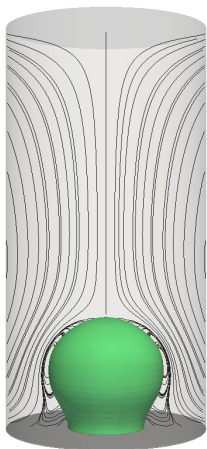
video with streamlines

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[Mokbel, Abels, Aland; 'A phase-field model for fluid-structure interaction'; *J. Comp. Phys.* (2018)]



# Simulation of a rubber ball with adhesion



video with streamlines

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[Mokbel, Abels, Aland; 'A phase-field model for fluid-structure interaction'; *J. Comp. Phys.* (2018)]



Phase field modeling

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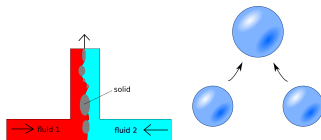
## Phase field model for FSI

- ▶ viscous, elastic and viscoelastic domains
- ▶ based on energy variation
- ▶ sharp interface limit shown
- ▶ rotations and translations without re-triangulation
- ▶ publication<sup>1</sup>



## Outlook

- ▶ complex deformations, topological changes
- ▶ simulation of solidification/fluidization
- ▶ elasticity + adhesion + contact line dynamics
- ▶ apply to describe mechanics of adhesive biological cells



<sup>1</sup> [Mokbel, Abels, Aland; 'A phase-field model for fluid-structure interaction'; J. Comp. Phys. (2018)]

# Advantages

w.r.t. ALE method

- ▶ inflow and outflow (in RT-DC case)
- ▶ interaction of multiple cells
- ▶ larger deformations, topological changes
- ▶ viscoelastic domains
- ▶ fluidization, solidification

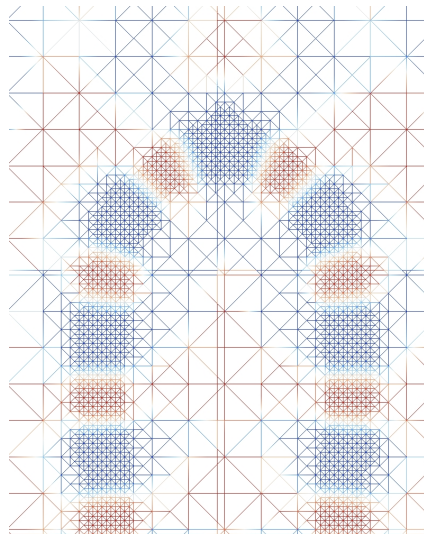
w.r.t. IB method

- ▶ adaptivity is easier
- ▶ parallelization is easier



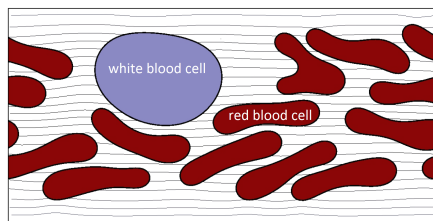
# Numerical treatment

- ▶ C++ FEM library AMDiS
- ▶ adaptive mesh
- ▶ P2 elements except for P1 for pressure
- ▶ 2D: direct solver UMFPACK
- ▶ 3D: Petsc based parallelization with problem-adapted preconditioners
- ▶ semi-implicit time discretization



# Simulation of blood flow

- ▶ Blood components
  - 55% Plasma (viscous fluid)
  - 44% red blood cells (RBC)
  - 1% white blood cells (WBC)
- ▶ multiple viscous fluid phases realized by multiple phase fields (for each cell)
- ▶ different viscosities in RBC, WBC and plasma <sup>1</sup>



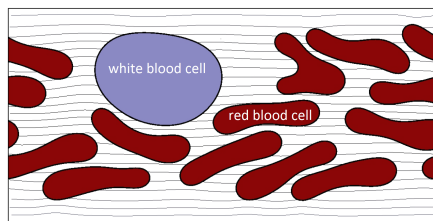
- ▶ faster margination for
  - ▶ higher WBC viscosity
  - ▶ higher RBC ratio
- ▶ agreement with approximative solutions<sup>2</sup> and experiments

<sup>1</sup>Marth, Aland, Voigt; JFM (2016)

<sup>2</sup>Fedosov & Gompper (2012, 2014)

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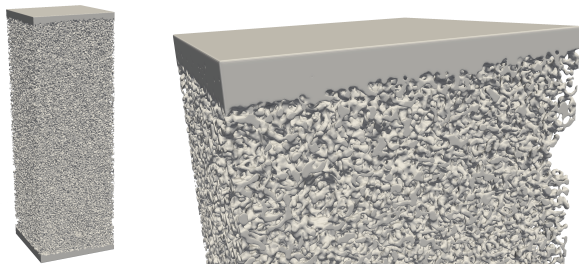
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elastic/stressless coupling

# Polymer foam<sup>1</sup>

- ▶ Phase 1: elastic solid material
- ▶ Phase 0: ambient air ( $S_0 = 0$ )



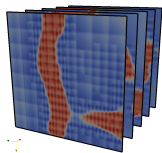
- ▶ How does the microstructure deform at a given outer force ?
- ▶ How does the elasticity of solid material determine the elastic response of the whole foam ?

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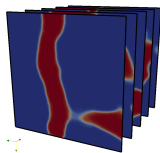
<sup>1</sup>Weissenborn et al. ECCM-17 (2016)

# Phasefield from tomography data

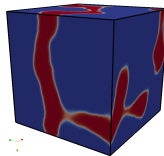
Tomographic / microscopic imaging data can be directly transferred into a phase field



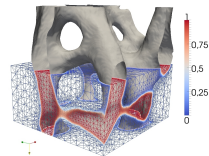
tomographic data



apply threshold



interpolate



use as phase field

- ▶ use for foam simulation
- ▶ calculate local stresses and strains to investigate foam stability

