TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Department of Mathematics, Institute of Scientific Computing

Collective cell behavior – a cell based parallelization approach for a phase field active polar gel model

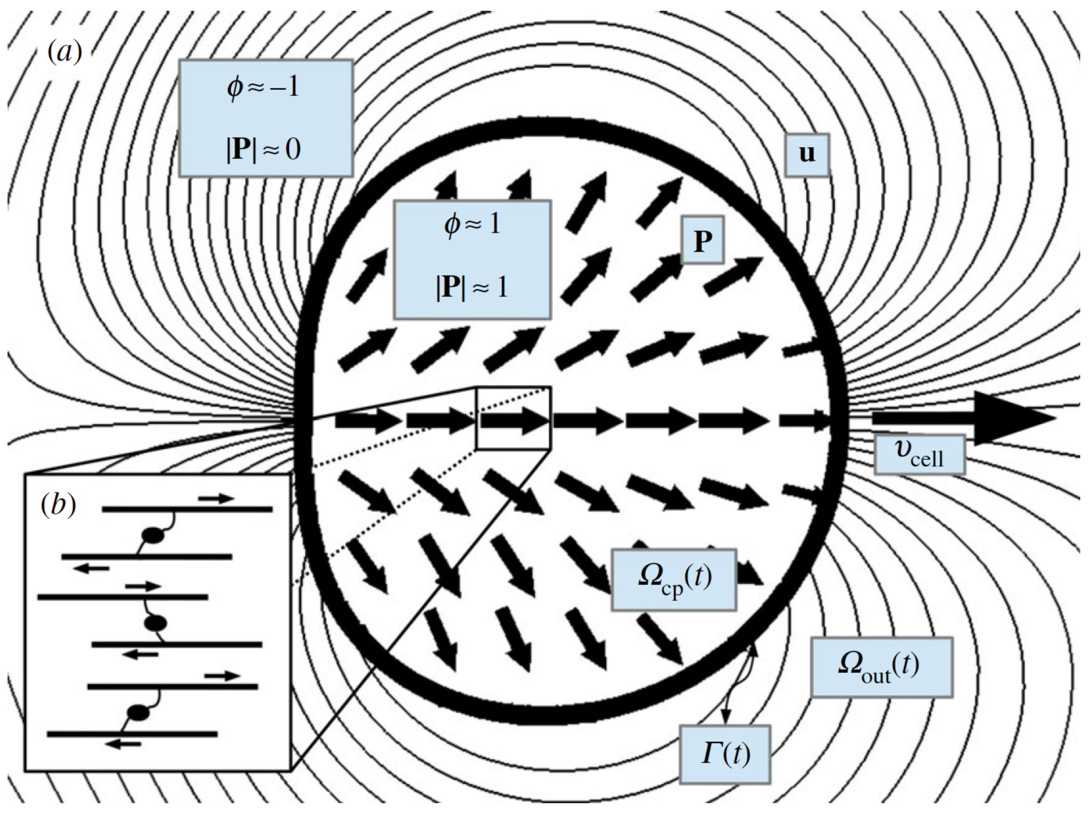
Simon Praetorius, Dennis Wenzel, Axel Voigt

Summary

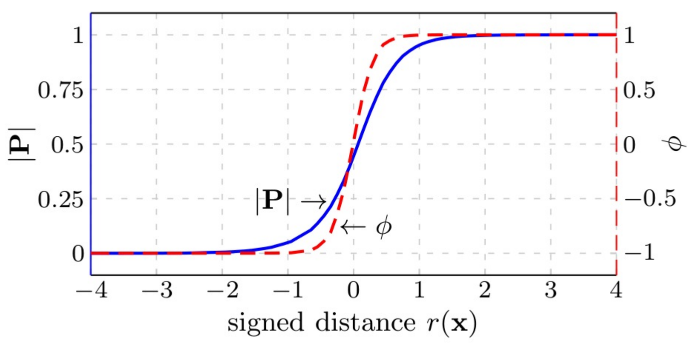
We consider a continuum model for collective cell movement. Each cell is modeled by a phase field active polar gel model and the cells interact via steric interactions. We provide a finite element implementation with a parallel efficiency of at least 0.5 in the number of cells. This is achieved by considering each cell on a different processor and various improvements to reduce the communication overhead to deal with the cell-cell interactions. We describe implementation details and demonstrate results for up to 768 cells.

Model for single cell

phase field model for cell motility – active polar gel within confinement



coupled model for phase field variable and polarization field, movement is result of splay instability within the cell



Model for multiple cell

consider one phase field variable for each cell and in addition interaction between cells

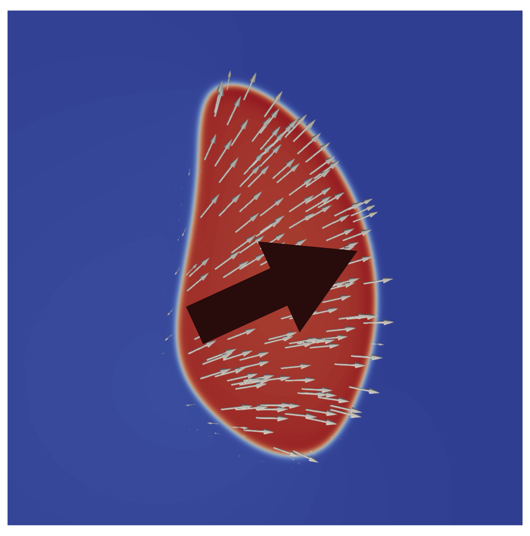
$$
\begin{aligned}
\partial_t\phi_i + v_0\nabla\cdot(\phi_i\mathbf{P}_i) &= \gamma\Delta\mu_i\,,\\
\mu_i := \frac{\delta\mathcal{F}}{\delta\phi_i} &= \frac{1}{Ca}\Big(-\epsilon\Delta\phi_i + \frac{1}{\epsilon}W'(\phi_i)\Big)\\
&\quad + \frac{1}{In}\Big(B'(\phi_i)\sum_{j\neq i} w(\phi_j) + w'(\phi_i)\sum_{j\neq i} B(\phi_j)\Big)\\
&\quad + \frac{1}{Pa}\Big(-\frac{c_1}{2}\|\mathbf{P}_i\|^2 - \beta\nabla\cdot\mathbf{P}_i\Big)\,,\\
\partial_t\mathbf{P}_i + (v_0\mathbf{P}_i\cdot\nabla)\mathbf{P}_i &= -\frac{1}{\kappa}\mathbf{H}_i\,,\\
\mathbf{H}_i := \frac{\delta\mathcal{F}}{\delta\mathbf{P}_i} &= \frac{1}{Pa}\Big(-c_1\phi_i\mathbf{P}_i + c_1\|\mathbf{P}_i\|^2\mathbf{P}_i - \Delta\mathbf{P}_i + \beta\nabla\phi_i\Big)
\end{aligned}
$$

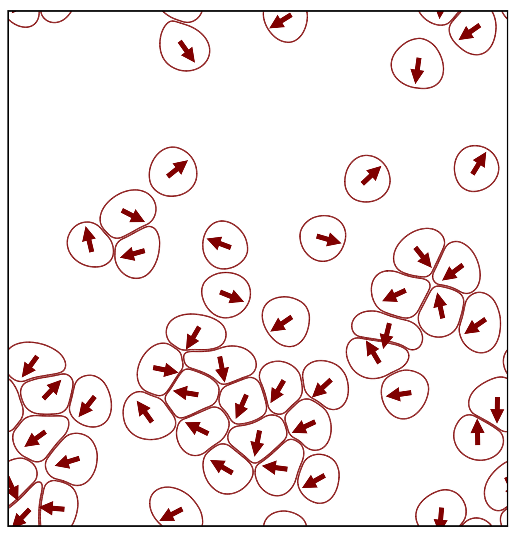
with the energy

$$
\begin{aligned}
\mathcal{F}[\{\mathbf{P}_i\},\{\phi_i\}] = \sum_i \frac{1}{Ca}\int_\Omega \frac{\epsilon}{2}\|\nabla\phi_i\|^2 + \frac{1}{\epsilon}W(\phi_i)\,\mathrm{d}\mathbf{x}\\
+ \frac{1}{In}\int_\Omega B(\phi_i)\sum_{j\neq i} w(\phi_j)\,\mathrm{d}\mathbf{x}\\
+ \frac{1}{Pa}\int_\Omega \frac{1}{2}\|\nabla\mathbf{P}_i\|^2 + \frac{c_1}{4}\|\mathbf{P}_i\|^2(-2\phi + \|\mathbf{P}_i\|^2) + \beta\mathbf{P}_i\cdot\nabla\phi_i\,\mathrm{d}\mathbf{x}
\end{aligned}
$$

and the short range interaction potential which can be computed from the phase field variables

$$
w(\phi_j) = \exp(-d_{\phi_j}^2/\epsilon^2), \quad \text{with} \quad d_{\phi_j}(\mathbf{x}) = -\frac{\epsilon}{\sqrt{2}}\ln\frac{1+\phi_j(\mathbf{x})}{1-\phi_j(\mathbf{x})}
$$



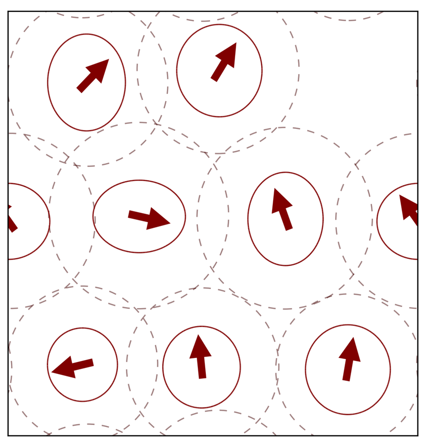


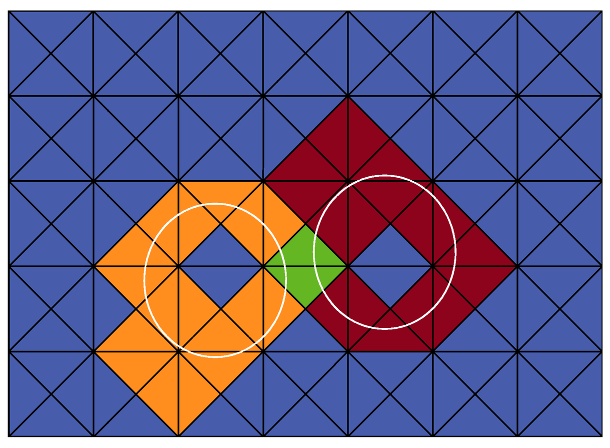
phase field of a single cell together with polarization field and net polarization and interaction of 48 cells

Implementational issues

AMDiS adaptive multidimensional simulations

reduce complexity resulting from interacting cells, introduce cut-off distance





only communicate ball center and radius and collect interface elements on coarse-grid to communicate

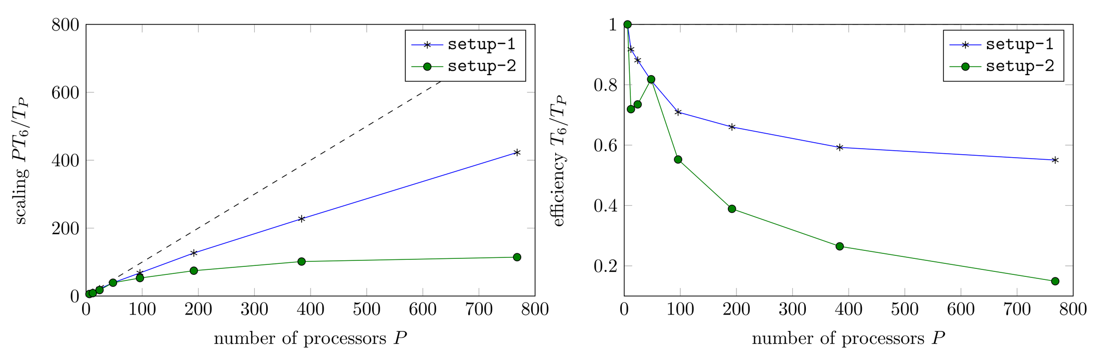
each phase field lives on its own adaptively refined mesh, only the coarse grids are common, communication of refinement by binary refinement tree

Scaling

two different setups for weak scaling

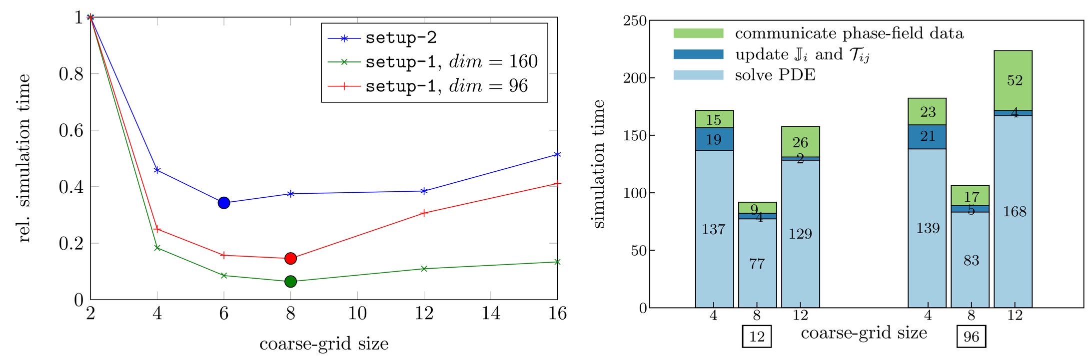
setup 1 – fixed size

setup 2 – fixed volume fraction



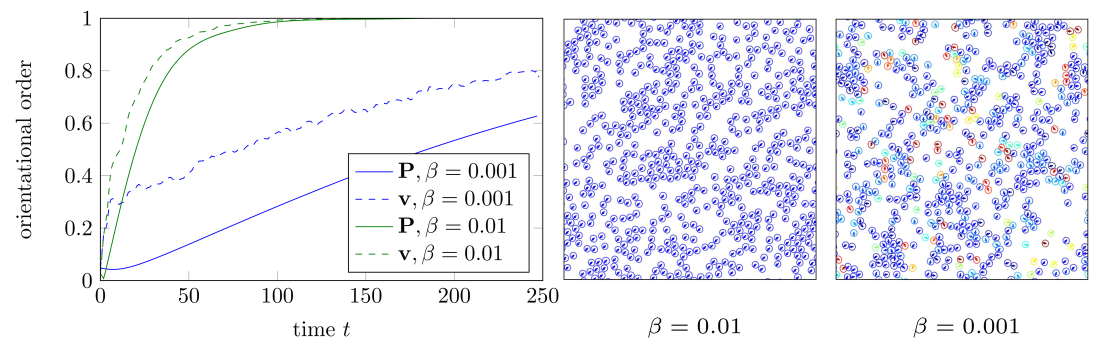
efficiency above 0.5 for setup 1 for up to 768 cells

efficiency depends on coarse grid level and can be maximized

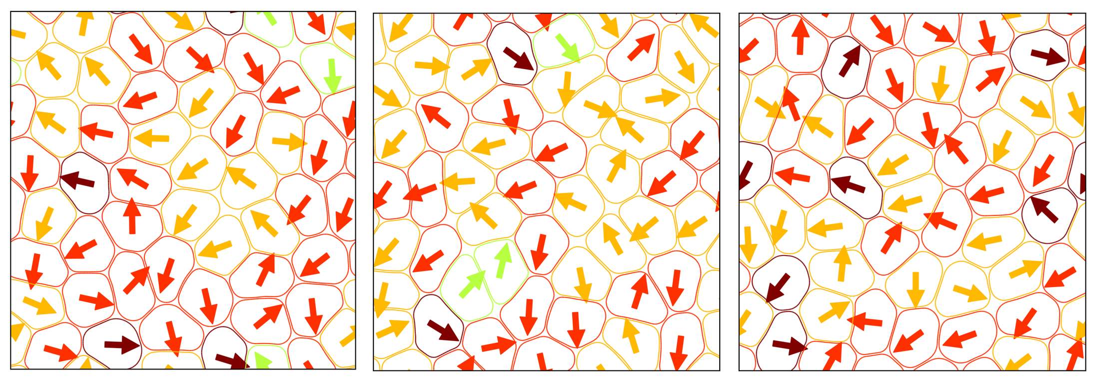


Physical results

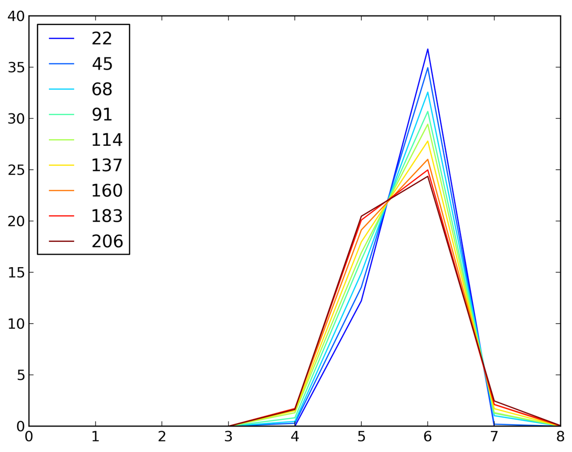
collective behavior resulting from cell-cell interaction, cluster formation and collective motion



high packing fraction leads to a model for tissue with characteristic neighbor distribution



color coding corresponds to the number of neighbors



Outlook

- consider other interaction potentials
- compare with discrete models, e.g. vertex model
- analyze liquid crystalline order in tissue
- compare with experimental data
- consider cell growth and division
- extension to three dimensions

References

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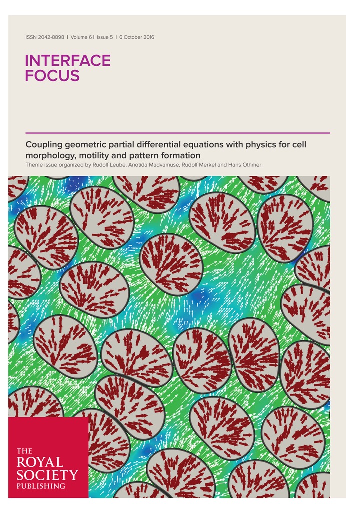

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Deutsche Forschungsgemeinschaft DFG

contact: Axel Voigt
e-mail: axel.voigt@tu-dresden.de