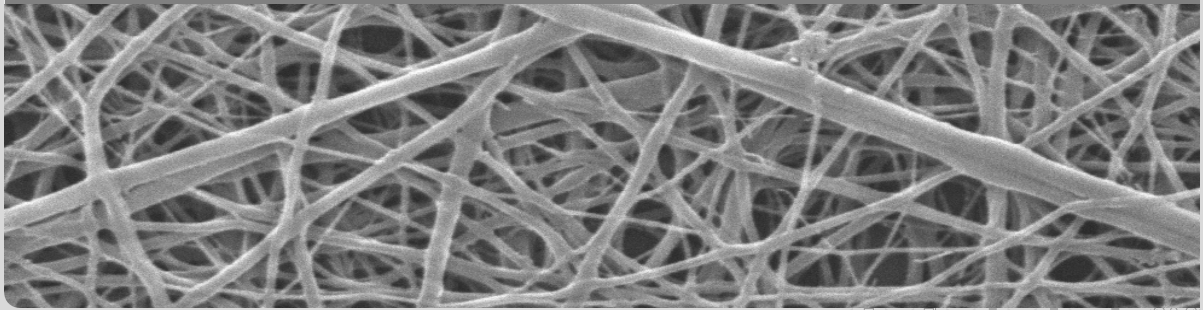
Karlsruhe Institute of Technology

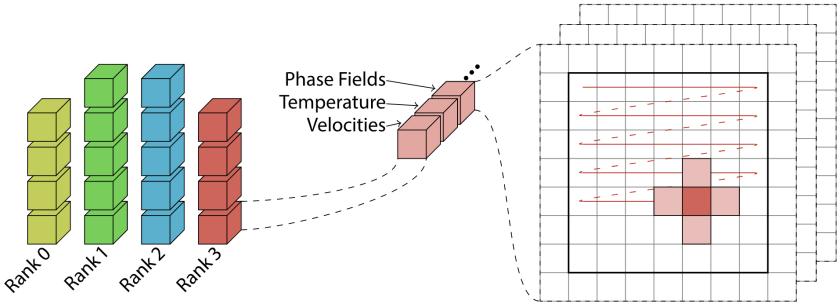
An ECM Model for Cells in Silico

Paul Brinkmeier

STEINBUCH CENTRE FOR COMPUTING



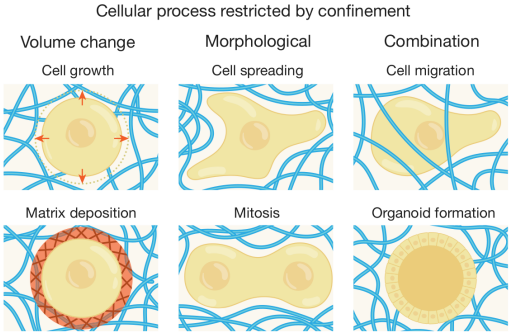
NAStJA: An MPI Stencil Code Solver



- CiS uses NAStJA under the hood
- NAStJA is a massively parallel stencil code solver

  $\Longrightarrow$ CiS extensions should be stencils

ECM Viscoelasticity: A Factor in Cell Behavior



- Collagen networks in the ECM mechanically restrict cells
- Collagen networks are *viscoelastic*
- ECM viscoelasticity influences cell behavior

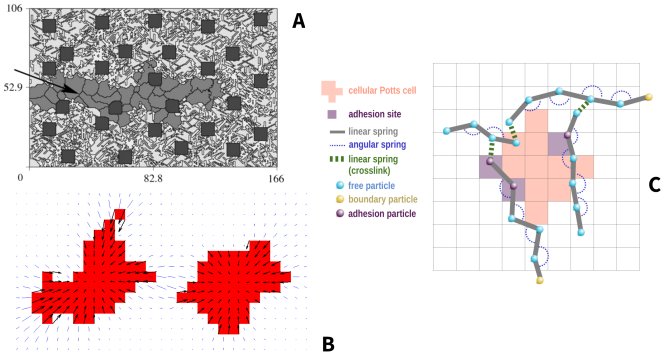
Modeling ECM Mechanics in CiS

How can we model ECM mechanics in CiS?

Two main requirements:

- Model exhibits viscoelastic properties
- Model can be implemented as a stencil in NAStJA

ECM Models in Literature



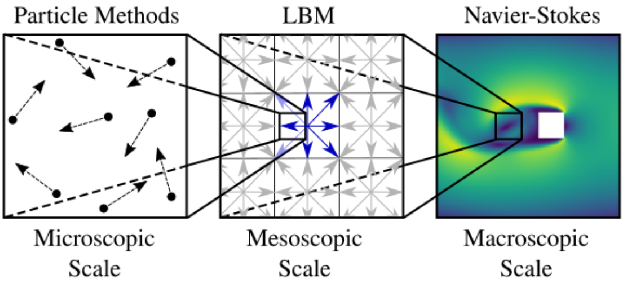
- A host of different ECM models exist
- Various foci, e.g. mechanics, growth factors
- Various approaches, e.g. FEM, Molecular Dynamics

My Approach

Two main requirements:

- Model exhibits viscoelastic properties
- Model can be implemented as a stencil in NAStJA

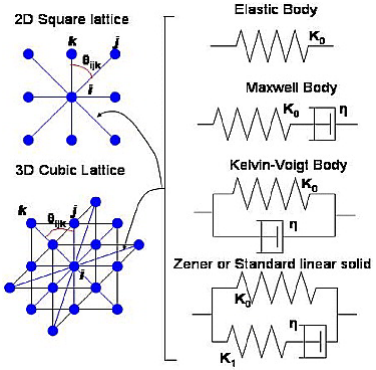
Lattice Boltzmann Method



$$f_i(\mathbf{x} + \mathbf{c}_i, t + 1) = f_i(\mathbf{x}, t) - \frac{1}{\tau}(f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t))$$

- Discretized particle velocities per lattice site
- Update Step: Streaming + Collision
- Usually used for hydrodynamics

Elastic Lattice Model



$$\mathbf{F}_{ij} = \mathbf{r}_{ij} K_{ij}(\mathbf{u}_{ij} \cdot \mathbf{x}_{ij}) + \frac{c\mathbf{u}_{ij}}{|\mathbf{x}_{ij}|^2} + \eta \mathbf{v}_{ij}$$

- A square lattice based discrete particle method
- Each lattice site represents a particle
- Particles are connected to neighbors by springs

My Approach

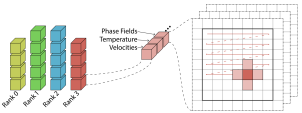
Two main requirements:

- Model exhibits viscoelastic properties ✓
- Model can be implemented as a stencil in NAStJA ✓

Challenges:

- How do we integrate the model with the CPM?
- How can it be implemented in NAStJA?
- How do we make it fast?

NAStJA: An MPI Stencil Code Solver



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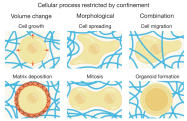
ECM Viscoelasticity: A Factor in Cell Behavior



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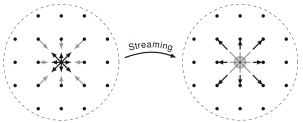

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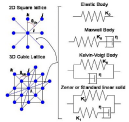

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