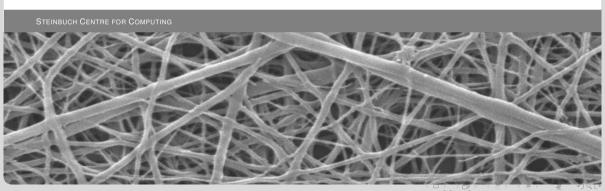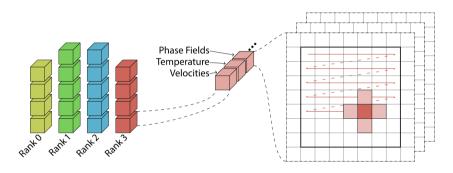# An ECM Model for Cells in Silico

Paul Brinkmeier

NAStJA: An MPI Stencil Code Solver
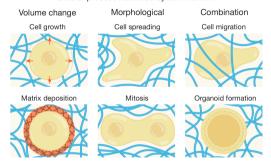

- CiS uses NAStJA under the hood
- NAStJA is a massively parallel stencil code solver
  $\implies$ CiS extensions should be stencils

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ECM Viscoelasticity:
A Factor in Cell Behavior

Cellular process restricted by confinement

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

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Modeling ECM Mechanics in CiS

How can we model ECM mechanics in CiS?
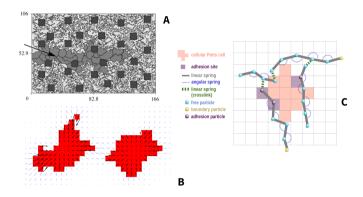
Two main requirements:

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

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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
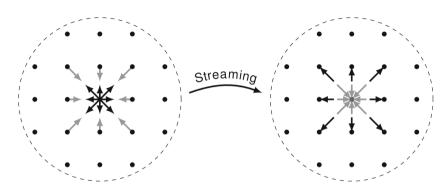
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My Approach

Two main requirements:

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

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Lattice Boltzmann Method

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

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Elastic Lattice Model

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

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Implementation

- Starting point: NAStJA + CiS
- Benchmark different implementations against each other
    - CPU
    - Vectorized
    - GPU
- Optimize for
    - Scaling behavior
    - Wall clock time
    - etc.

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NAStJA: An MPI Stencil Code Solver

Phase Fields, Temperature, Velocities

Rank 0, Rank 1, Rank 2, Rank 3

- CiS uses NAStJA under the hood
- NAStJA is a massively parallel stencil code solver
  $\implies$ CiS extensions should be stencils

ECM Viscoelasticity: A Factor in Cell Behavior

Cellular process restricted by confinement

Volume change / Cell growth   Morphological / Cell spreading   Combination / Cell migration

Matrix deposition   Mitosis   Organoid formation

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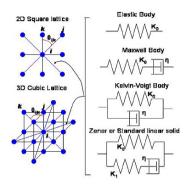
Lattice Boltzmann Method

Streaming

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

Elastic Lattice Model

2D Square lattice   Elastic Body

3D Cubic Lattice   Maxwell Body   Kelvin-Voigt Body   Zener or Standard linear solid

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