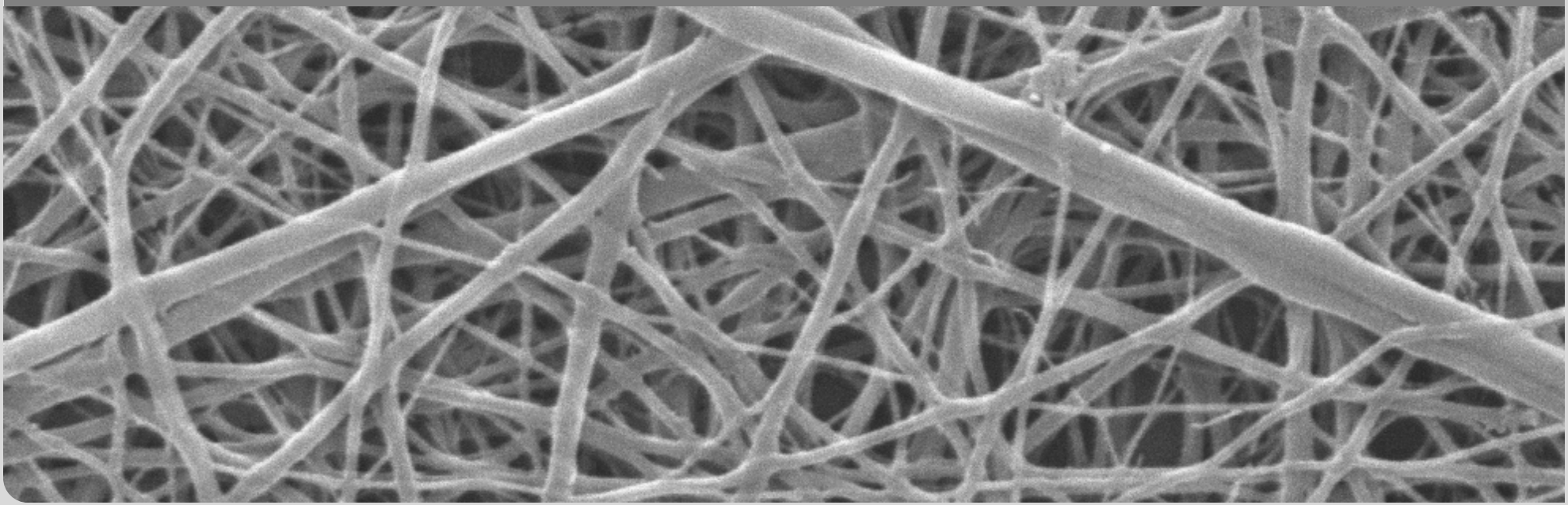
Karlsruhe Institute of Technology

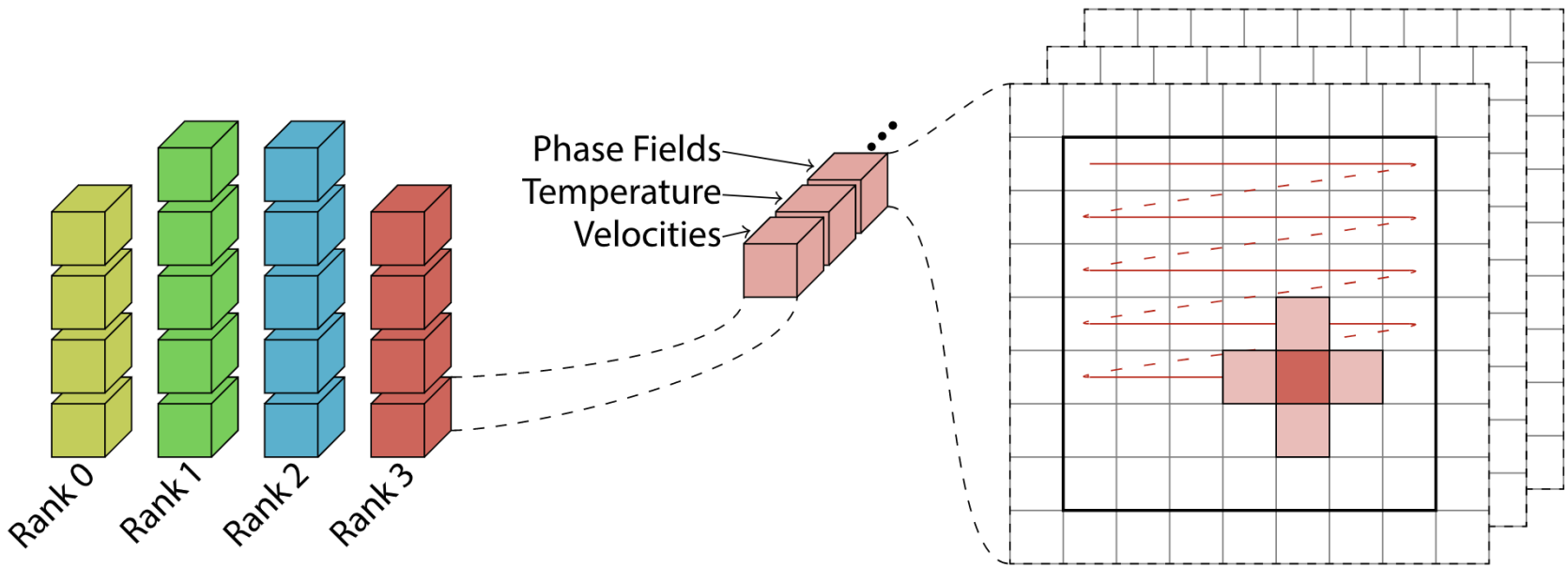
An ECM Model for Cells in Silico

Paul Brinkmeier

STEINBUCH CENTRE FOR COMPUTING

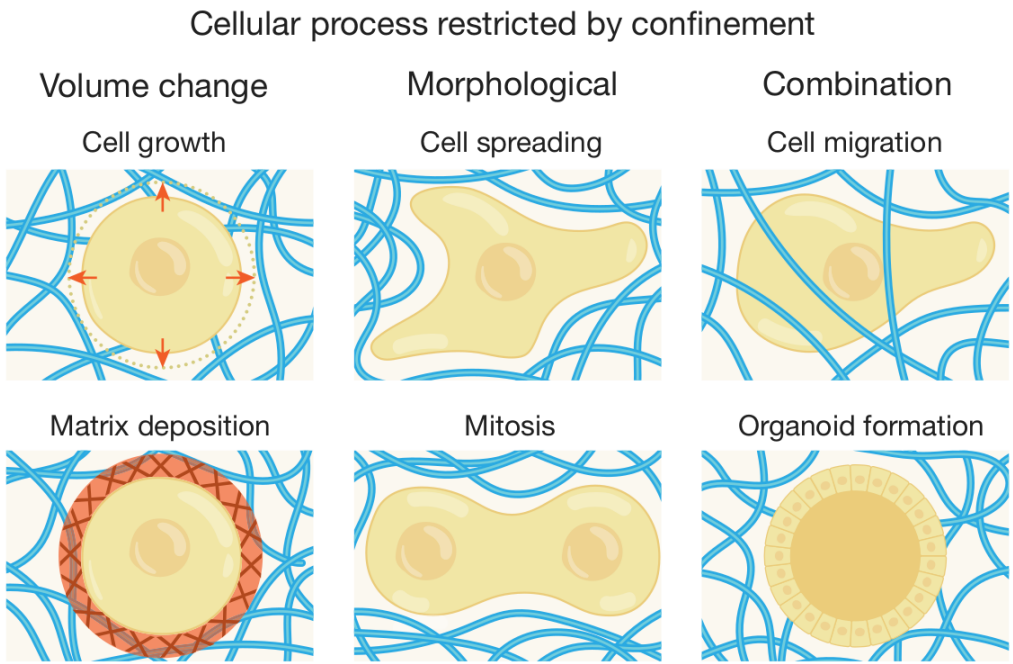


NAStJA: An MPI Stencil Code Solver



- 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

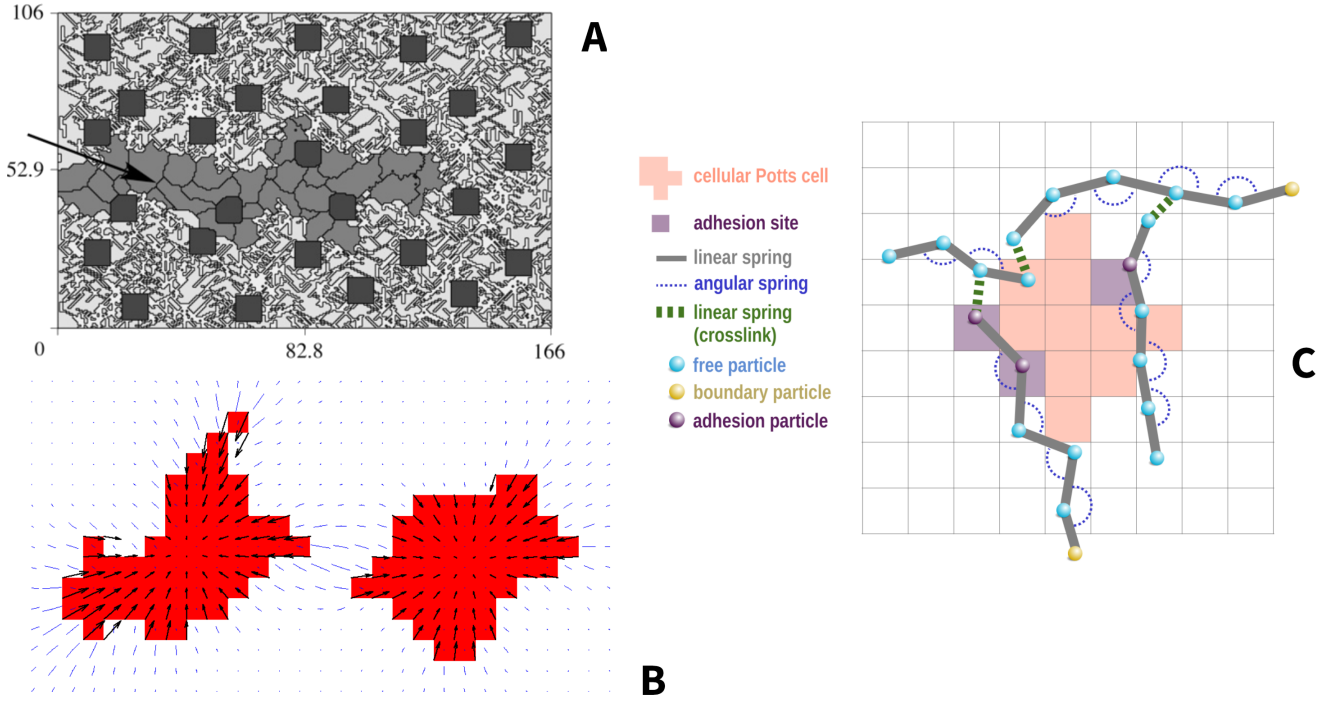
Modeling ECM Mechanics in CiS

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



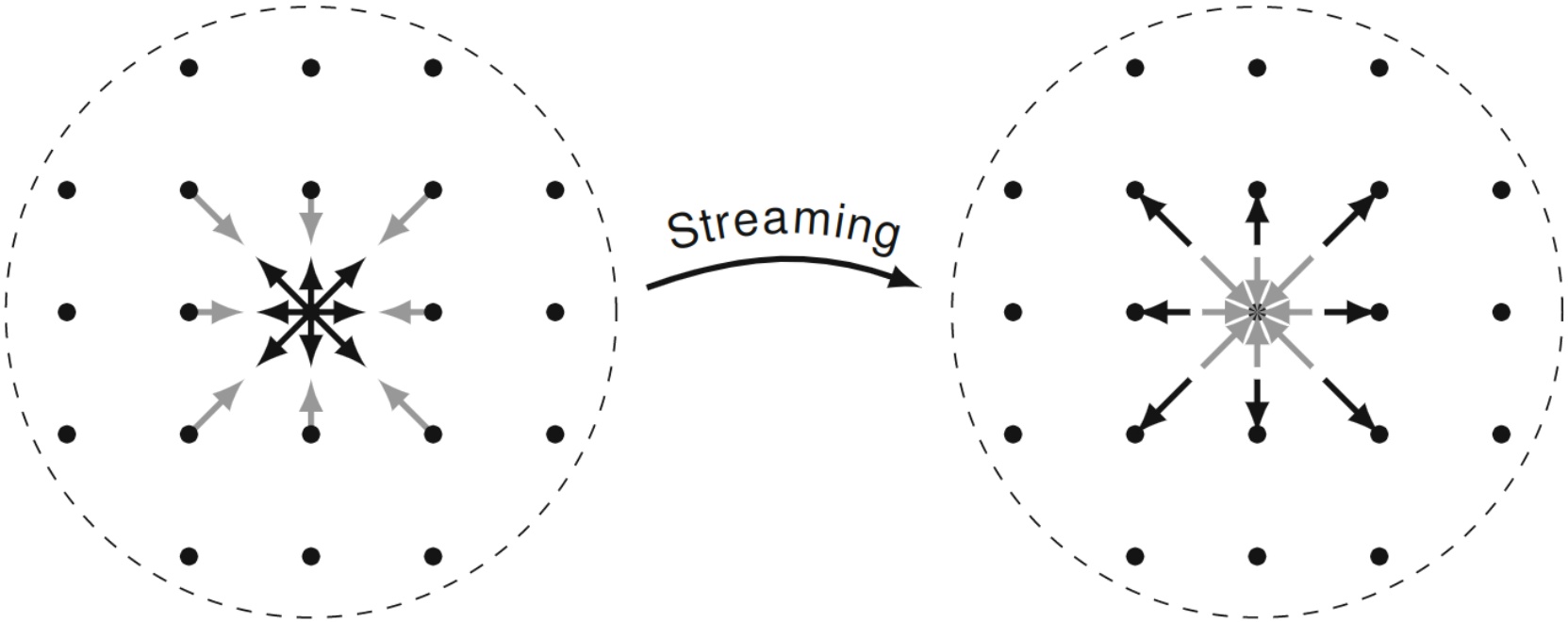
- A host of different ECM models exist
- Various foci, e.g. mechanics, growth factors
- Various approaches, e.g. FEM, Molecular Dynamics
- But: So far no approach is suitable as a stencil

My Approach

Two main requirements:

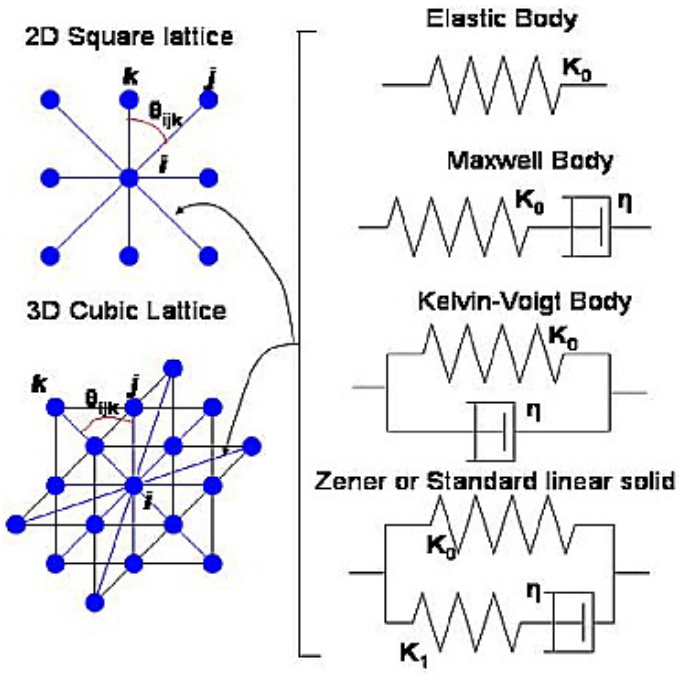
- Model exhibits viscoelastic properties
- Model can be implemented as a stencil in NAStJA

Lattice Boltzmann Method



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

Elastic Lattice Model

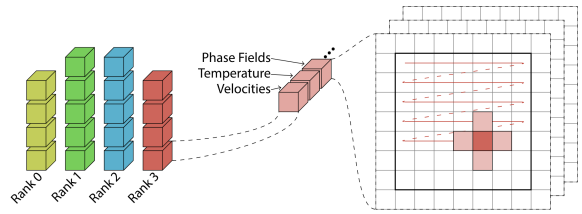


- A square lattice based discrete particle method
- Each lattice site represents a particle
- Particles are connected to neighbors by springs

Implementation

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

NAStJA: An MPI Stencil Code Solver



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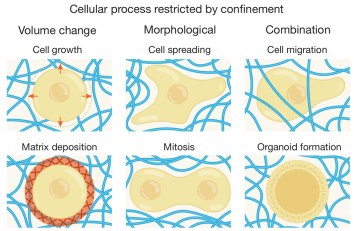

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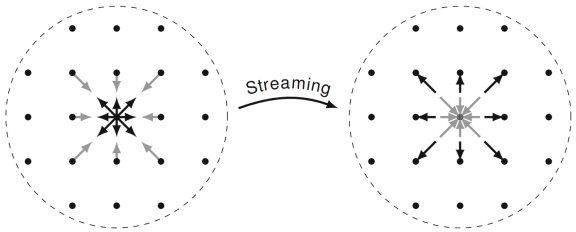

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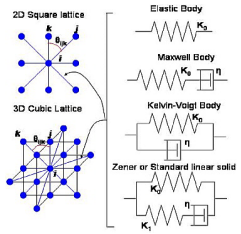

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