MFBM-CT06

Methods for Biological Modeling – Subgroup Contributed Talks

- **Miroslav Phan ETH Zurich, Department of Biosystems Science and Engineering, Basel, Switzerland**
  A Rejection Based Gillespie Algorithm for non-Markovian Stochastic Processes with Individual Reactant Properties
- **Elba Raimundez University of Bonn**
  Efficient sampling by marginalization of scaling parameters for mechanistic models with relative data
- **Aden Forrow Mathematical Institute, University of Oxford**
  Learning stochastic dynamics with measurement noise
- **Marco Berghoff Karlsruhe Institute of Technology**
  Cells In Sillico – Parallel Tissue Development Simulation

This session will be recorded and made available on the SMB 2021 website for up to a week after the conference concludes, unless a speaker has previously expressed that they wish not to be recorded.
We invite non-speakers to turn off their cameras if they wish and we ask all non-speakers to mute their microphone.
If you have a question for the speaker, please either type it in the chat or wait until the Q&A time after the presentation to ask your question live using the 'Raise you hand' reaction.

Cells In Sillico – Parallel Tissue Development Simulation

Steinbuch Center for Computing – Scientific Computing & Mathematics

Marco Berghoff | June 16th | virtual SMB 2021

High-performance Computing
How to Increase the Performance

- Reality/Experiments
- Physical Parameter
- Mathematical Model

- Numerical Scheme
- Application Program
- Parallel Computing (MPI, …)
- Hardware Architecture

- First group is hardly application-driven.
- Second group is computational performance-driven.
- Interdisciplinary collaboration with Jakob Rosenbauer (Alexander Schug's Lab)

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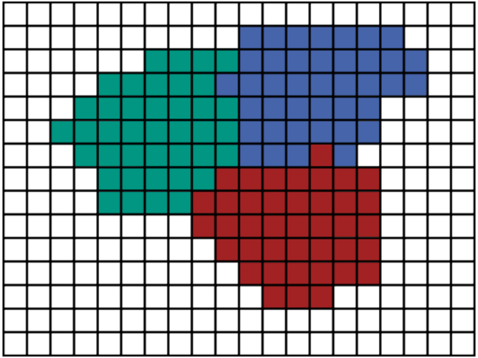
In this talk

- Tissue Development Model
- Node/single core performance
- Scalable communication
- Introduce *NAStJA* framework with *Cells in Silico*
- Applications

Cellular Potts Model
Introduction

- Grid based cell dynamic simulation
- François Graner and James Glazier (1992)
- Mostly applied in 2D, only few cells in 3D
- Energie states on $\mathcal{H}_{\text{CPM}}$
- Metropolis Monte Carlo acceptance of new states



$$\mathcal{H}_{\text{CPM}} = \lambda_{\text{v}} \sum_{i \in \Omega} \left(v(\varsigma_i) - V(\tau(\varsigma_i))\right)^2 + \lambda_{\text{s}} \sum_{i \in \Omega} \left(s(\varsigma_i) - S(\tau(\varsigma_i))\right)^2 + \sum_{i \in \Omega} \sum_{j \in N(i)} J_{\tau(\varsigma_i),\tau(\varsigma'_j)} \left(1 - \delta(\varsigma_i, \varsigma'_j)\right) + \cdots$$

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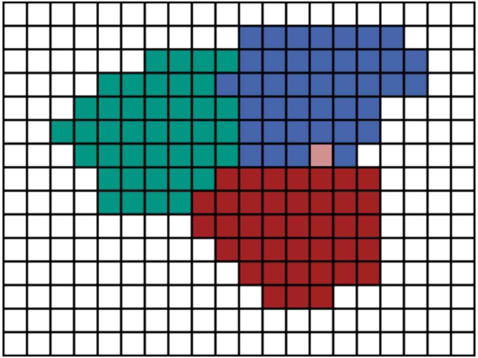

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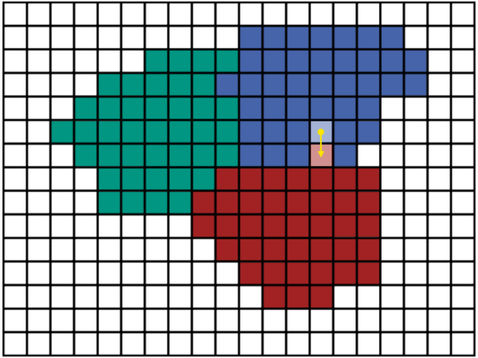

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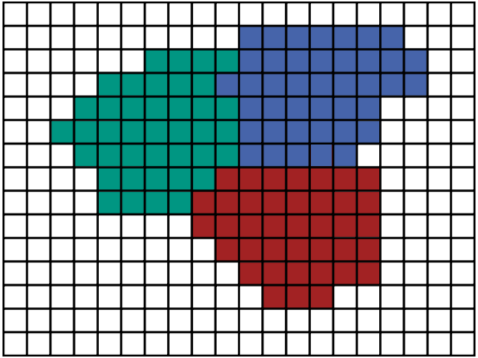

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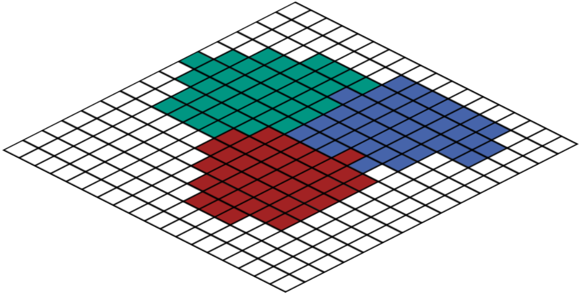
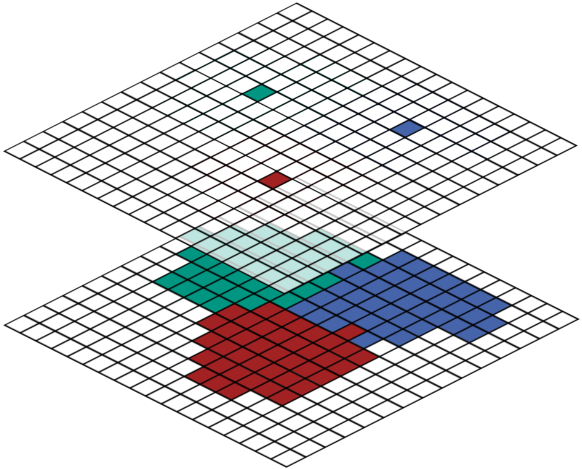
Multi Scale – Multi Level Model
From Microscale to Macroscale



- Celluar Potts Model (microscale)

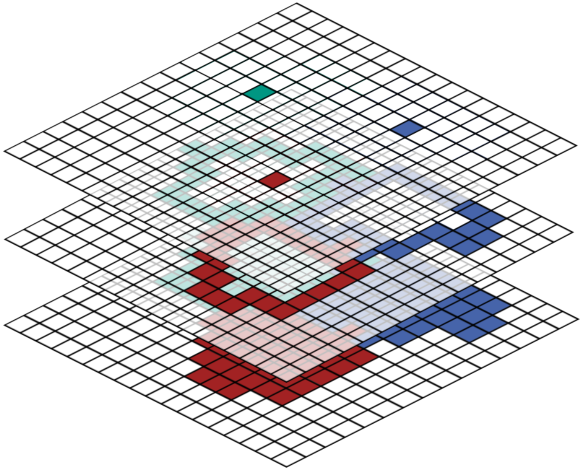
Multi Scale – Multi Level Model
From Microscale to Macroscale

- Agend-based (macroscale)
  - Properties on cell level
  - Signaling (drugs, nutrient)
  - Processing of signals
  - Cell divison
- Celluar Potts Model (microscale)

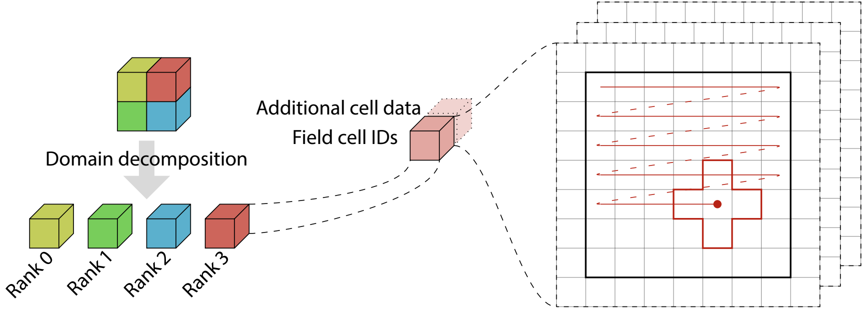


Multi Scale – Multi Level Model
From Microscale to Macroscale

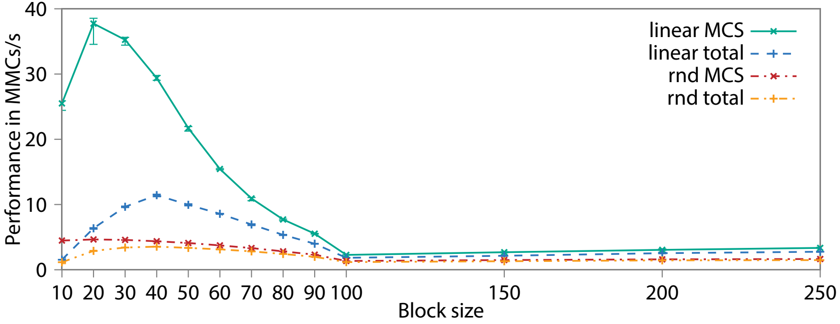
- Agend-based (macroscale)
  - Properties on cell level
  - Signaling (drugs, nutrient)
  - Processing of signals
  - Cell divison
- Diffusion (mesoscale)
  - Signals
  - According to surface
- Celluar Potts Model (microscale)



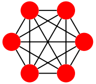
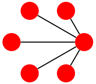
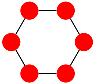
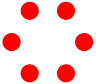
Parallelization using NAStJA
Spread Data and Computation



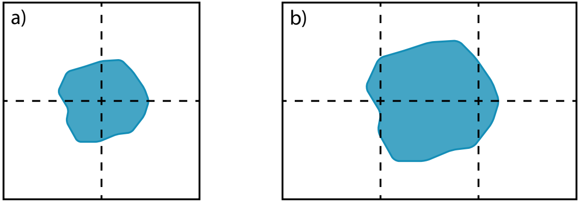
Results
Cache Optimization

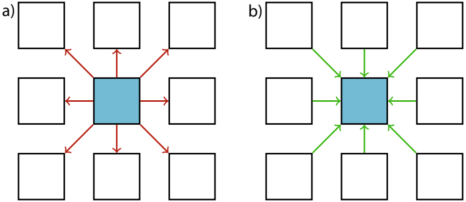


Scalable Parallel Communication
Overview

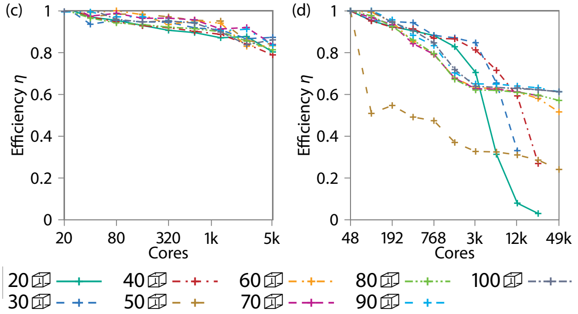
 All-to-All	$\mathcal{O}(N^2)$	matrix transpose, fast Fourier-transformation, residuum calculations
 One-to-All, All-to-One	$\mathcal{O}(N)$	master–worker, broadcasting
 Point-to-Point	$\mathcal{O}(1)$	halo exchange
 no communication	0	best communication (not HPC anymore)

Scalable Parallel Communication
Preconditions to Allow Point-to-point Communication





Results
Scalability on ForHLR II and JUWELS



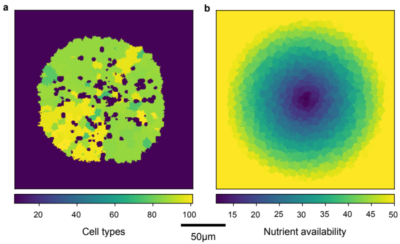
[Berghoff et al.: Cells in Silico – introducing a high-performance framework for large-scale tissue modeling, BMC Bioinformatics 2020]

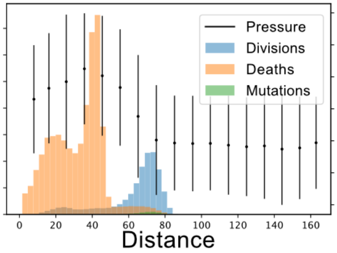
Application
Mutation and Evolution

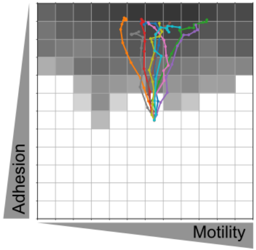
Karlsruhe Institute of Technology

Talk by Jakob Rosenbauer

In silico model of evolution in heterogeneous tumors and the influence of the microenvironment
in Mathematical Oncology (CT06-ONCO)

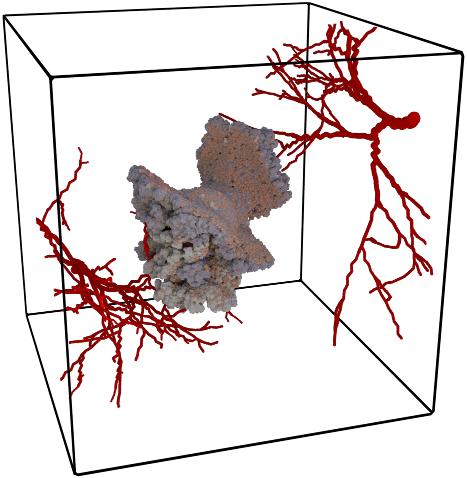


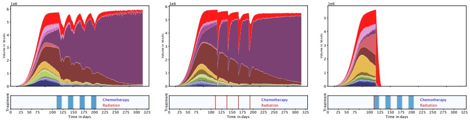




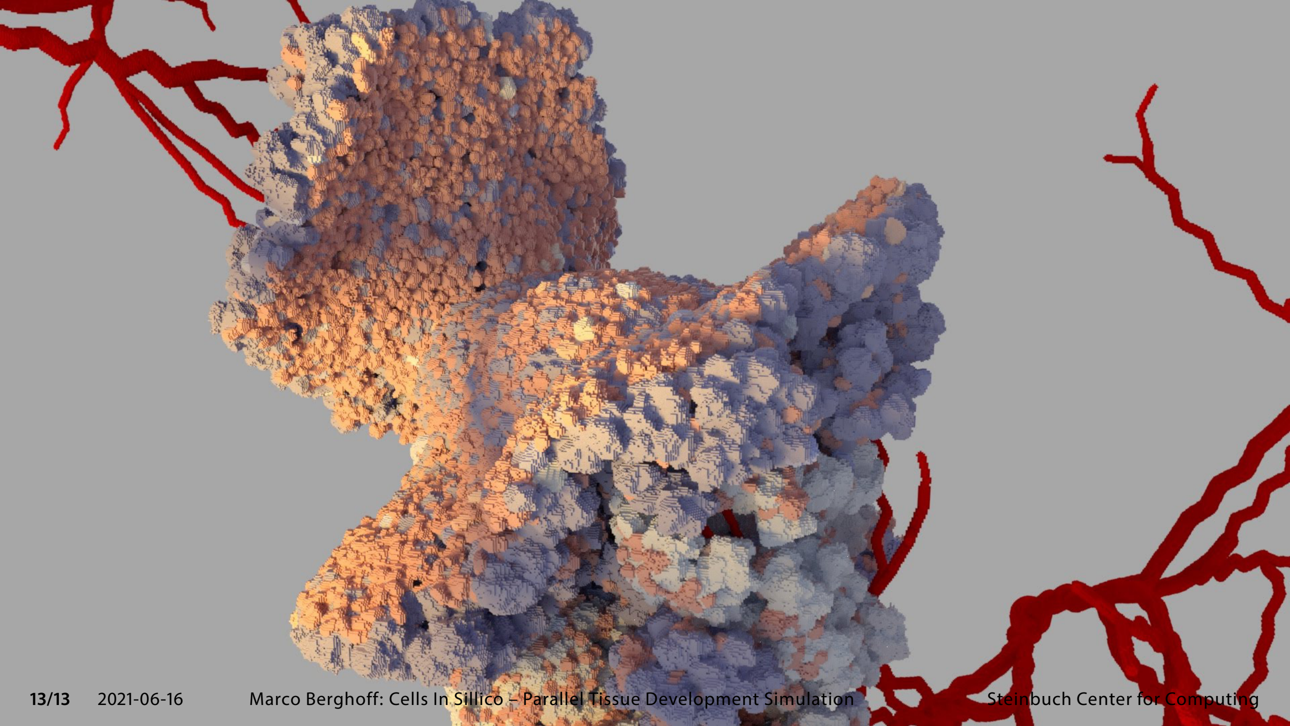
Application
Cancer Growth and Treatments

- 1000^3 Voxels
- ~ 1.5 mio Cells
- 24h 1000 cores simulation
- 1 mm^3 1 year real





[Rosenbauer, Berghoff, Schug: Emerging Tumor Development by Simulating Single-cell Events, bioRxiv 2020]



Take Home Message

- Cells in Silico is a NAStJA module for tissue development
- High-performance computing ready
- Modular
  - Energie functions
  - Signal functions
  - Treatments
  - …
- Input via config files (GUI in development)
- nastjaviewer for fast quasi 3D visualisation
- Paraview and python dataframe compatible for further analysis
- Open source and available under gitlab.com/nastja

Contact marco.berghoff@kit.edu or @NAStJAsolver