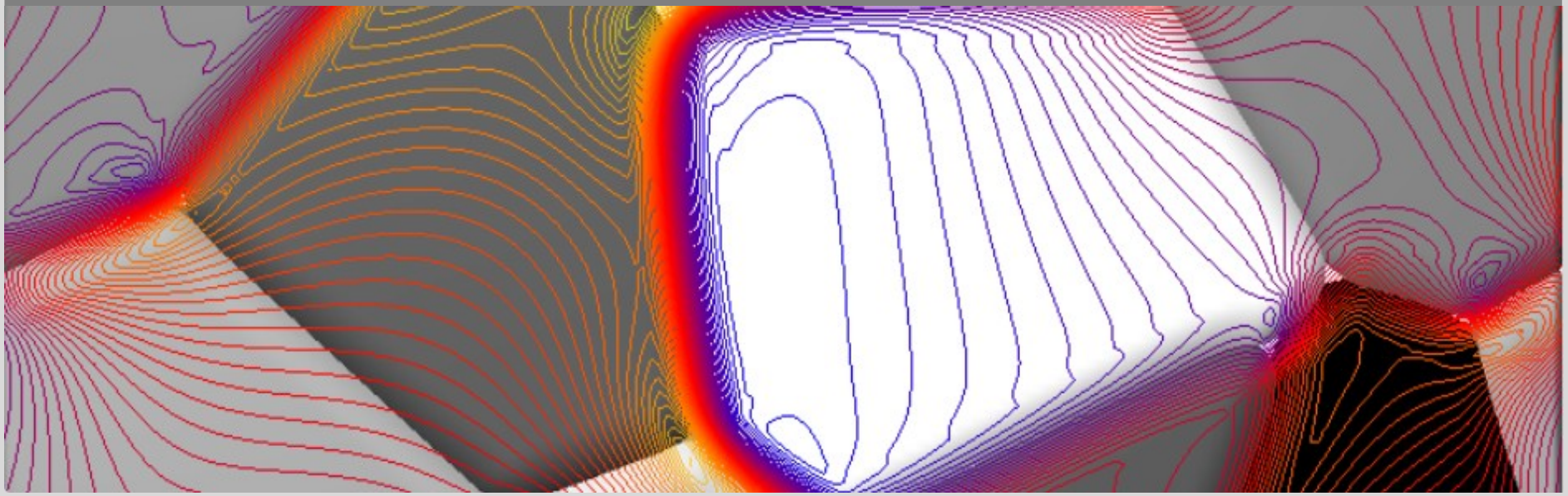
Karlsruher Institut für Technologie

Impulsvortrag: Phasenfeldmethode und High-Performance Computing

Michael Selzer

Institute of Applied Materials – Computional Materials Science (IAM-CMS)

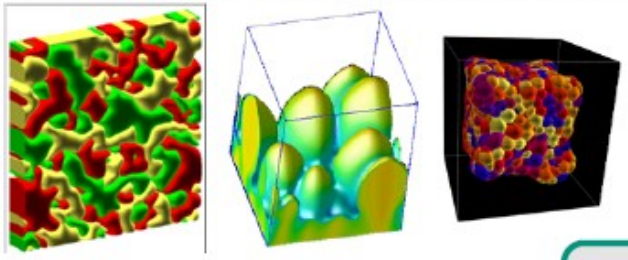


Overview: Microstructure Simulations

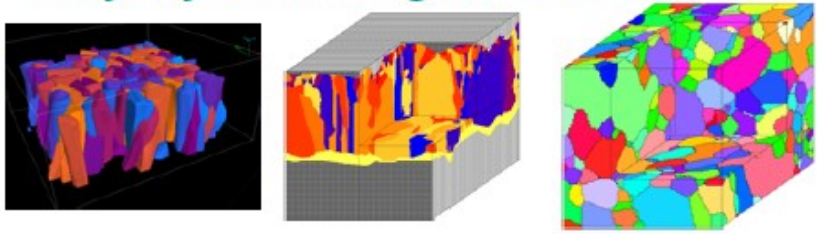
Britta Nestler and her group

Karlsruher Institut für Technologie

Solidification Microstructures

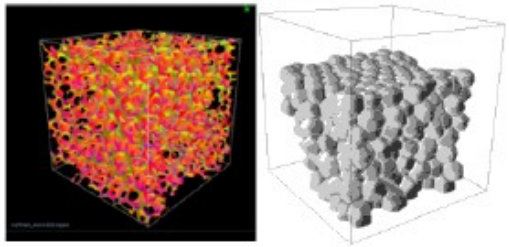


Polycrystalline grainstructures

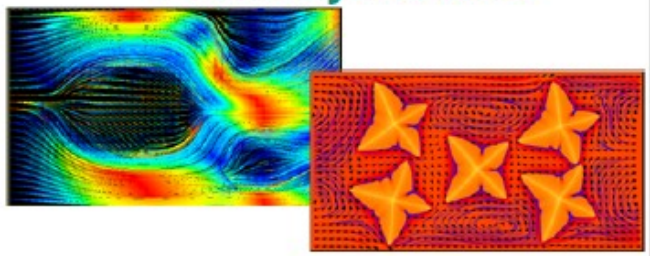


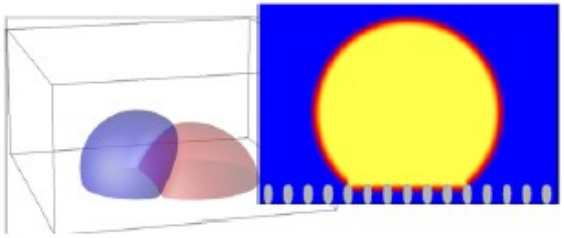
Microstructure simulations in material engineering

Porous structures

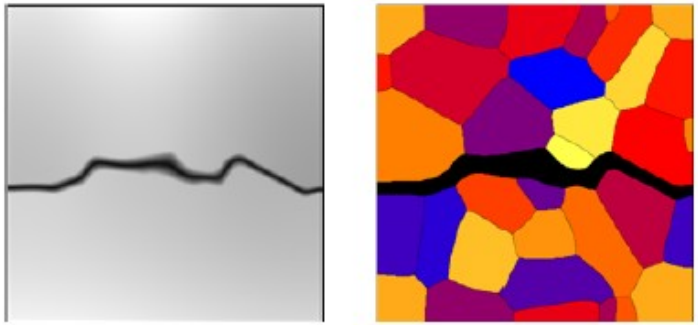


Fluid dynamics





Wetting at surfaces



Crack propagation in grain structures

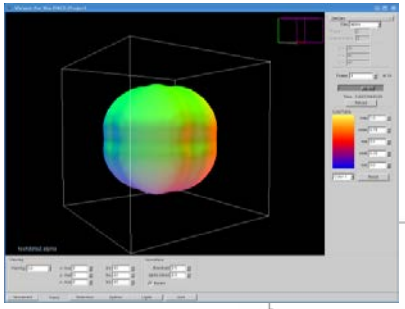
General workflow

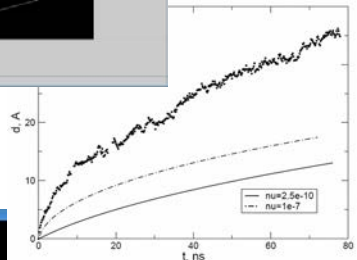
Model development → **Simulation** → **Visualization and data analyses**

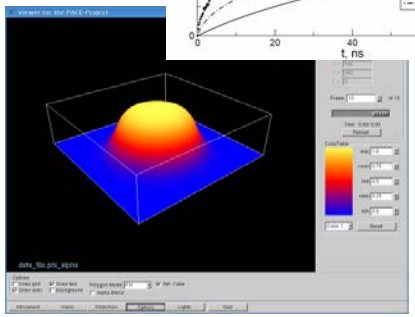
$$\frac{\partial e}{\partial t} = -\nabla \cdot \left(L_{00} \nabla \frac{1}{T} + \sum_{j=1}^{K} L_{0j} \nabla \left(\frac{-\mu_j}{T} \right) \right)$$

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \left(L_{i0} \nabla \frac{1}{T} + \sum_{j=1}^{K} L_{ij} \nabla \left(\frac{-\mu_j}{T} \right) \right)$$

$$\frac{\partial \phi_\alpha}{\partial t} = \varepsilon (\nabla \cdot a_{,\nabla \phi_\alpha} - a_{,\phi_\alpha}) - \frac{1}{\varepsilon} w_{,\phi_\alpha} - \frac{f_{,\phi_\alpha}}{T} - \lambda$$



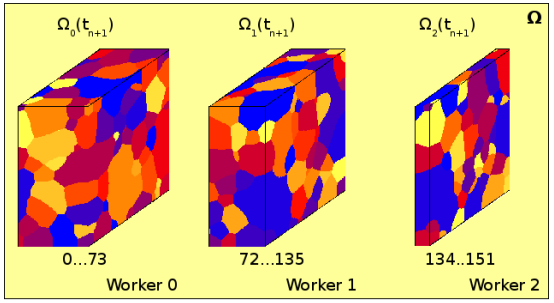




- High performance computing
- Vectorisation
- Model optimization

Pace3D – Parallel Algorithms for Crystal Evolution

- the Pace3D - package contains modules for the solution of various applications:
  - phase-field models for microstructure formations in multicomponent and multiphase materials
  - CFD solvers for modelling fluid flow processes based on the Navier-Stokes equations and on the Lattice-Boltzmann method
  - Solid Mechanics
  - Micromagnetism
  - Grand chemical potential, Grand elastic potential



- Implementation in C, C++ for Linux, > 600.000 l.o.c.
- simulations can be run sequentially or parallely using MPI and OpenMP on high performance computers
- performance-optimization of the software is achieved by adaptive meshes, computing time and memory saving algorithms, dynamical domain decomposition and data compression
- Framework for easy access of the pre- and postprocessing features
- Hugh package of pre- and postprocessing methods

Dokumentation des Softwareframeworks Pace3D

- Mehr als 600 Einstellmöglichkeiten
- Annotationsprache, die im Code Beschreibungen, Kommentare und physikalische Einheiten hinterlegt
- Generierung einer Benutzer-dokumentation aus den Annotationen
- Typsichere Benutzeroberfläche
- Latex-Dokumentationskonzept zur Komposition einzelner Dokumente zu einem Benutzerhandbuch

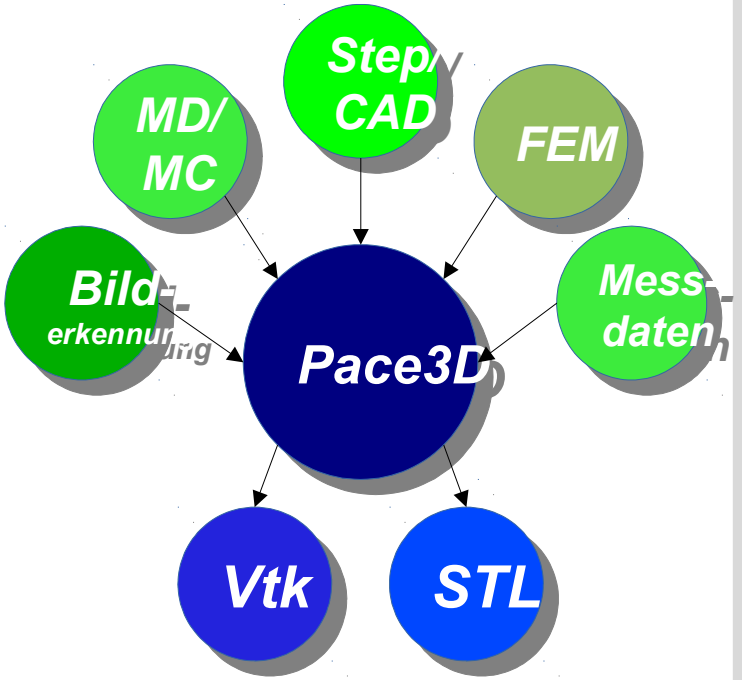
Titelseite des Benutzerhandbuchs

Interoperabilität von Pace3D

- Pace3D verfügt über die Möglichkeit verschiedene Formate zu verarbeiten.

- Es existieren Exporter für vtk und STL. Das Pace3D-Framework ermöglicht eine einfache und schnelle Entwicklung von weiteren Exportern.

- Pace3D kann auch verschiedene Formate importieren. Es existieren Importer für Molekulardynamikdaten (MD Daten), Monte-Carlo Daten (MC Daten), Calphad-Daten, Bild-erkennungsverfahren und Messdaten, z.B. Electron Backscatter Diffraction (EBSD) und Finite Element (FEM) Daten.

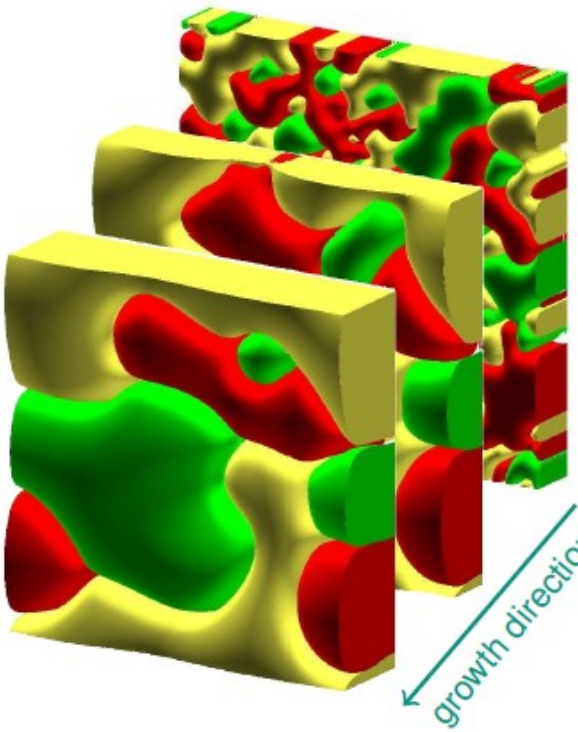


- Für CAD-Anwendungen (z.B. Pro-E) steht ein Importer für das Stepdatenformat zur Verfügung. Aus dem Gesamtumfang des Stepformats ist eine Untermenge mit den wichtigsten Elementen vorhanden.

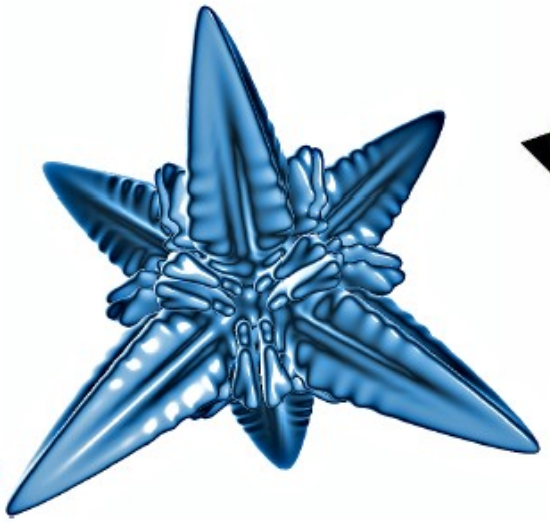
Phase-field model for phase transitions in multiphase and multi-component systems

Application to solidification

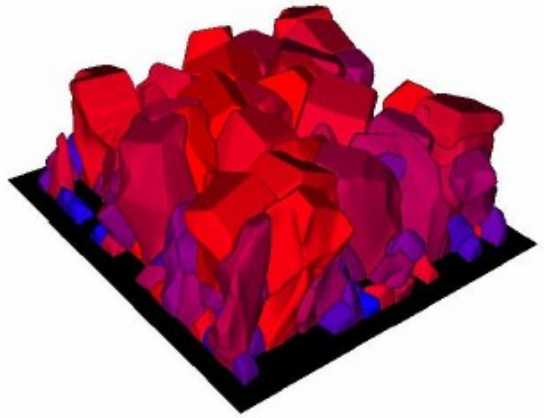
- 3D ternary eutectics
- liquid $\rightarrow \alpha + \beta + \gamma$
- f.e. Al-Cu-Ag



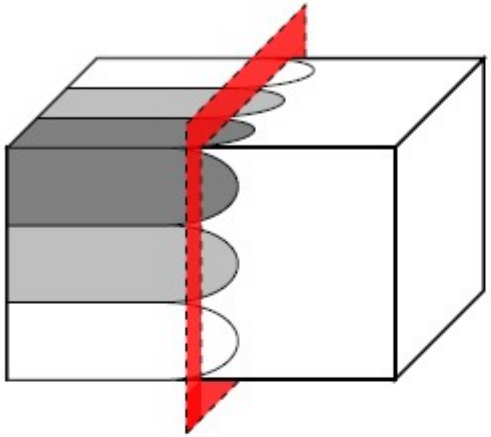
- Ni-dendrit
- $\Delta T \approx 250K$
- $3nm$ nucleus
- diameter $\approx 2\mu m$

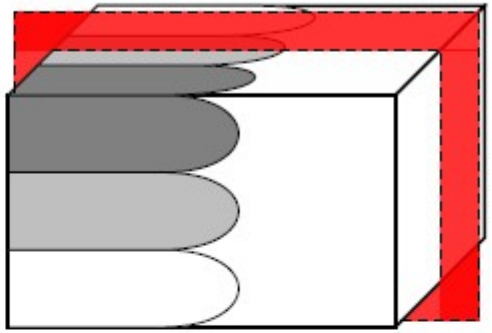


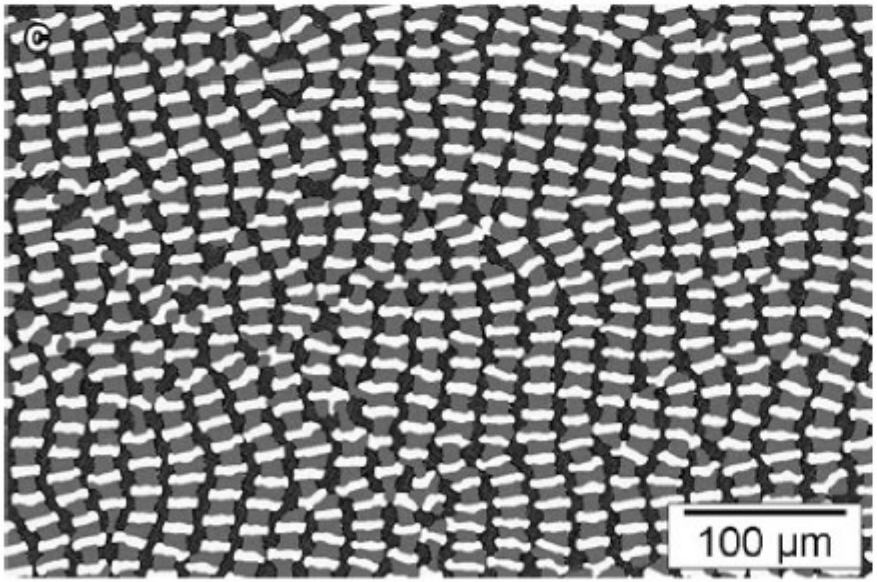
- Calcite crystals
- growth competition
- constant driving force

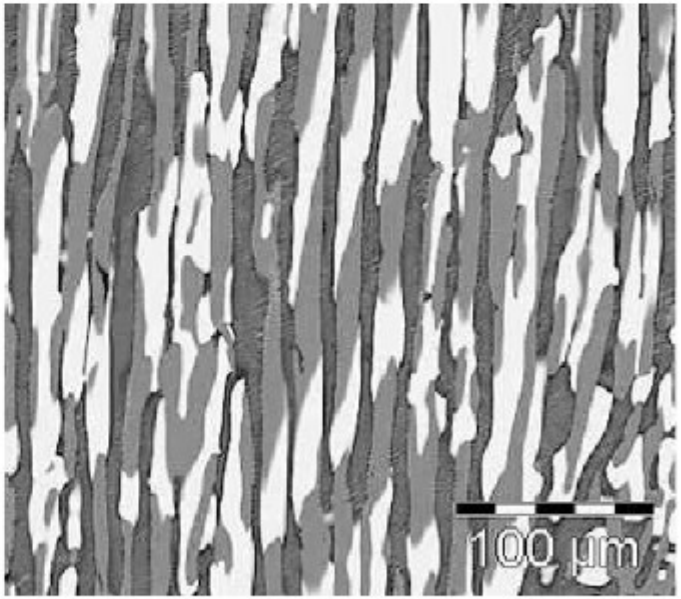


Experimental patterns









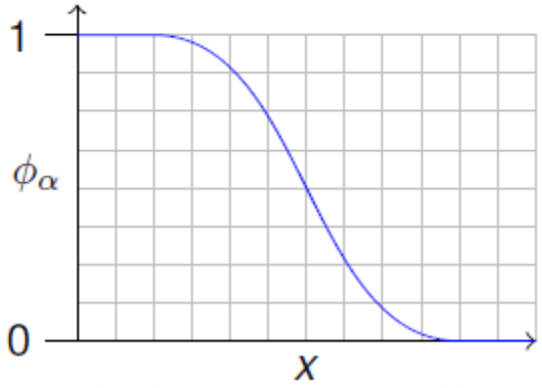
Dennstedt, A., & Ratke, L. (2012). Transactions of the Indian Institute of Metals, 65(6), 777-782.
Genau, A., & Ratke, L. (2012). International Journal of Materials Research, 103(4), 469-475.

Phase-field model derivation

- Grand chemical potential functional:

$$\Psi(\phi, \mu, T) = \int_\Omega \underbrace{\left(\epsilon a(\phi, \nabla\phi) + \frac{1}{\epsilon}\omega(\phi) \right)}_{\text{surface energy}} + \underbrace{\psi(\phi, \mu, T)}_{\text{bulk potential}} \, d\Omega$$

- phase-field vector $\phi = (\phi_1, \phi_2, ..., \phi_N)^T$
- order parameter ϕ_α represents the volume fraction of each phase
- volumetric interface at the surface
- smooth transition between the order parameters
- Allen-Cahn type variational differentiation of the functional
- $\rightarrow$ **no interface tracking needed**



Nestler, B., Garcke, H., & Stinner, B. (2005). Physical Review E, 71(4), 041609

Evolution equations for multiphases/components

$$\omega\varepsilon\partial_t\phi_\alpha = \varepsilon\left(\nabla\cdot a_{,\nabla\phi_\alpha}\left(\boldsymbol{\phi},\nabla\boldsymbol{\phi}\right) - a_{,\phi_\alpha}\left(\boldsymbol{\phi},\nabla\boldsymbol{\phi}\right)\right) - \frac{1}{\varepsilon}w_{,\phi_\alpha}\left(\boldsymbol{\phi}\right) - \Psi\left(T,\boldsymbol{\mu},\boldsymbol{\phi}\right)_{,\phi_\alpha} - \Lambda,$$

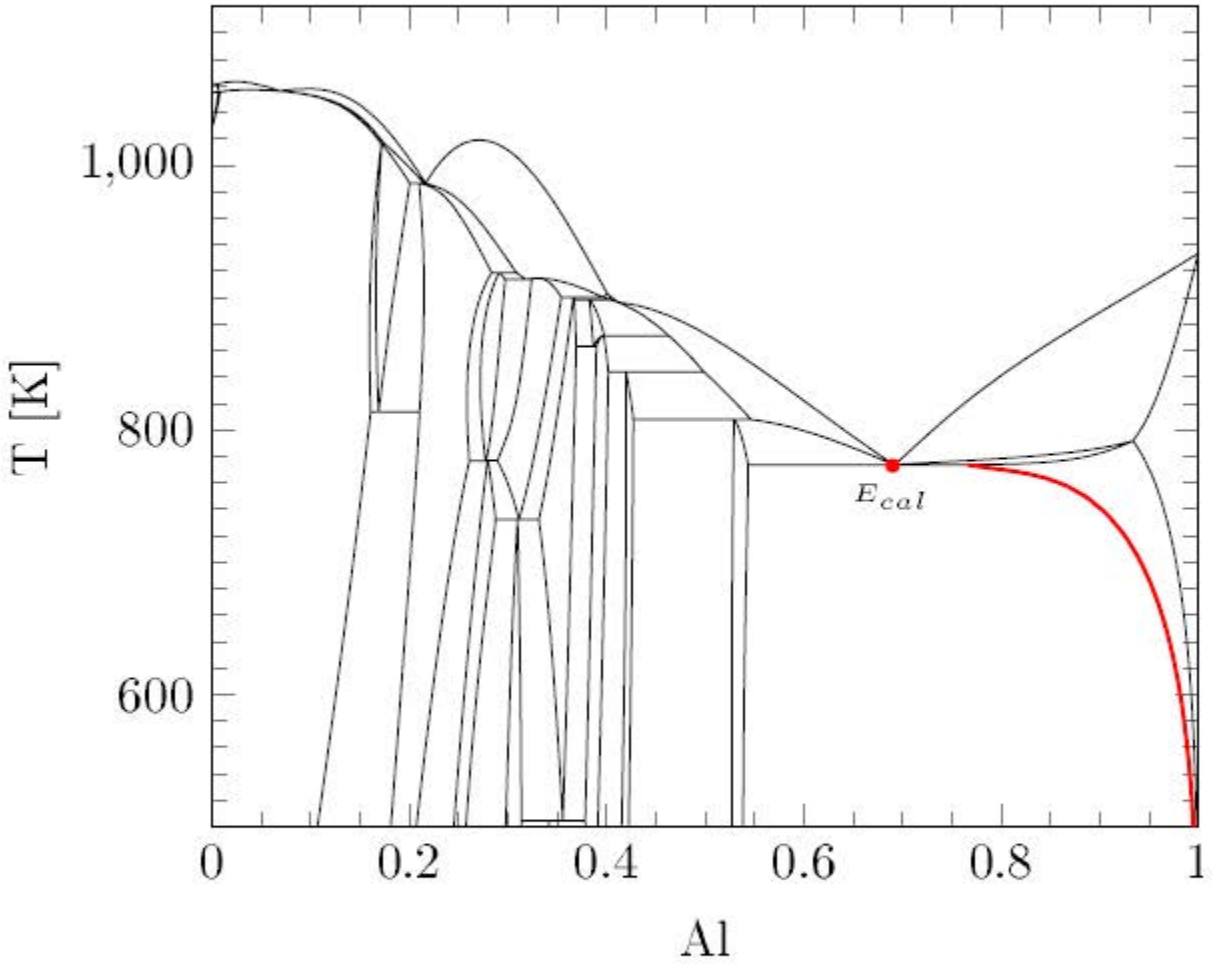
where Λ is the Lagrange parameter to maintain the constraint $\sum_{\alpha=1}^{N}\phi_\alpha = 1$ and ω is a relaxation constant.

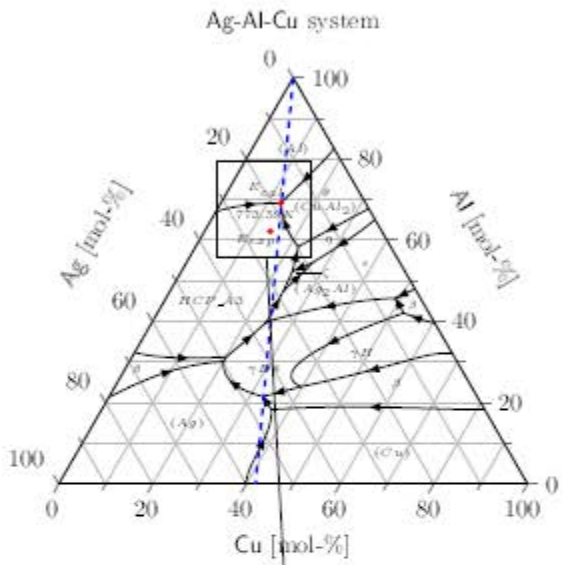
$$\left\{\frac{\partial\mu_i}{\partial t}\right\} = \left[\sum_{\alpha=1}^{N} h_\alpha\left(\boldsymbol{\phi}\right)\frac{\partial c_i^\alpha\left(\boldsymbol{\mu},T\right)}{\partial\mu_j}\right]_{ij}^{-1} \left\{\nabla\cdot\sum_{j=1}^{K-1} M_{ij}\left(\boldsymbol{\phi}\right)\nabla\mu_j - \sum_{\alpha}^{N} c_i^\alpha\left(\boldsymbol{\mu},T\right)\frac{\partial h_\alpha\left(\boldsymbol{\phi}\right)}{\partial t}\right\}$$

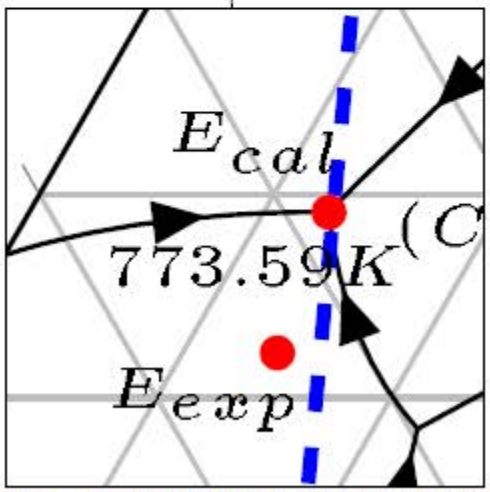
with mobilities $M_{ij}\left(\boldsymbol{\phi}\right) = \sum_{\alpha=1}^{N} M_{ij}^\alpha g_\alpha\left(\boldsymbol{\phi}\right), \quad M_{ij}^\alpha = D_\alpha^{ij}\frac{\partial c_i^\alpha\left(\boldsymbol{\mu}\right)}{\partial\mu_j}$

D_α^{ij}: Inter-diffusivities of the independent components

Phase diagram Al-Ag-Cu

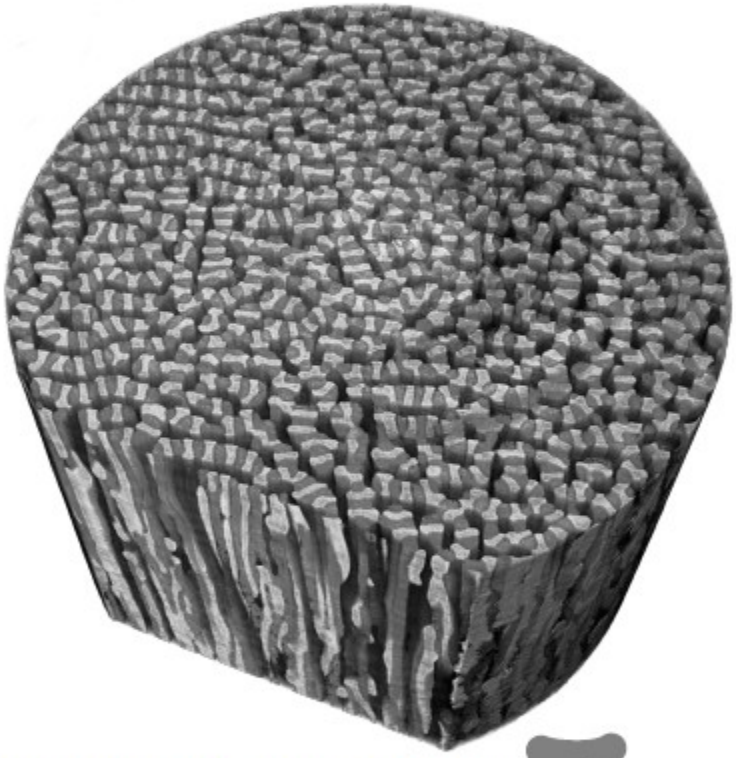




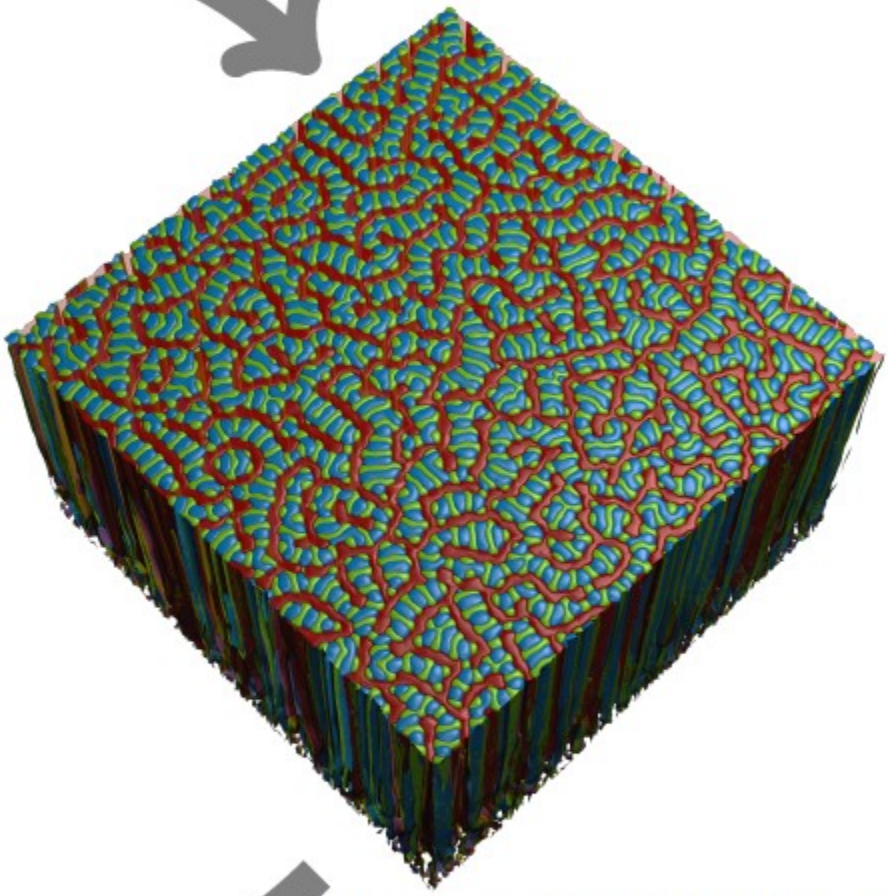


Data derived from: Witusiewicz, VT and Hecht, U and Fries, SG and Rex, S,Journal of alloys and compounds, 385, 2004 and 387, 2005

Microstructure prediction for Al-Ag-Cu

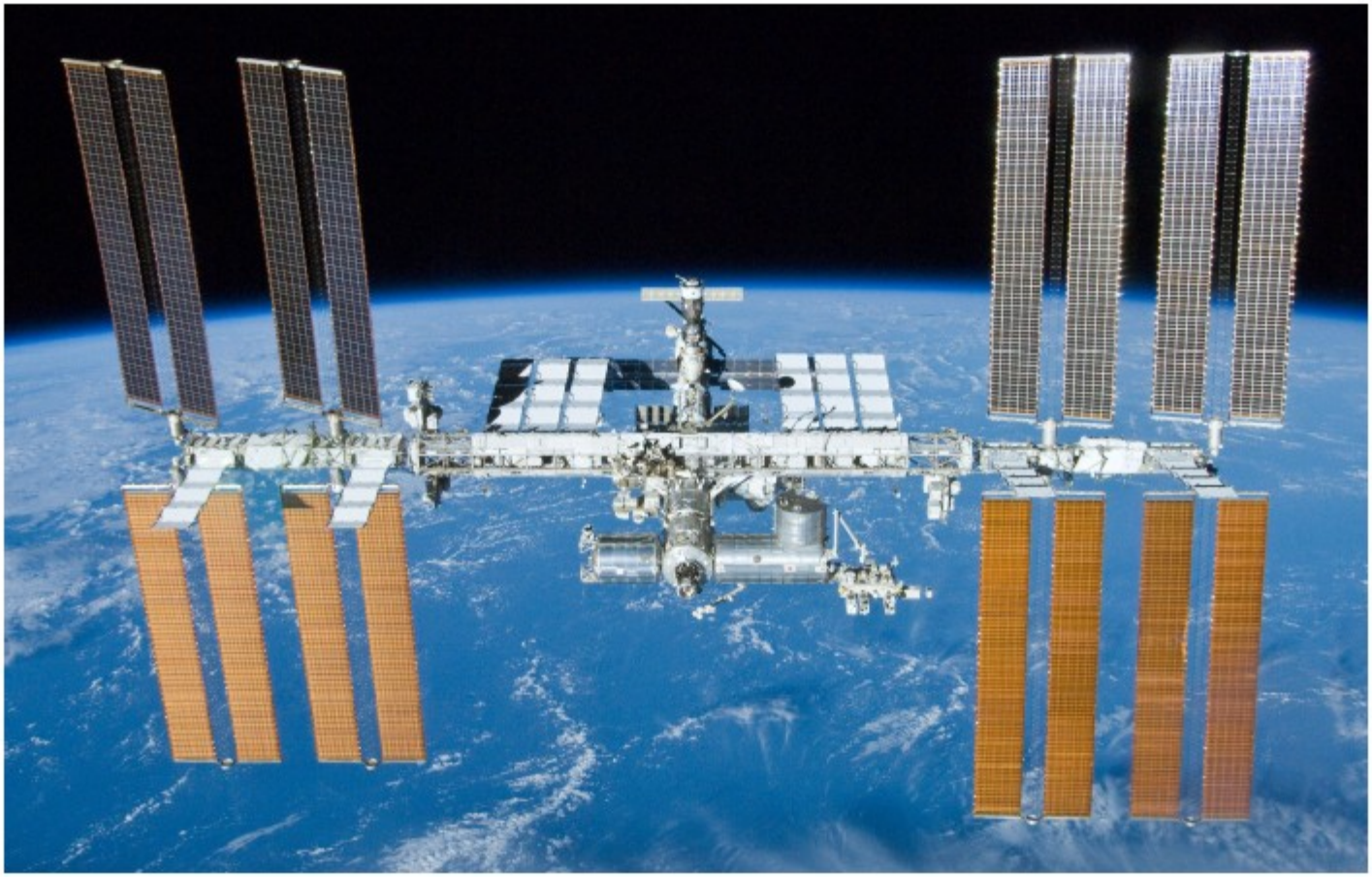


tomography of experimental Al-Ag-Cu structure of A. Dennstedt from DLR



3D phase-field simulation of Al-Ag-Cu of $2420 \times 2420 \times 1474$ voxels on 84700 cores

Disruptive technologies / HPC transforms



https://upload.wikimedia.org/wikipedia/commons/0/04/International_Space_Station_after_undocking_of_STS-132.jpg

Optimizations Layer

Parameter Layer

Model Layer

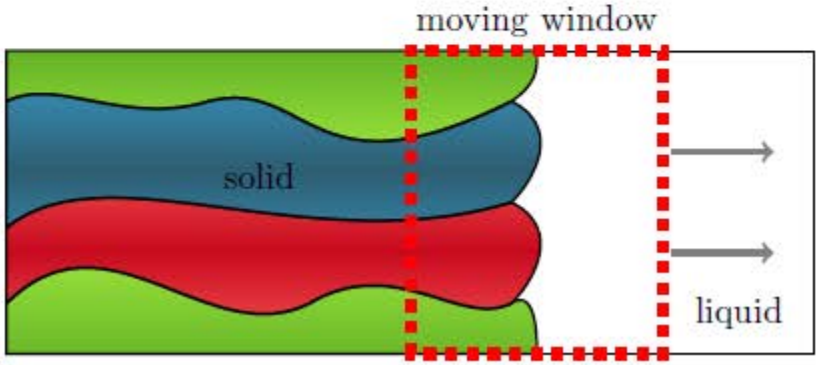
Algorithm Layer

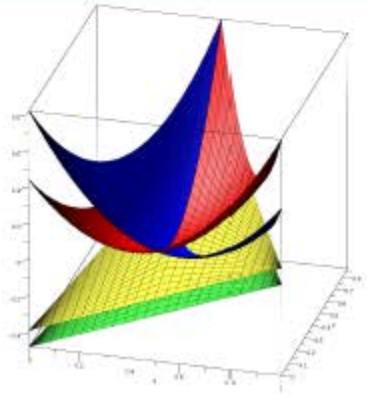
Hardware Layer

Optimizations I

Parameter Layer

- moving window technique
  - diffusion in solid is multiple magnitudes lower than in liquid
    ⟶solid diffusion neglected
- temperature diffusion magnitudes higher than in concentration
  ⟶analytic temperature gradient
- fitting of Gibbs energies with parabolic approach for Calphad database





Optimizations I

Model Layer

- simplifications due to defined setup
- classification of regions (solid, liquid, interface) $\longrightarrow$ skip terms
- classification of cells (number of active phases) $\longrightarrow$ skip terms
- pre-calculation of multiple required values (temperature depended terms)

Optimizations II

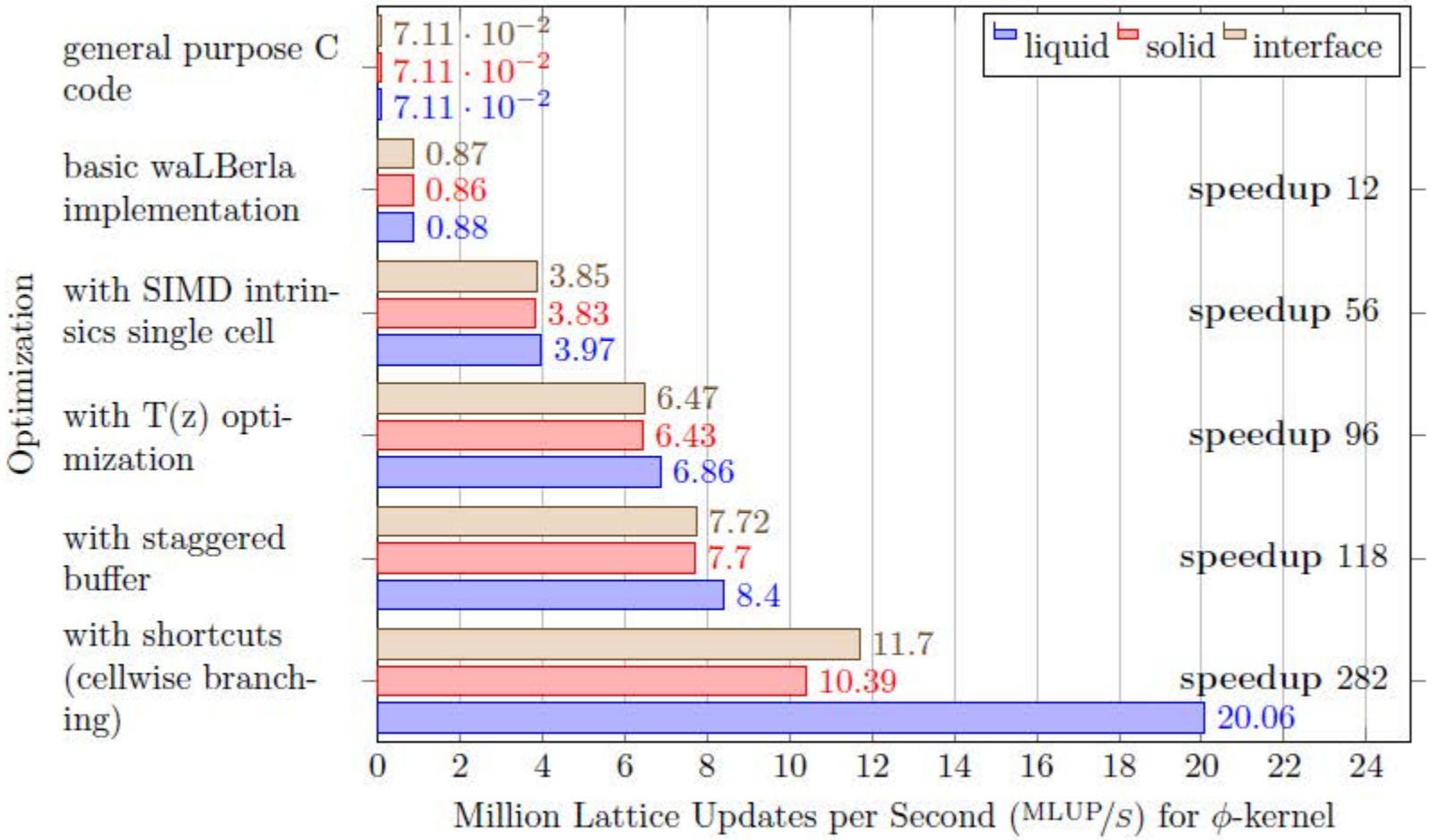
Algorithm Layer

- access patterns / stencils
- overlapping computation and communication
- block structured grid and static load balancing
- eliminate of common subexpressions / buffering techniques

Hardware Layer

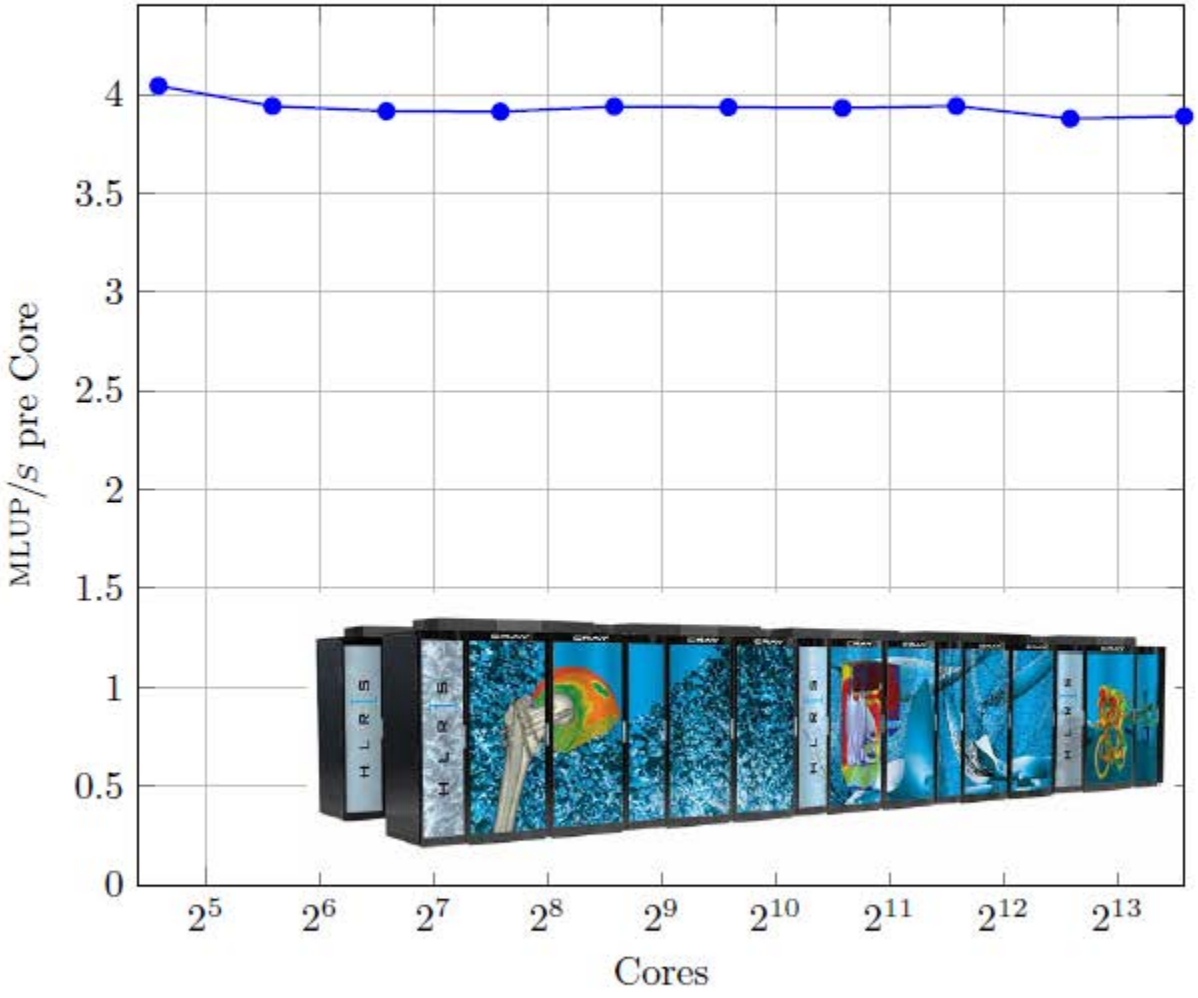
- explicit kernel SIMDification
- Memory layout (AoS vs. SoA)

Optimization results – ϕ-kernel – Hornet



- $60 \times 60 \times 60$ cells per block

Weak Scaling - Hornet / Hazel Hen

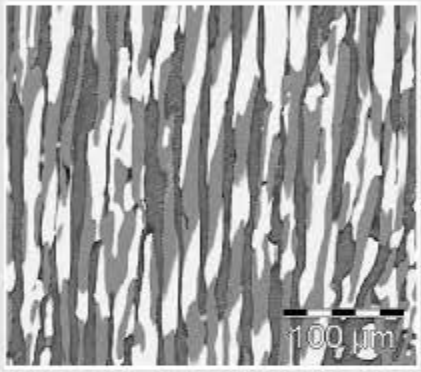


Bauer, Hötzer, Steinmetz, Jainta, Berghoff, Schornbaum, Godenschwager, Köstler, Nestler, and Rüde: SuperComputing, (2015)

Spiral growth in ternary systems

Motivation

- Assumption, 2D tilt leads to spirals in 3D



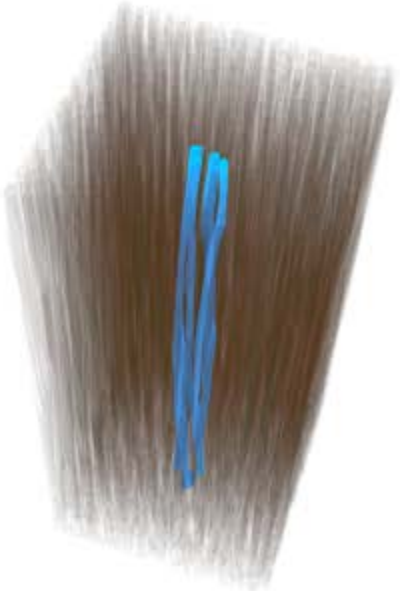
Genau, A., & Ratke, L. (2012). IJMR, 103(4), 469-475.

System parameters

- $940 \times 940 \times 2080$ cells
- system with largest 2D tilt angle

Result

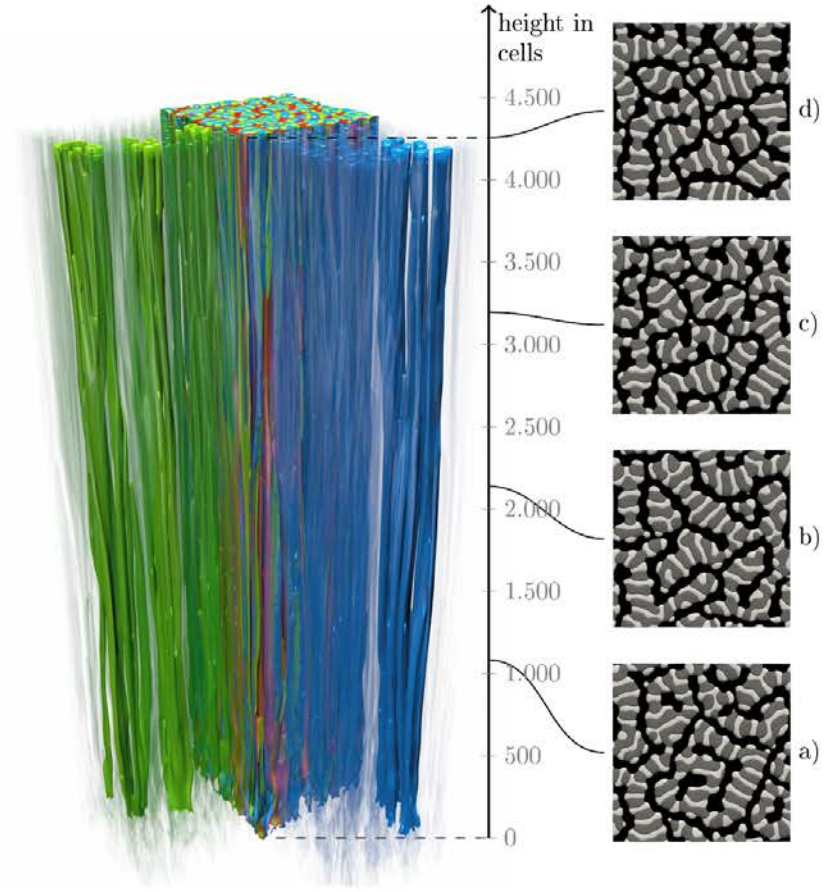
- multiple spirals
- spirals part of chain
- large domains are necessary



Hötzer, Steinmetz, Jainta, Schulz, Kellner, Nestler, Genau, Dennstedt, Bauer, Köstler, and Rüde: Acta Materialia, (2015) (submitted

Storage needs for average phase-field simulations

- used cores: 13 600 on Hornet/Hazel Hen/SuperMuc
- duration: 18h
- calculation domain size: $800 \times 800 \times 256$ voxel
- total domain size: $800 \times 800 \times 4\,500$ voxel
- voxel size per frame: 7 GB
- number of frames: ≈ 100
- total mesh size: 393 GB
- reduced mesh size: ≈ 30 MB

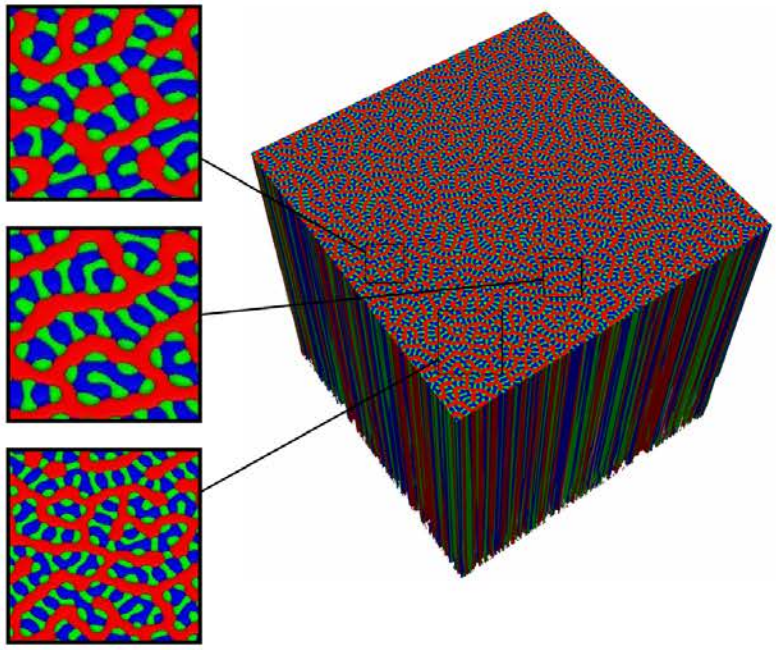


- phase-field simulation of Al-Ag-Cu

Hötzer, J., 2017. Massiv-parallele und großskalige Phasenfeldsimulationen zur Untersuchung der Mikrostrukturentwicklung(Vol. 70). KIT Scientific Publishing.

Storage needs for large scale phase-field simulations

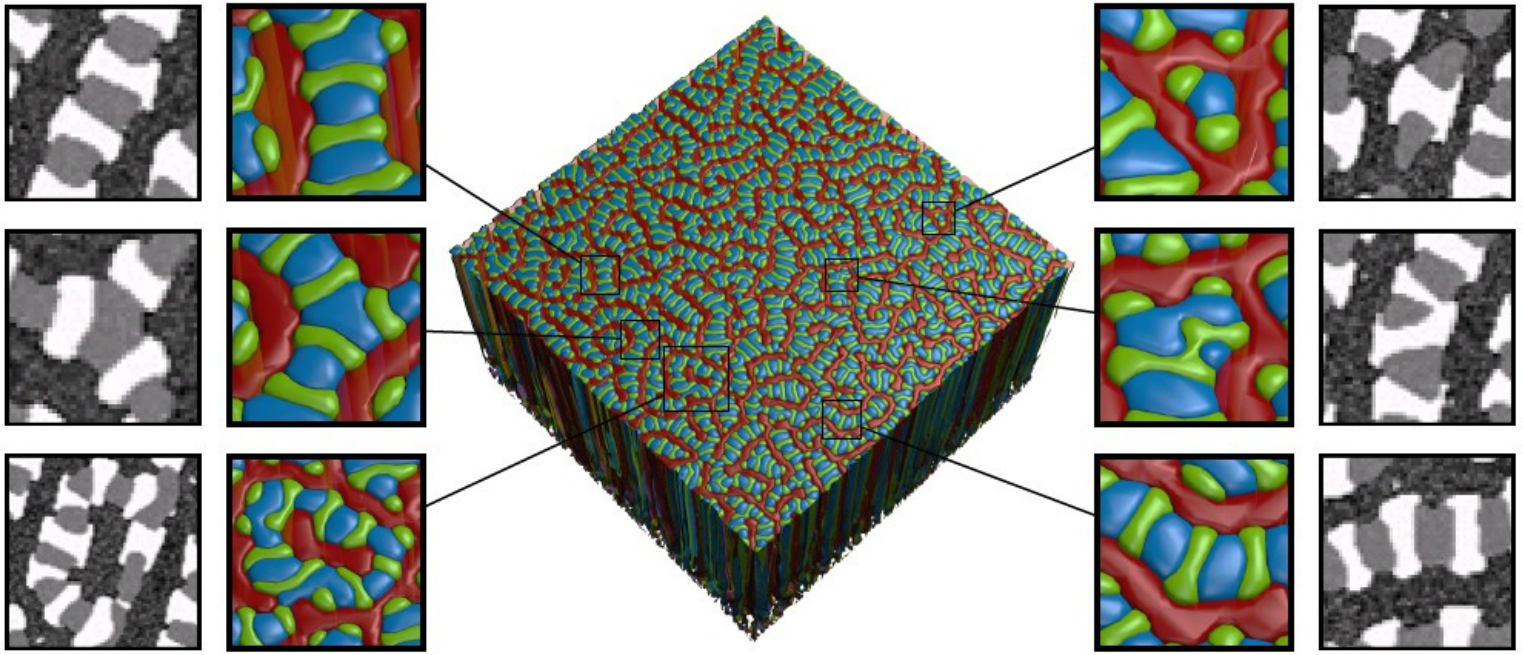
- used cores: 171 696 on Hazel Hen (2015)
- duration: 6, 7h
- calculation domain size: $4\,116 \times 4\,088 \times 256$ voxel
- total domain size: $4\,116 \times 4\,088 \times 4\,325$ voxel
- voxel size per frame: 192 GB
- number of frames: ≈ 30
- total mesh size: 1 486 GB
- reduced mesh size: $\approx$ 100 MB



- phase-field simulation of Al-Ag-Cu with $4\,116 \times 4\,088 \times 4\,325$ cells $\hat{=} 1.6 \times 1.6 \times 1.7$ mm on 171 696 cores of Hazel Hen (2015)
  $\longrightarrow$ **performance of 1,0401 $^{\text{PFLOP}}/_{\text{s}}$**

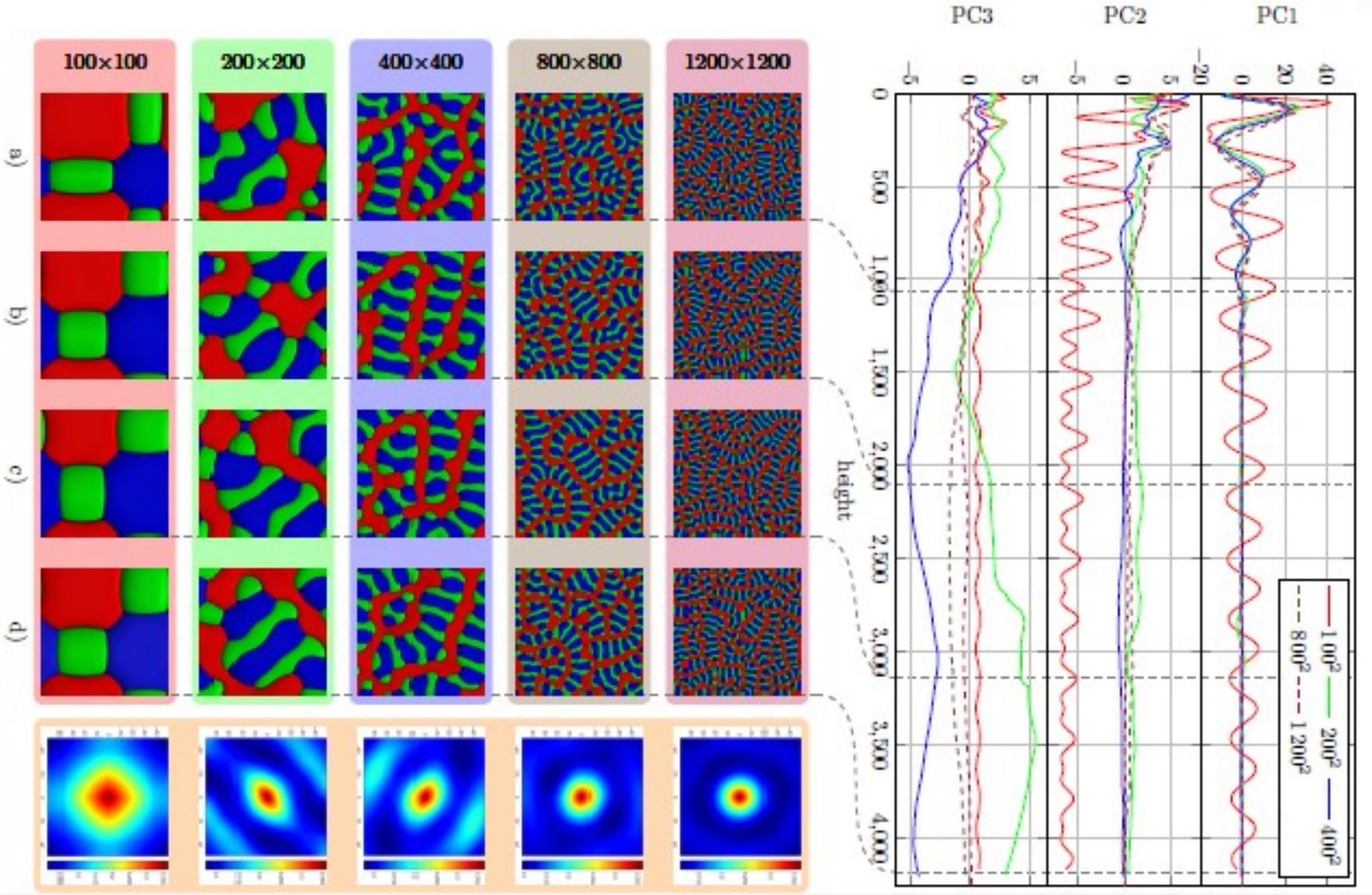
Hötzer, J., 2017. Massiv-parallele und großskalige Phasenfeldsimulationen zur Untersuchung der Mikrostrukturentwicklung(Vol. 70). KIT Scientific Publishing.

Microtomography and simulations of directional solidification microstructures in a ternary eutectic Al-Ag-Cu alloy

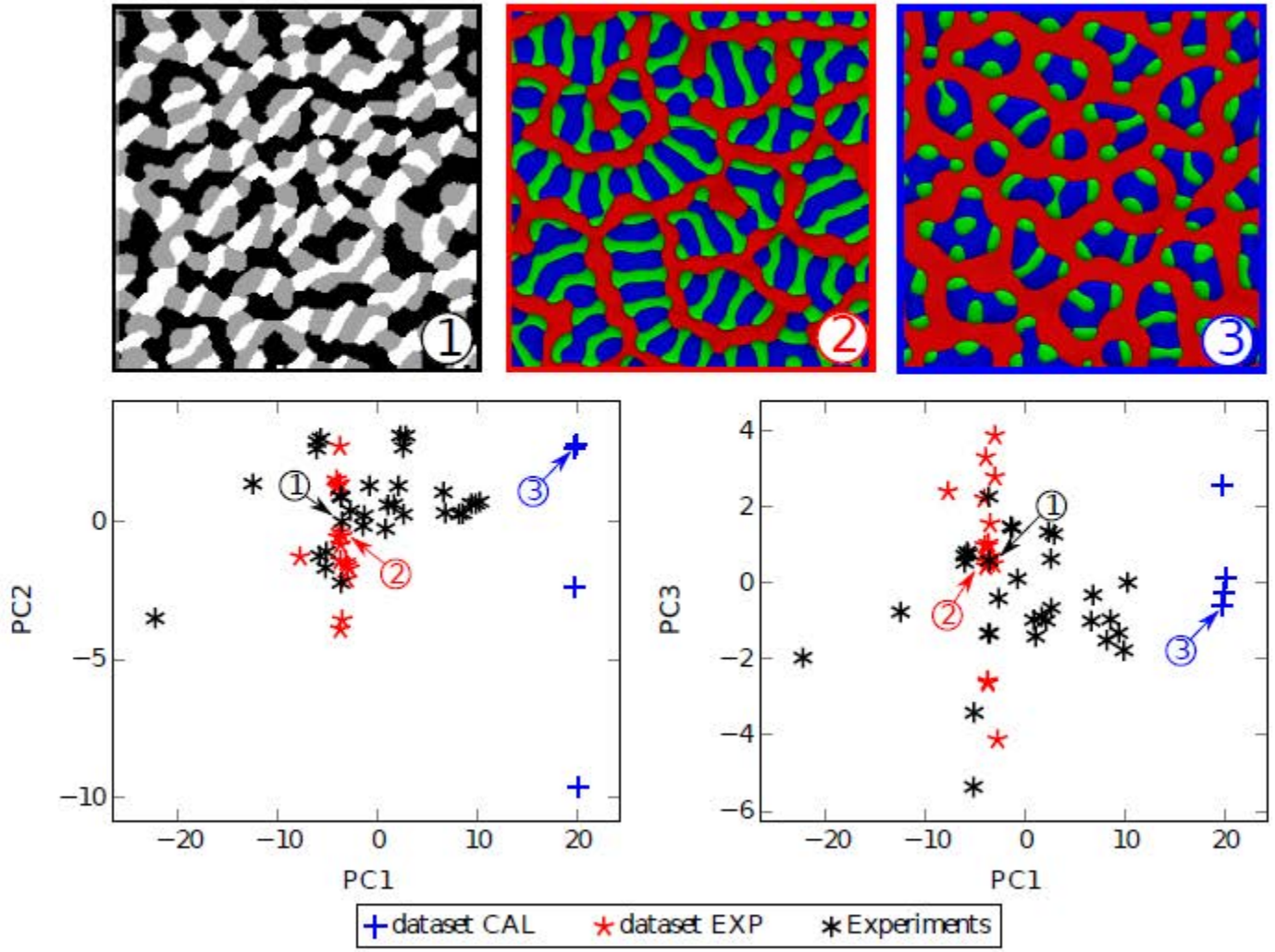


- Massiv Parallel Microstructure Simulation on high computer systems
- Pattern characterization, derivation of morphology diagrams
- Cooperation with A. Dennstedt, L. Ratke, DLR Cologne
- Cooperation with S. Kalidinid, Georgia Tech., USA

Influence of domain size with PCA



Quantitative comparison of simulations and experiments with PCA



Steinmetz, Yabansu, Hötzer, Jainta, Nestler and Kalidindi: Acta Materialia, (2015)

Ausblick

- In Vorbereitung: Positionspapier ,,Roadmap zu einer Digitalisierung der Materialwissenschaften“ in Zusammenarbeit mit DFG, DGM und Gesprächen mit dem BMBF

- DFG-Projekt:
  Sustainable Lifecycle Management for Scientific Software (SuLMaSS)

- Weitere Projektanträge mit Rechenzentrum (SCC, RDM) und Bibliothek in Planung zum Thema Datenmangement und Datenflussmanagement