Karlsruhe Institute of Technology

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Hochschule Karlsruhe Technik und Wirtschaft
UNIVERSITY OF APPLIED SCIENCES

HLRS

IAM Institute for Applied Materials

Large-scale and massively parallel phase-field simulations of pattern formation in ternary eutectic alloys

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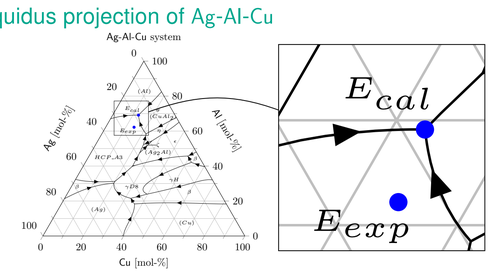
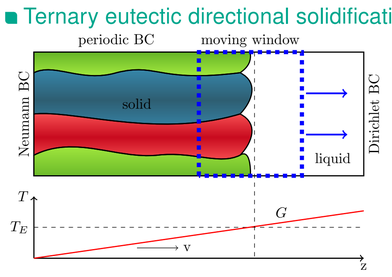
Motivation

- Liquidus projection of Ag-Al-Cu



- E_{cal} from thermodynamic database CALPHAD (→**high** temperature patterns)
- E_{exp} phase-fractions below solubility shift (→**low** temperature patterns)

- Ternary eutectic directional solidification

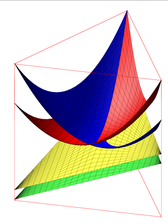


- one liquid phase →three solid phases
- frozen temperature approach

Phase-field model

- Phase-field evolution equation: →940 FLOPs per cell and timestep

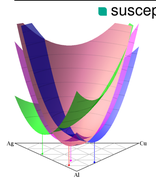
$$\tau_\alpha \epsilon \frac{\partial \phi_\alpha}{\partial t} = \underbrace{-\epsilon T \overbrace{\left(\frac{\partial a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})}{\partial \phi_\alpha} + \nabla \cdot \frac{\partial a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})}{\partial \nabla \phi_\alpha} \right)}^{\text{D3C7}} - \frac{1}{\epsilon} T \overbrace{\frac{\partial \omega(\boldsymbol{\phi})}{\partial \phi_\alpha}}^{\text{D3C1}}}_{\text{surface contribution}} \underbrace{- \overbrace{\frac{\partial \psi(\boldsymbol{\phi}, \boldsymbol{\mu}, T)}{\partial \phi_\alpha}}^{\text{D3C1}}}_{\text{driving force}} + \frac{1}{N} \sum_{\beta=1}^{N} \text{rhs}_\beta}_{:=\text{rhs}\ \alpha}$$

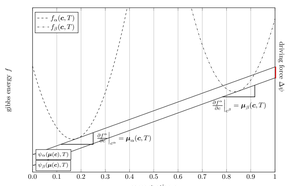


- Chemical potential evolution equation: →2214 FLOPs per cell and timestep

$$\frac{\partial \boldsymbol{\mu}}{\partial t} = \underbrace{\overbrace{\left[\sum_{\alpha=1}^{N} h_\alpha(\boldsymbol{\phi}) \left(\frac{\partial \boldsymbol{c}^\alpha(\boldsymbol{\mu}, T)}{\partial \boldsymbol{\mu}} \right) \right]^{-1}}^{\text{D3C1}}}_{\text{susceptibility}} \left(\underbrace{\overbrace{\nabla \cdot \left(\boldsymbol{M}(\boldsymbol{\phi}, \boldsymbol{\mu}, T) \nabla \boldsymbol{\mu} \right)}^{\text{D3C7}} - \overbrace{\boldsymbol{J}_{\text{at}}(\boldsymbol{\phi}, \boldsymbol{\mu}, T)}^{\text{D3C19}}}_{\text{flux of } \mu \text{ depending on the mobility } \boldsymbol{M}} \right.$$

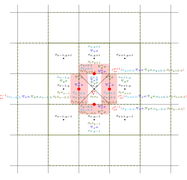
$$\left. - \underbrace{\overbrace{\sum_{\alpha=1}^{N} \boldsymbol{c}_\alpha(\boldsymbol{\mu}, T) \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial t}}^{\text{D3C1}}}_{\text{contribution of the phase change}} - \underbrace{\overbrace{\sum_{\alpha=1}^{N} h_\alpha(\boldsymbol{\phi}) \left(\frac{\partial \boldsymbol{c}_\alpha(\boldsymbol{\mu}, T)}{\partial T} \right) \frac{\partial T}{\partial t}}^{\text{D3C1}}}_{\text{contribution of the temperature change}} \right)$$





- Antitrapping-current

$$\boldsymbol{J}_{\text{at}} = \frac{\pi \epsilon}{4} \sum_{\substack{\alpha=1 \\ (\alpha \neq \ell)}}^{N} \frac{g_\alpha(\boldsymbol{\phi}) h_\ell(\boldsymbol{\phi})}{\sqrt{\phi_\alpha \phi_\ell}} \frac{\partial \phi_\alpha}{\partial t} \left(\frac{\nabla \phi_\alpha}{|\nabla \phi_\alpha|} \cdot \frac{\nabla \phi_\ell}{|\nabla \phi_\ell|} \right) \left(\left(\boldsymbol{c}^\ell(\boldsymbol{\mu}) - \boldsymbol{c}^\alpha(\boldsymbol{\mu}) \right) \otimes \frac{\nabla \phi_\alpha}{|\nabla \phi_\alpha|} \right)$$



- **thermodynamic consistent** phase-field model of **Allen–Cahn** type
- **finite differences** scheme in space and **forward euler** in time
- coupling with thermodynamic **CALPHAD**-database

[1] Choudhury: KIT Scientific Publishing, (2013)

Implementation

- ϕ update

$$\phi(\mathbf{x}, t) \xrightarrow{\text{D3C7}} \phi(\mathbf{x}, t + \Delta t)$$
$$\mu(\mathbf{x}, t) \xrightarrow{\text{D3C1}} \phi(\mathbf{x}, t + \Delta t)$$

- μ update

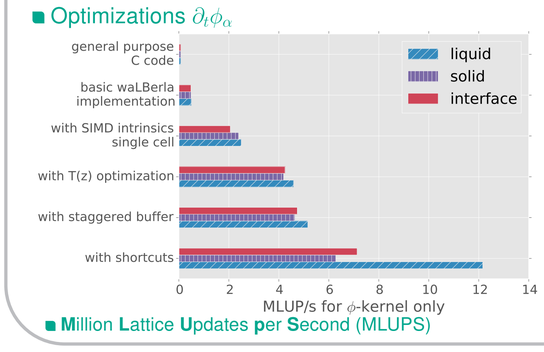
$$\phi(\mathbf{x}, t) \xrightarrow{\text{D3C19}} \phi(\mathbf{x}, t + \Delta t) \xrightarrow{\text{D3C19}}$$
$$\mu(\mathbf{x}, t) \xrightarrow{\text{D3C7}} \mu(\mathbf{x}, t + \Delta t)$$

- massive parallel **waLBerla** framework based on block structured grids
- **buffering** and **classification** techniques to reduce calculation time
- explicit **vectorization** by using intrinsics for SSE, AVX, QPX

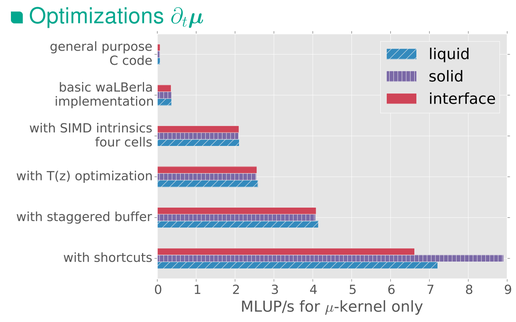
Reality/Experiments
Physical Parameter
Mathematical Model
Numerical Scheme
Application Program
Parallel Programming Models (MPI, Cuda)
Hardware Architecture

Optimization & Scaling

- Optimizations $\partial_t \phi_\alpha$

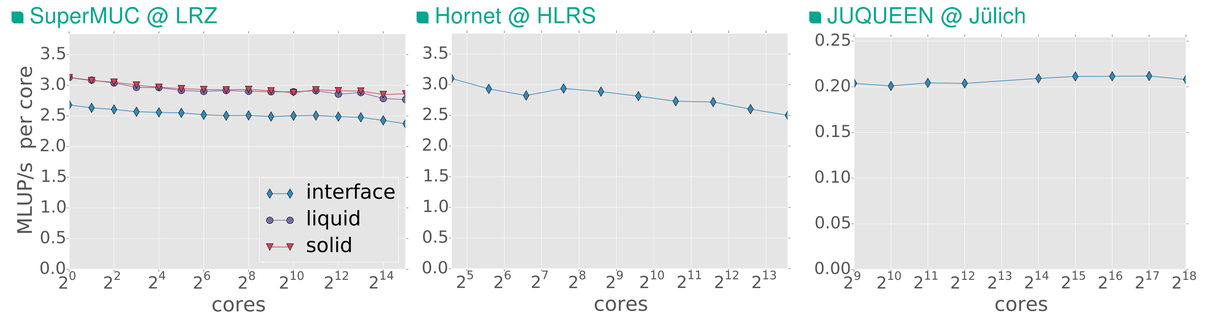


- Optimizations $\partial_t \boldsymbol{\mu}$



- **M**illion **L**attice **U**pdates **p**er **S**econd (MLUPS)

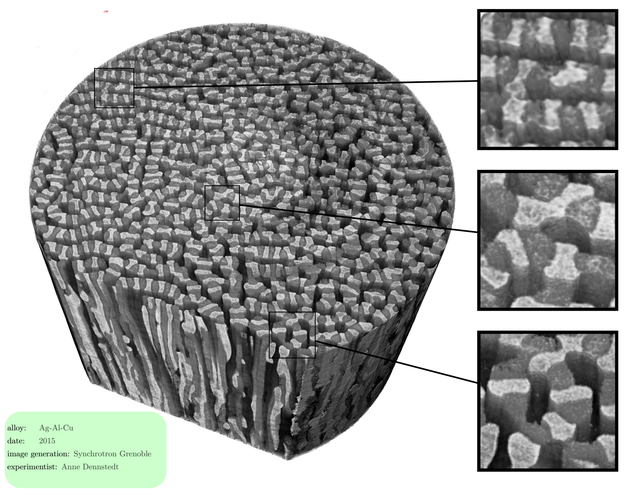
- SuperMUC @ LRZ
- Hornet @ HLRS
- JUQUEEN @ Jülich



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

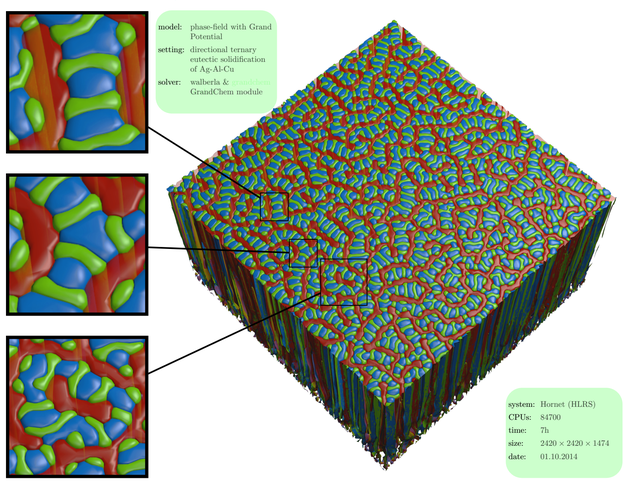
Ternary eutectic directional solidification

- Experiment (Ag-Al-Cu)



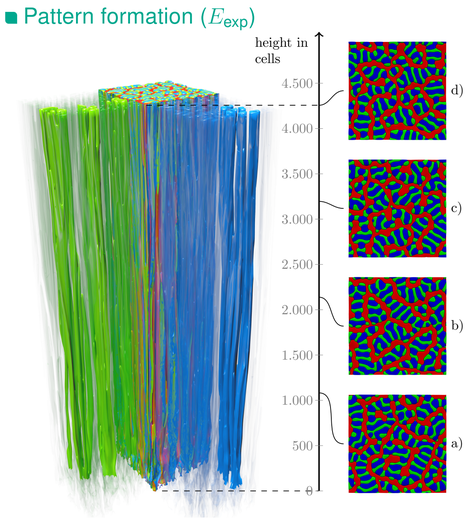
- synchrotron tomography

- Simulation (E_{exp})



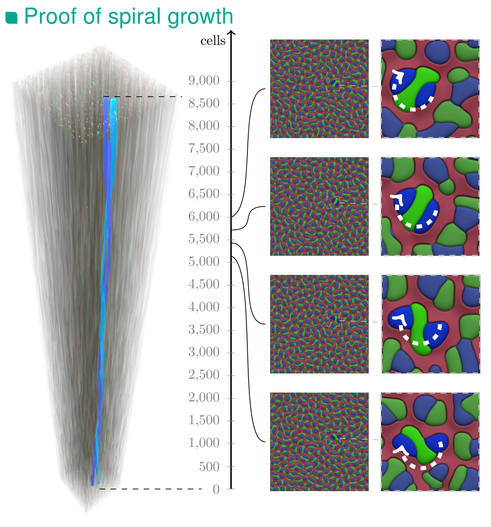
- $2420 \times 2420 \times 1474$ voxel cells
- 84 700 cores @Hornet

- Pattern formation (E_{exp})



- $800 \times 800 \times 4256$ voxel cells
- 13 600 cores @Hornet

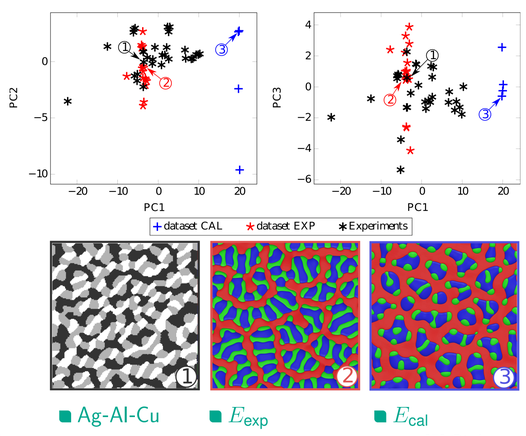
- Proof of spiral growth



- $800 \times 800 \times 8520$ voxel cells
- 13 600 cores @Hornet

[3] Hötzer, Steinmetz, Jainta, Schulz, Kellner, Nestler, Genau, Dennstedt, Bauer, Köstler, and Rüde: Acta Materialia, (2015) (submitted) , [4] Hötzer, Jainta, Steinmetz, Nestler, Dennstedt, Genau, Bauer, Köstler, and Rüde: Acta Materialia, (2015)

Quantitative comparison using PCA



- Ag-Al-Cu
- E_{exp}
- E_{cal}

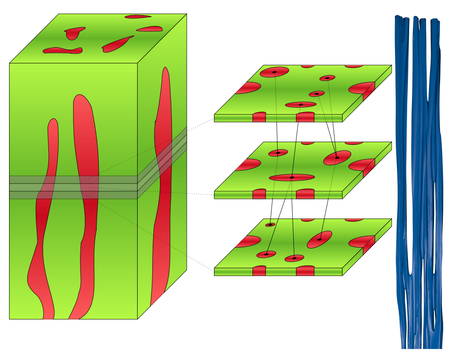
- **principal component analysis** (PCA) based on **two-point correlations**
- **quantitative comparison** of simulations and experimental micrographs
- determination of **representative volume elements** (RVE)
- determination of necessary simulation time

- good agreement of E_{exp} simulation (red) with experimental micrographs (black)
- deviation of E_{cal} (blue) due to solubility shift after solidification

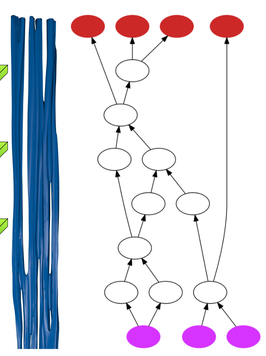
[5] Steinmetz, Yabansu, Hötzer, Jainta, Nestler and Kalidindi: Acta Materialia, (2015)

Graph based analysis

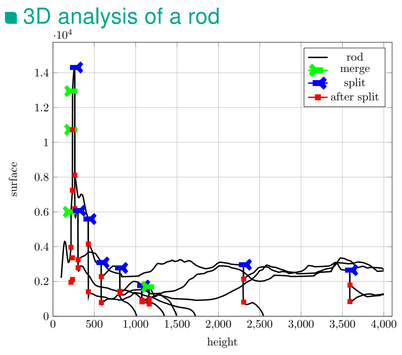
- Implementation



- Minimal graph of a rod



- 3D analysis of a rod



- events and volume change during growth
- reduction of 3D data

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