

Datenfluss und Datenanalyse in der Materialforschung

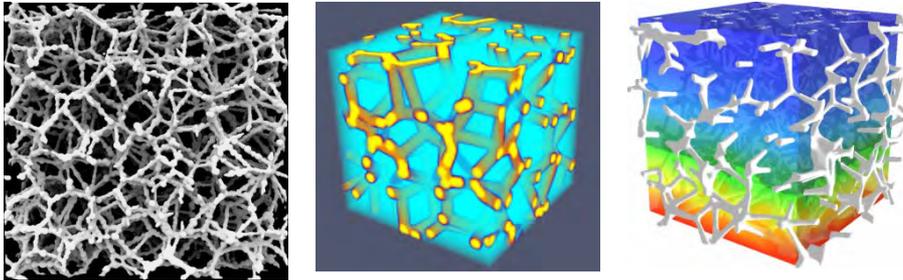
Britta Nestler, Institute of Applied Materials (IAM-CMS)

P3-Treffen 5.+ 6. März 2018, KIT, Campus Nord

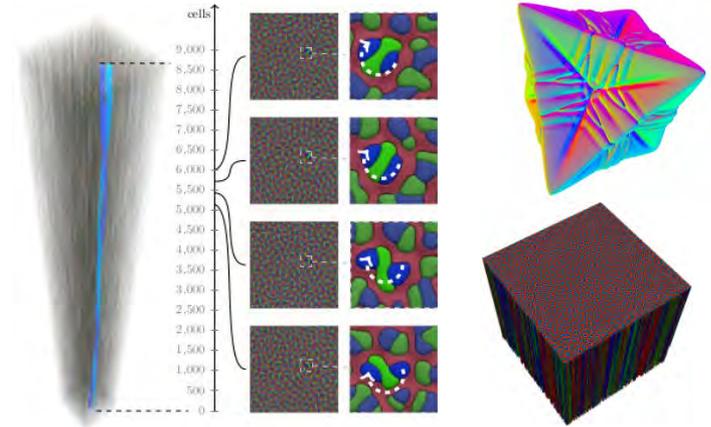


Overview – Microstructures Simulations

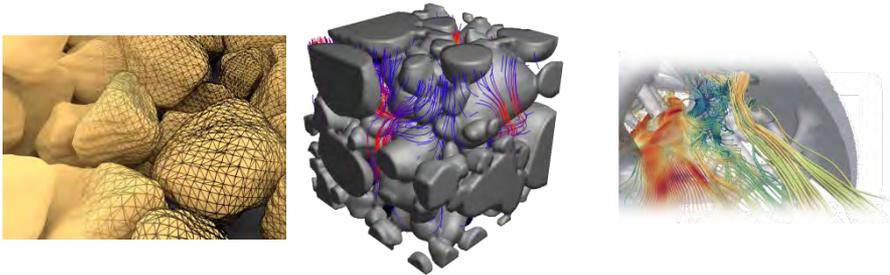
heat transport



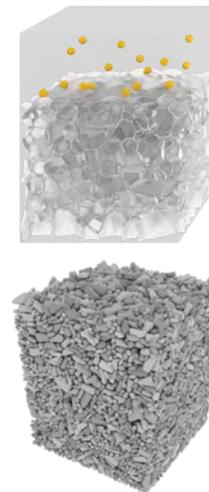
solidification



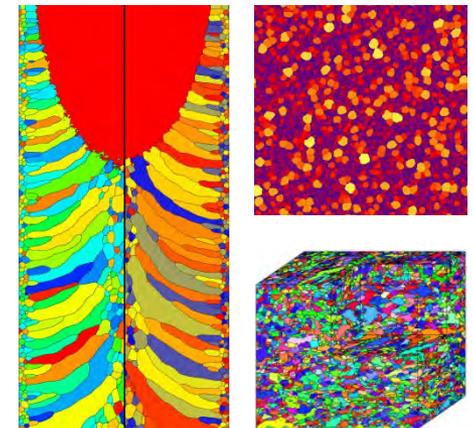
fluid dynamics



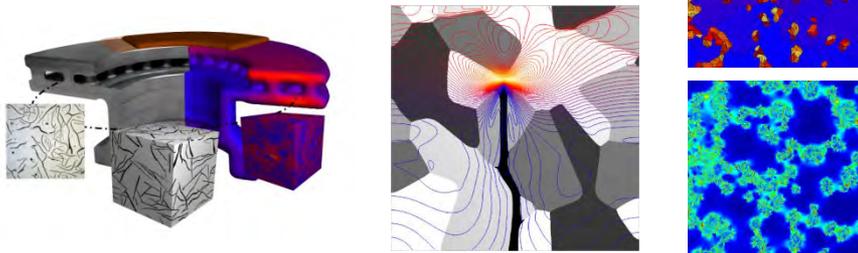
sintering



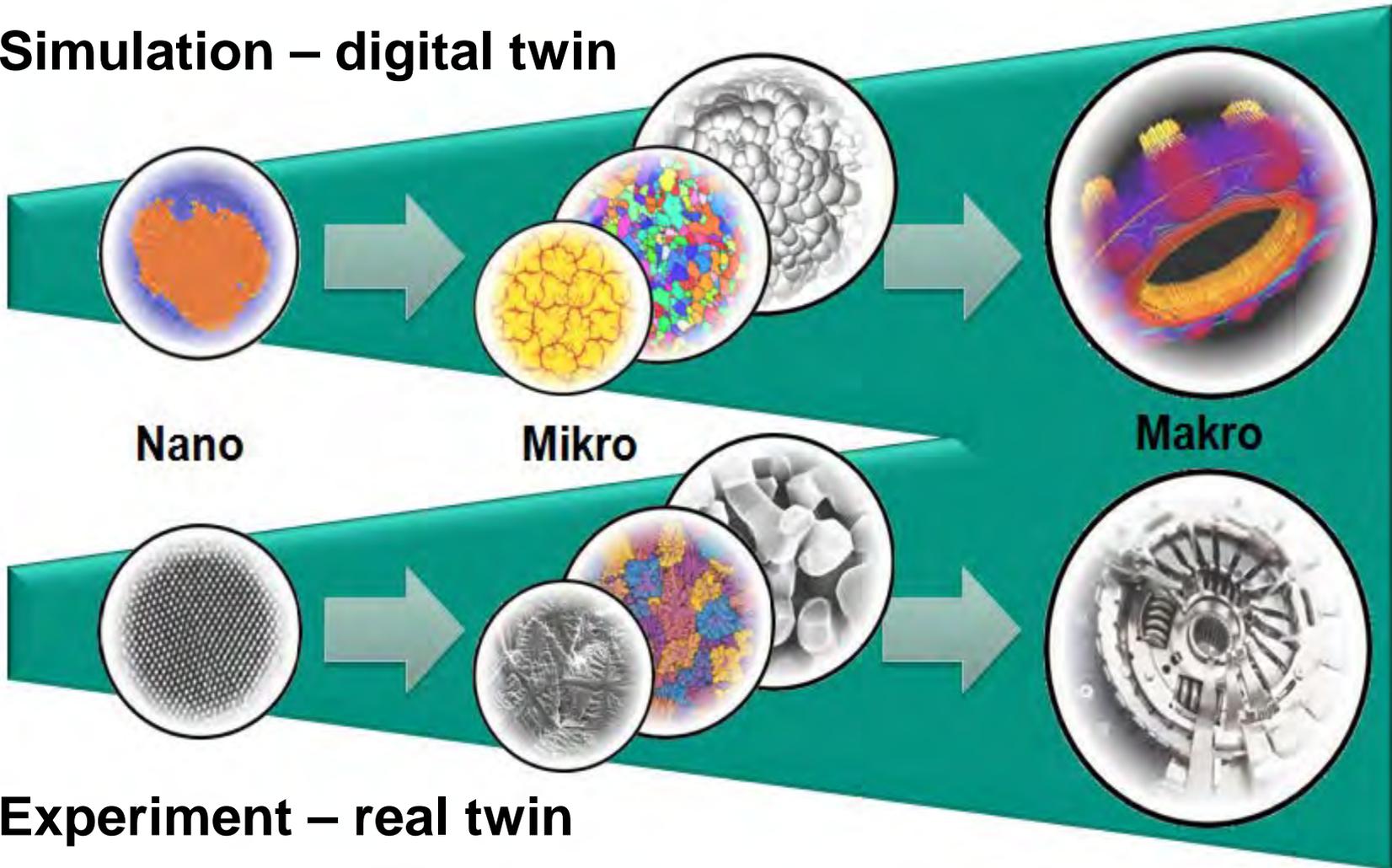
grain growth



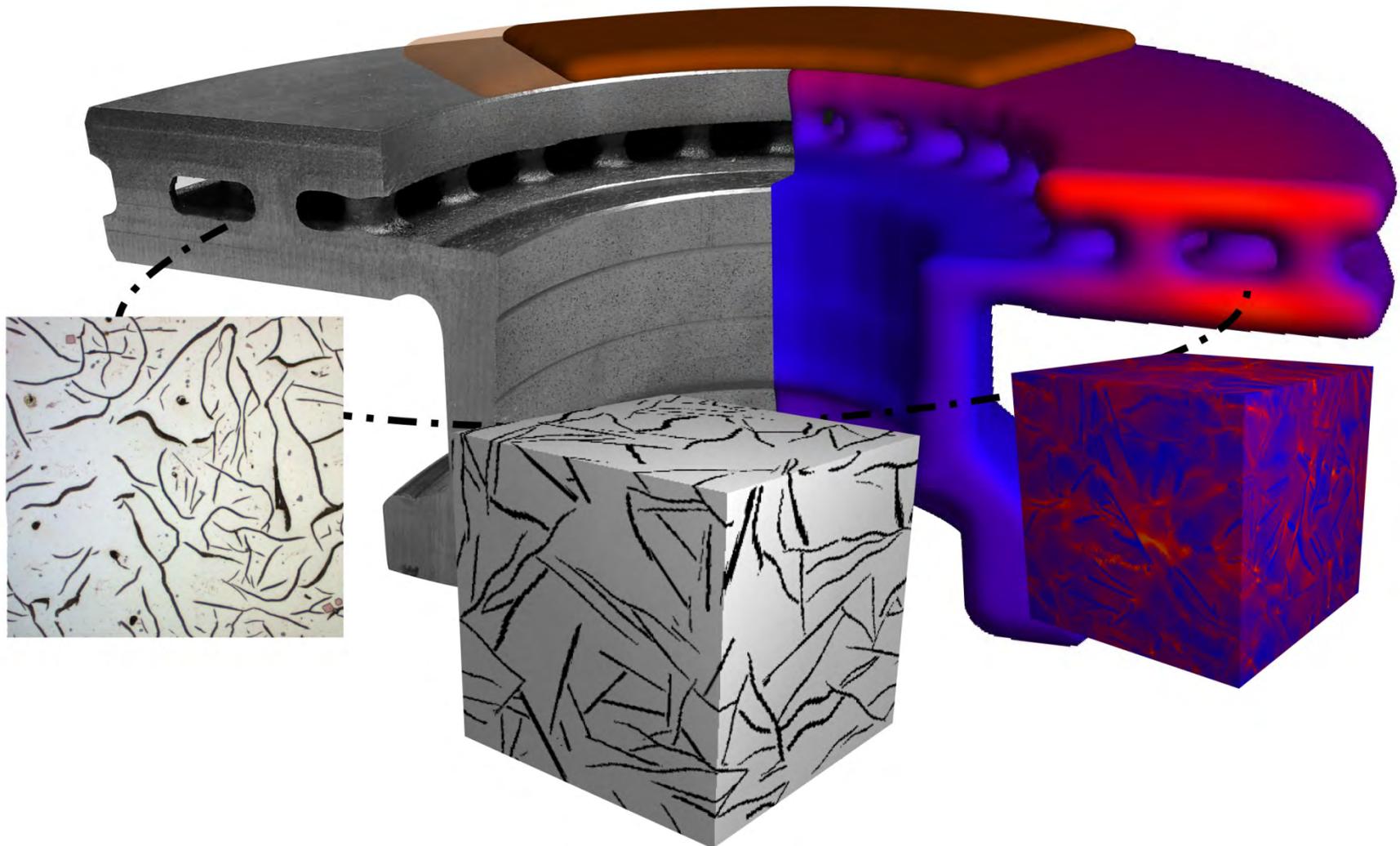
mechanical forces



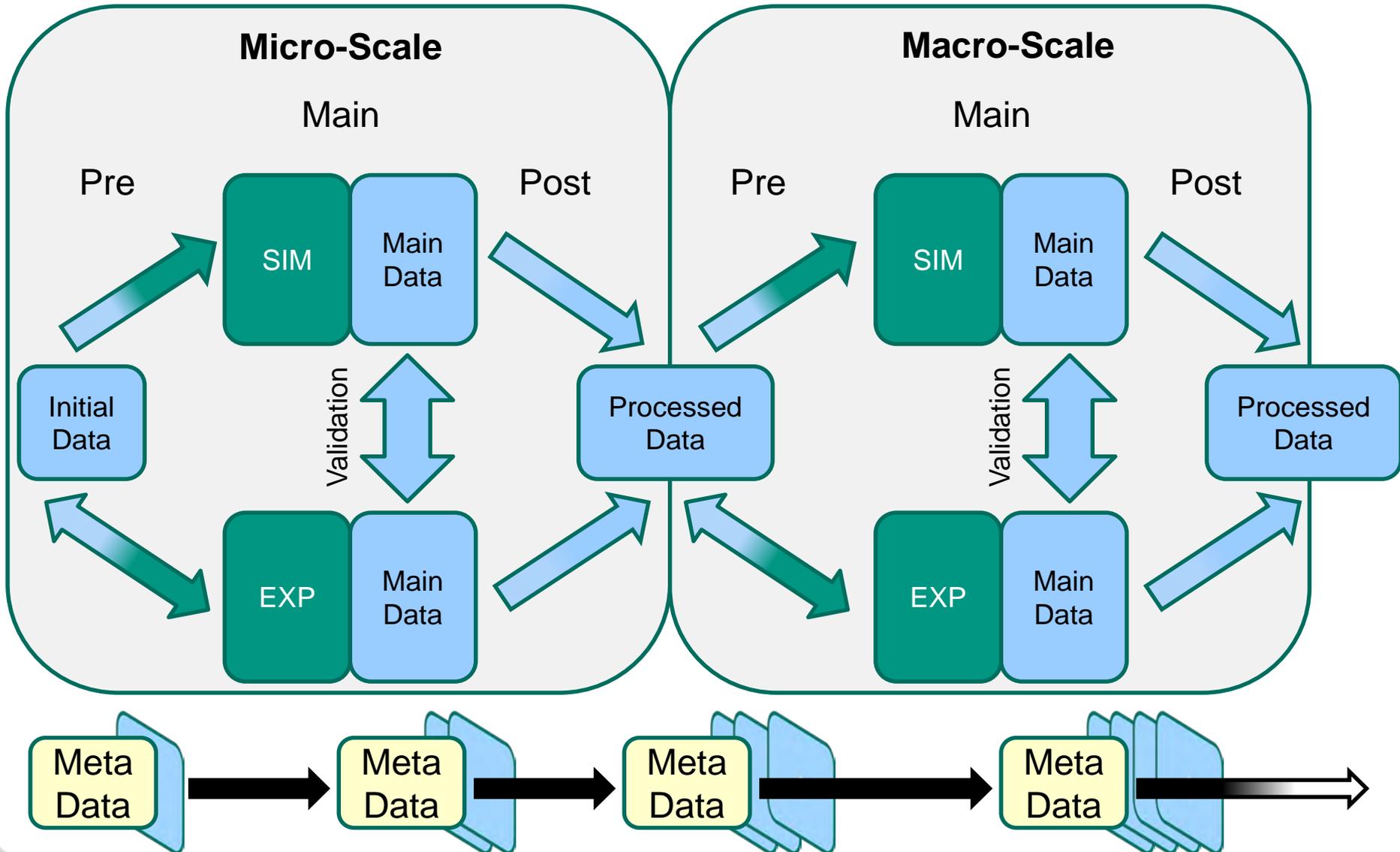
Simulation – digital twin



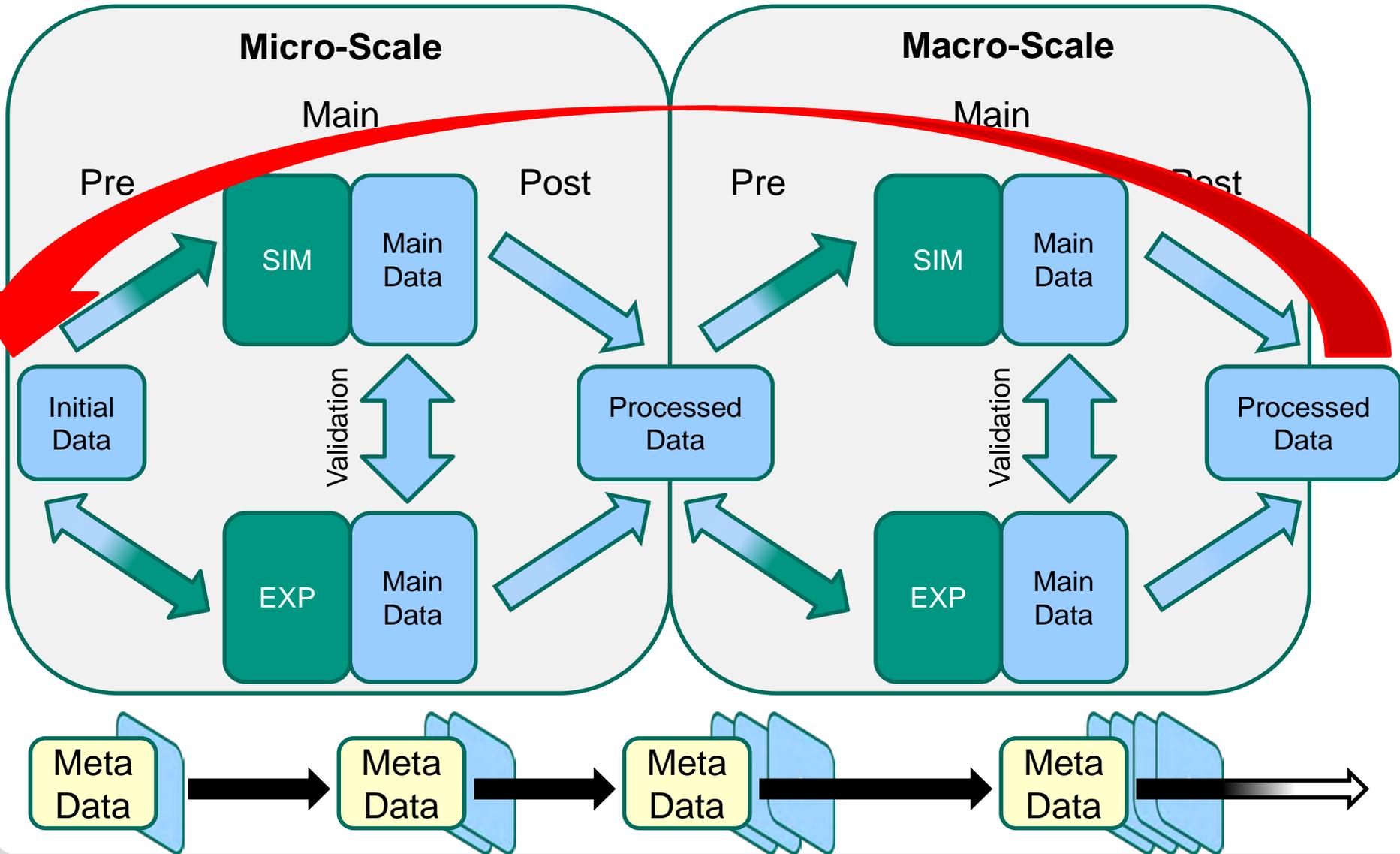
Multiscale simulation of thermomechanical load in brake discs



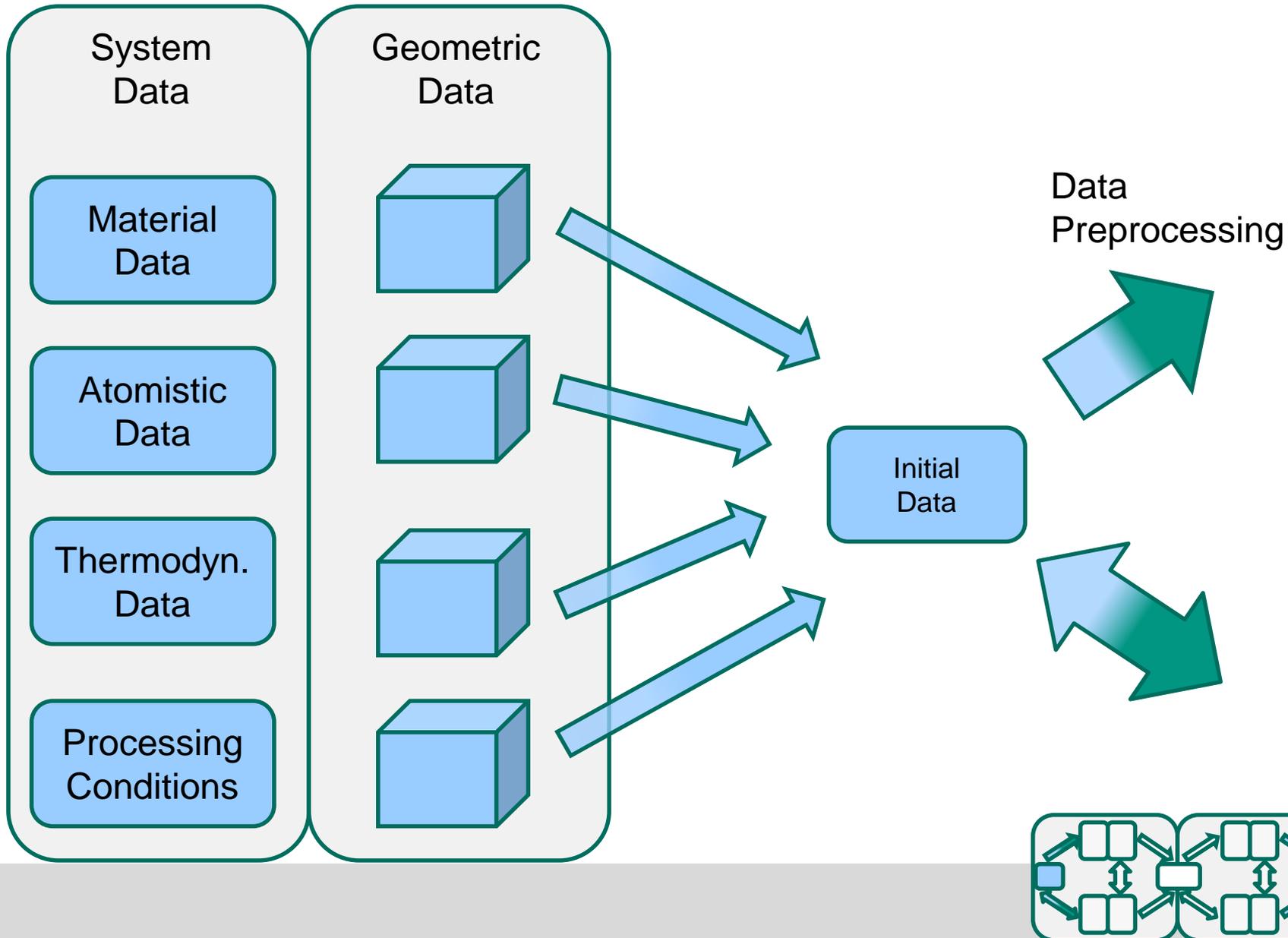
Data flow of Pre-, Main- and Post-Processing



Data flow of Pre-, Main- and Post-Processing

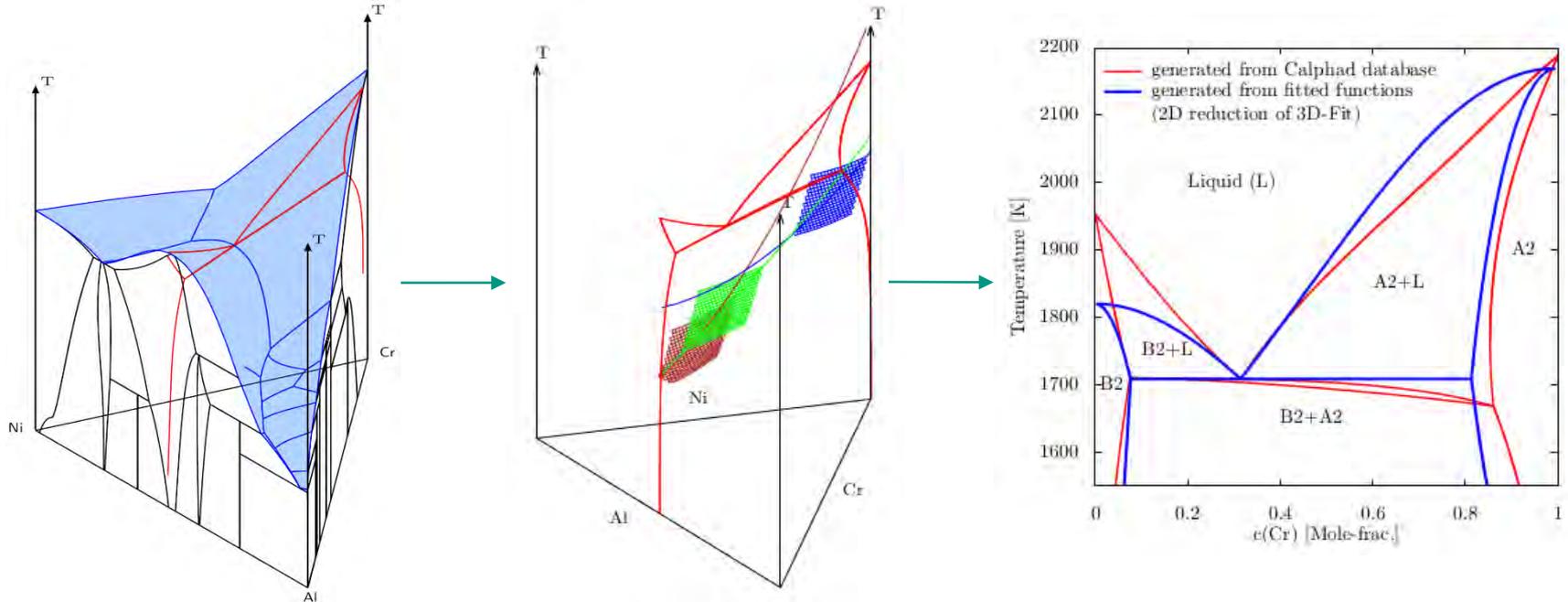


Data flow of Pre-Processing

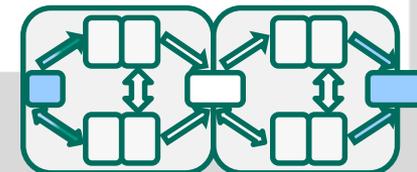


Data flow: From thermodynamic modelling to microstructure simulation

- Transfer of thermodynamic information from Calphad-databases to phase-field simulations for the directional solidification of NiAl-34Cr



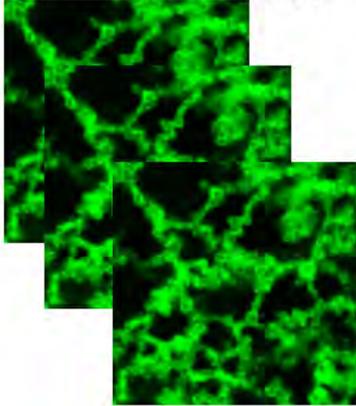
- Ternary phase diagram provided by Calphad database
- Fitted Gibbs energy curves for the eutectic system NiAl-34Cr
- Rebuild phase diagram (blue) as input for phase-field simulations



Data flow: From experimental images to microstructure simulation

Experiment

Confocal laser scanning microscopy



Binarization

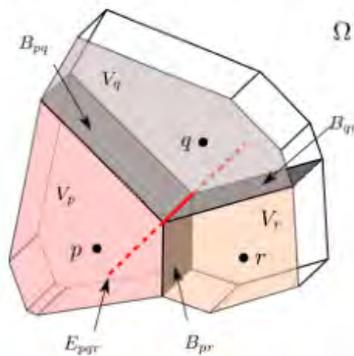


Reconstruction
size: $50 \times 50 \times 50 \mu\text{m}$

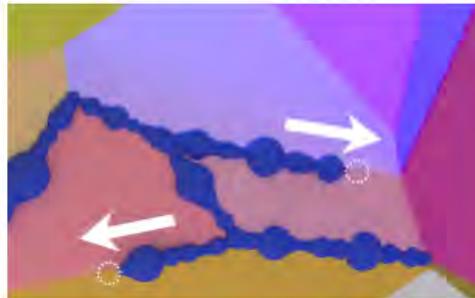


Algorithm

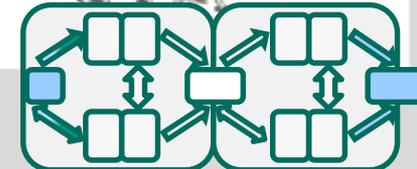
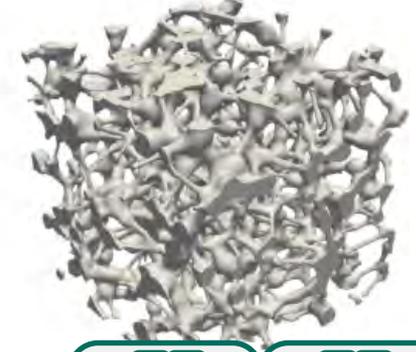
Voronoi tessellation



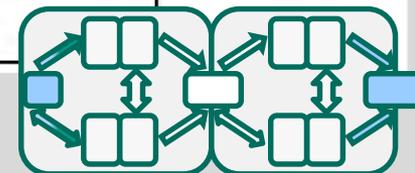
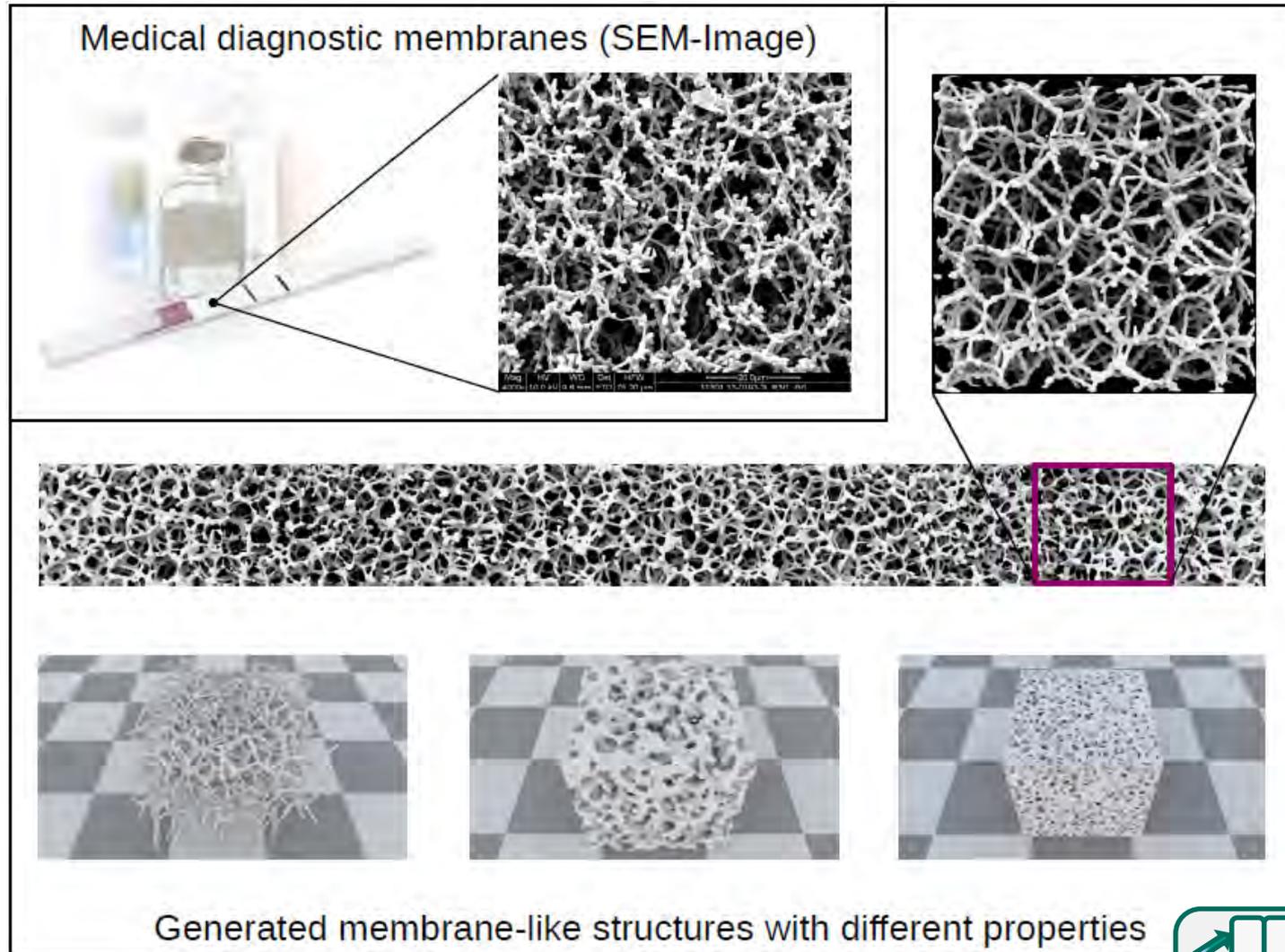
Drawing
microstructure



Generated



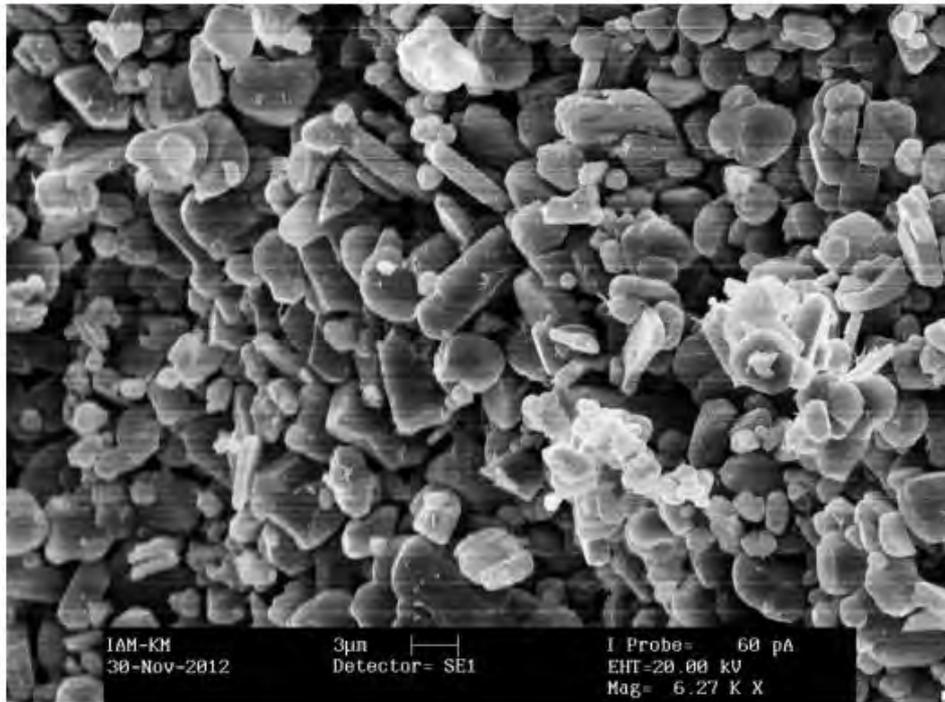
Data flow: From experimental images to algorithmically generated microstructures



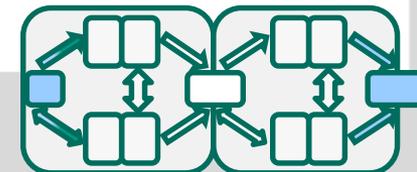
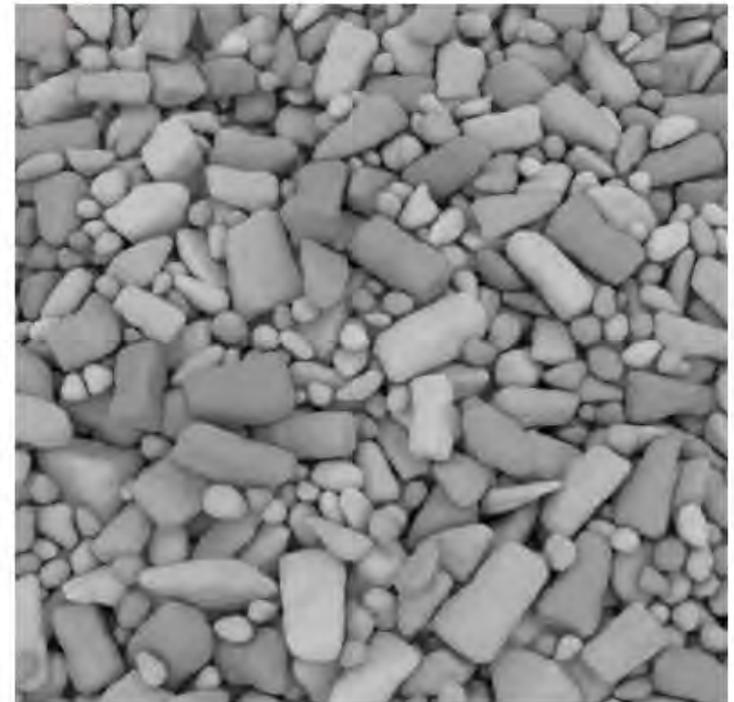
Data flow: From experimental images to algorithmically generated microstructures

Green body for sintering

■ Experiment

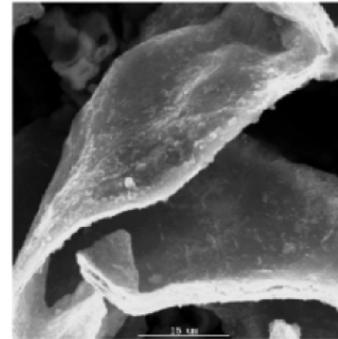


■ Generated

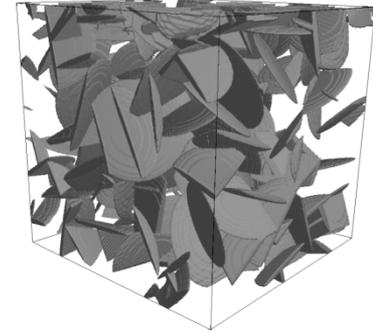


Data flow: From literature (DIN) to algorithmically generated microstructures

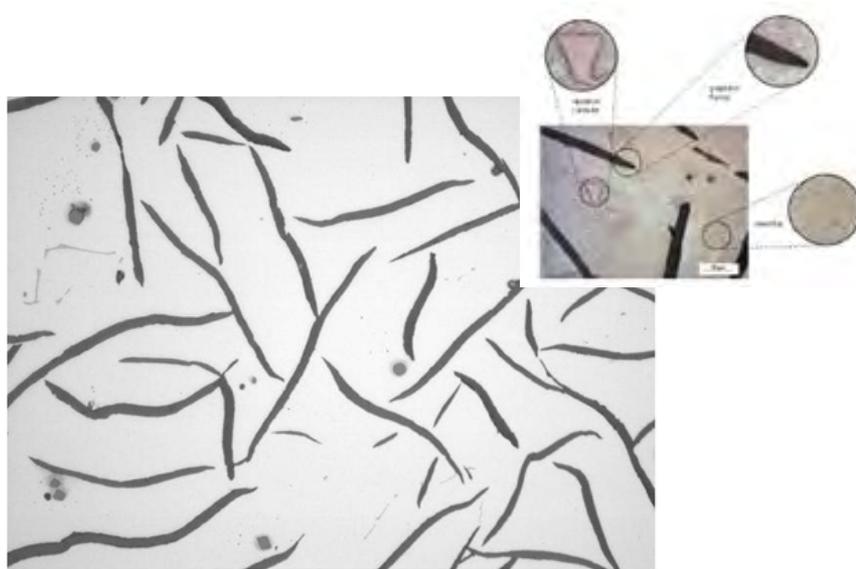
- Filling of graphite inclusions
- Random distribution
- Variation of phase fractions, shape factors etc.



Graphite flake



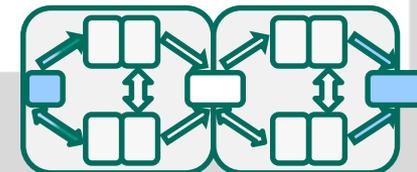
3D- domain



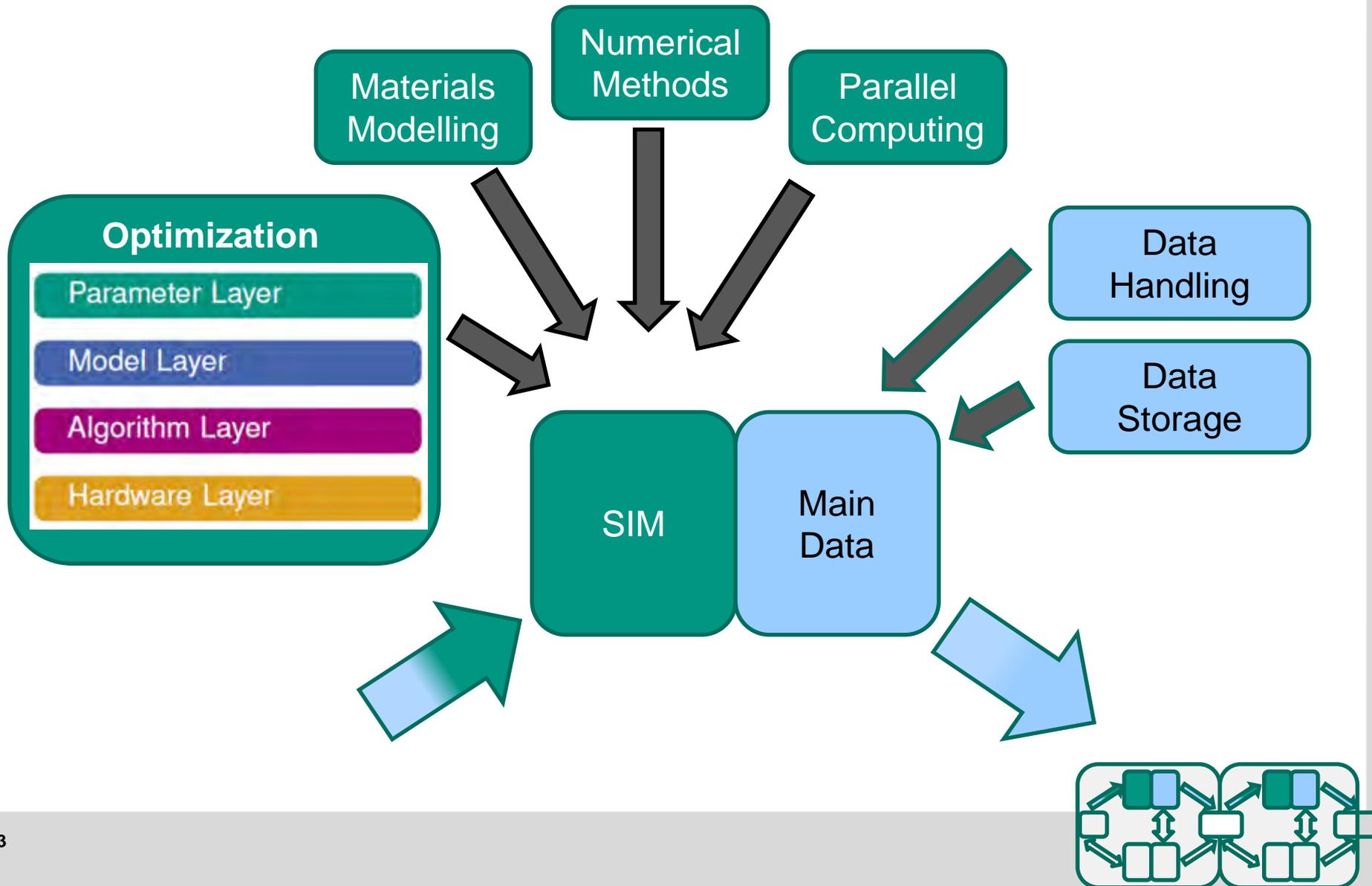
micrograph



*2-D cut through
filled domain*

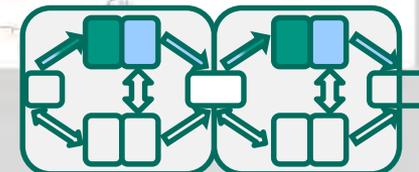
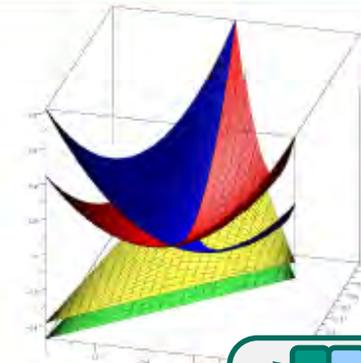
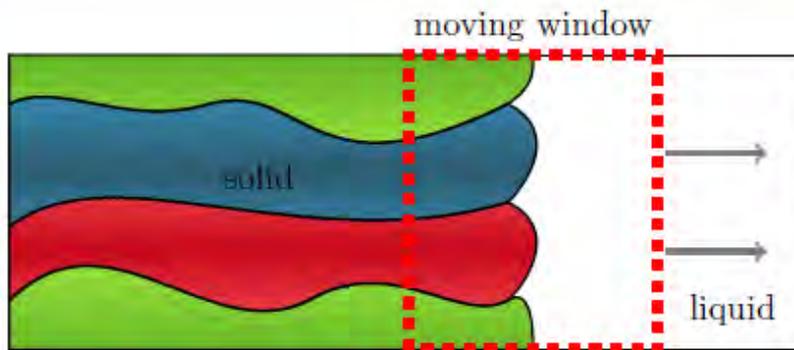


Main-Processing



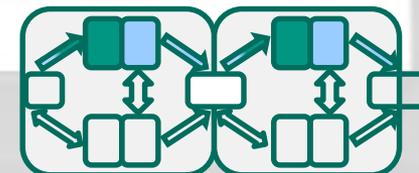
Parameter Layer

- 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



Model Layer

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

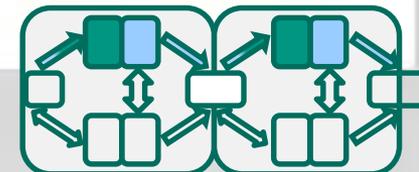


Algorithm Layer

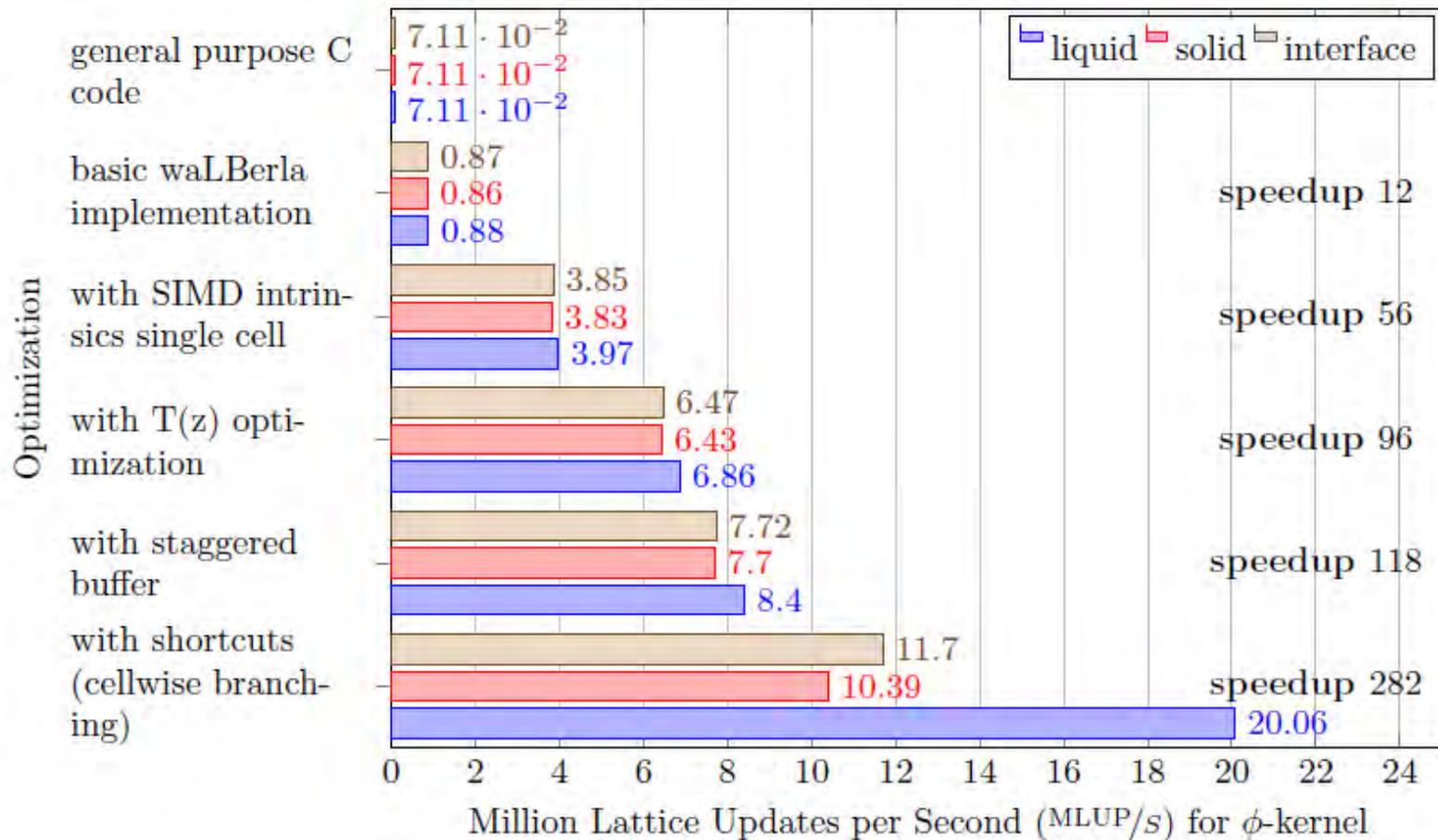
- access patterns / stencils
- overlapping computation and communication
- block structured grid and static load balancing
- eliminate of common subexpressions / buffering techniques

Hardware Layer

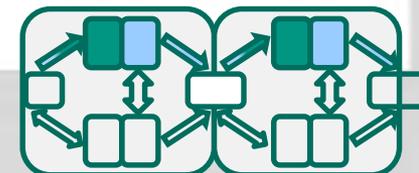
- explicit kernel SIMDification
- Memory layout (AoS vs. SoA)



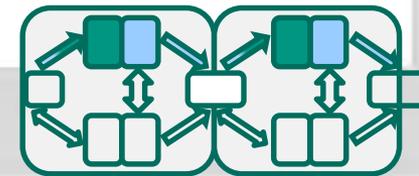
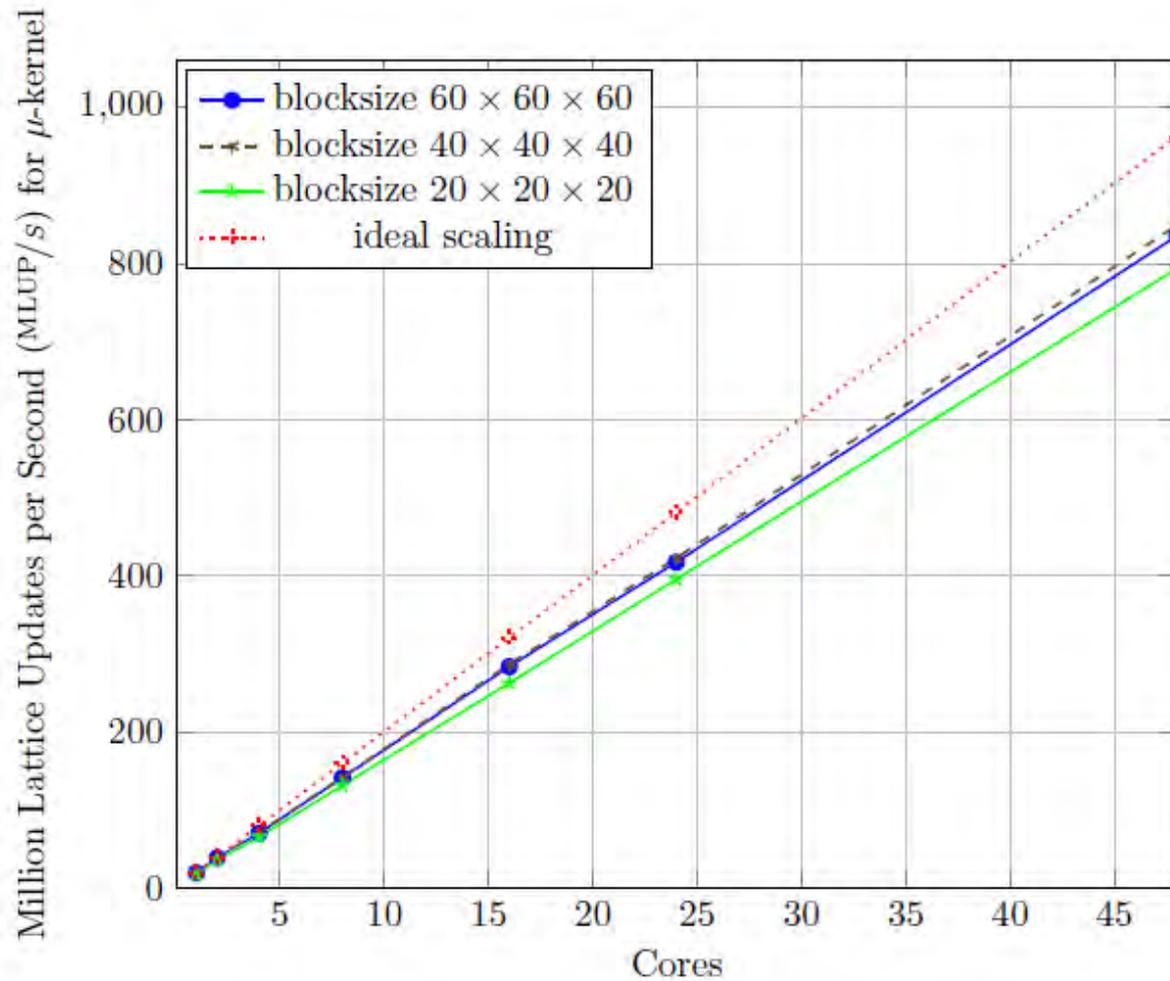
Optimization results – ϕ -kernel – Hornet



■ $60 \times 60 \times 60$ cells per block



Single node scaling – Hornet



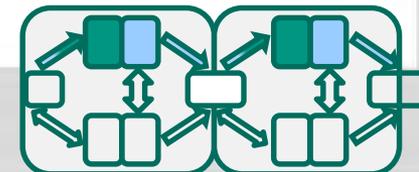
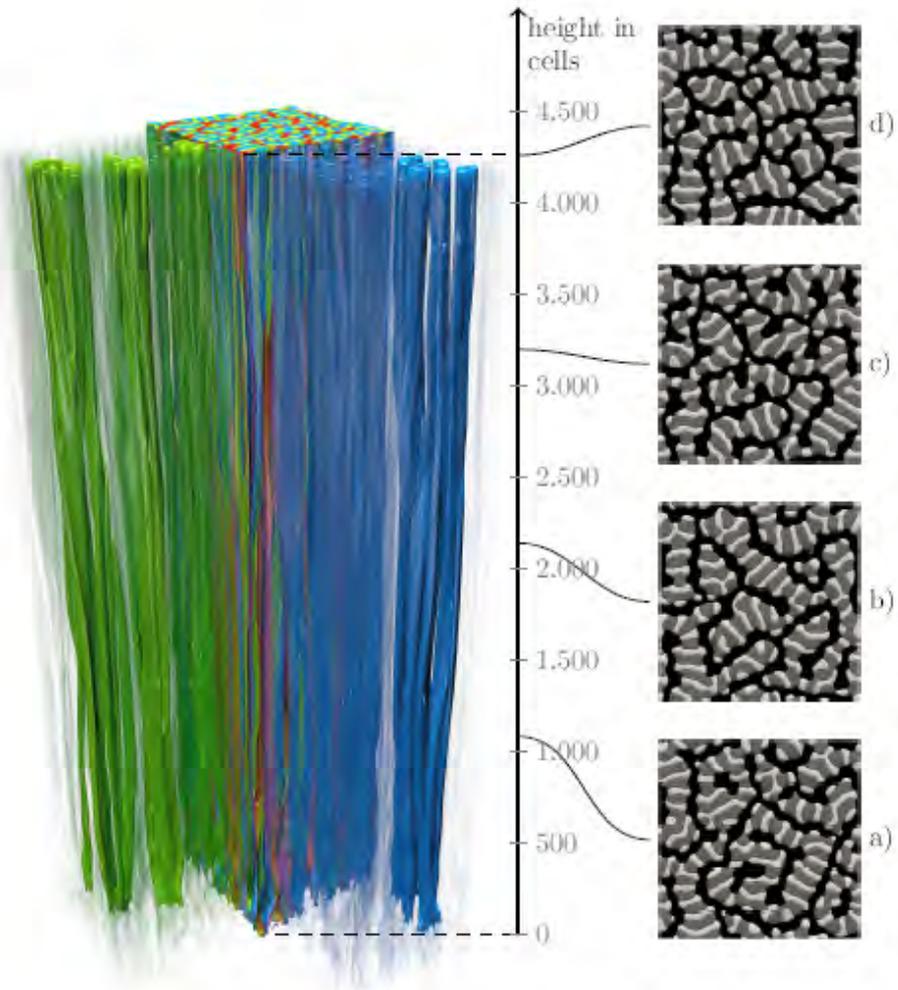
Large 3D Simulation for Al-Ag-Cu

System parameters

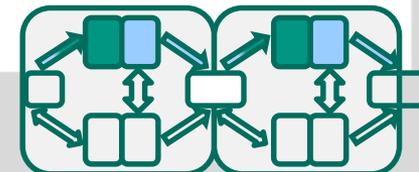
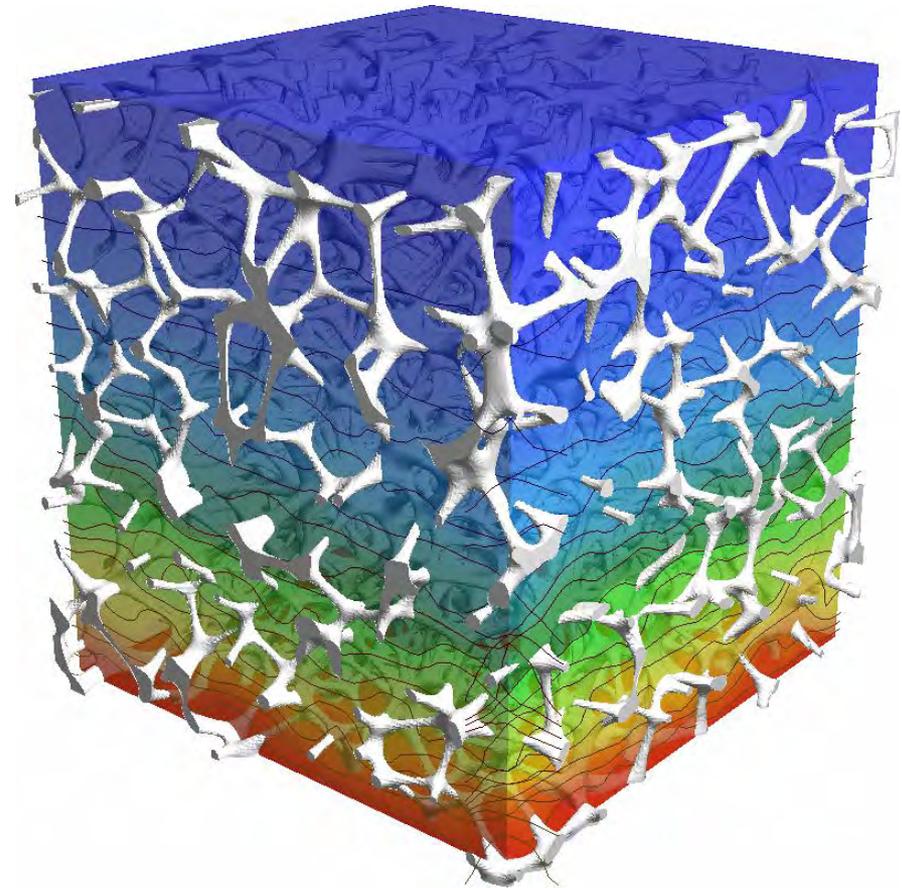
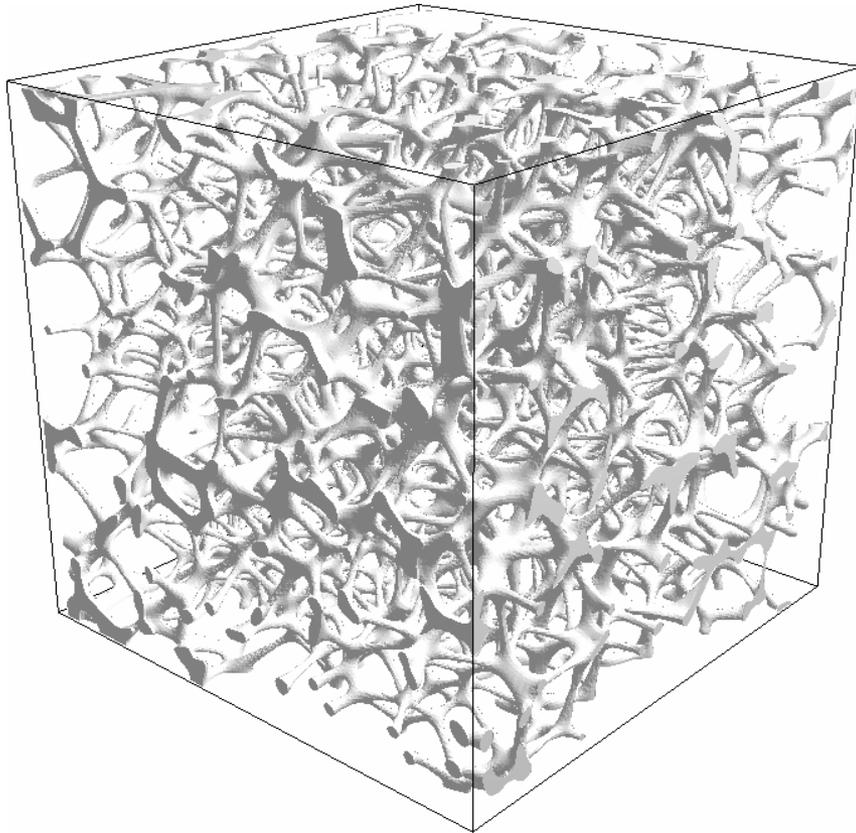
- Ternary eutectic point: E_{exp}
- $800 \times 800 \times 4256$ cells
- 15,9h on 13600 CPUs

Result

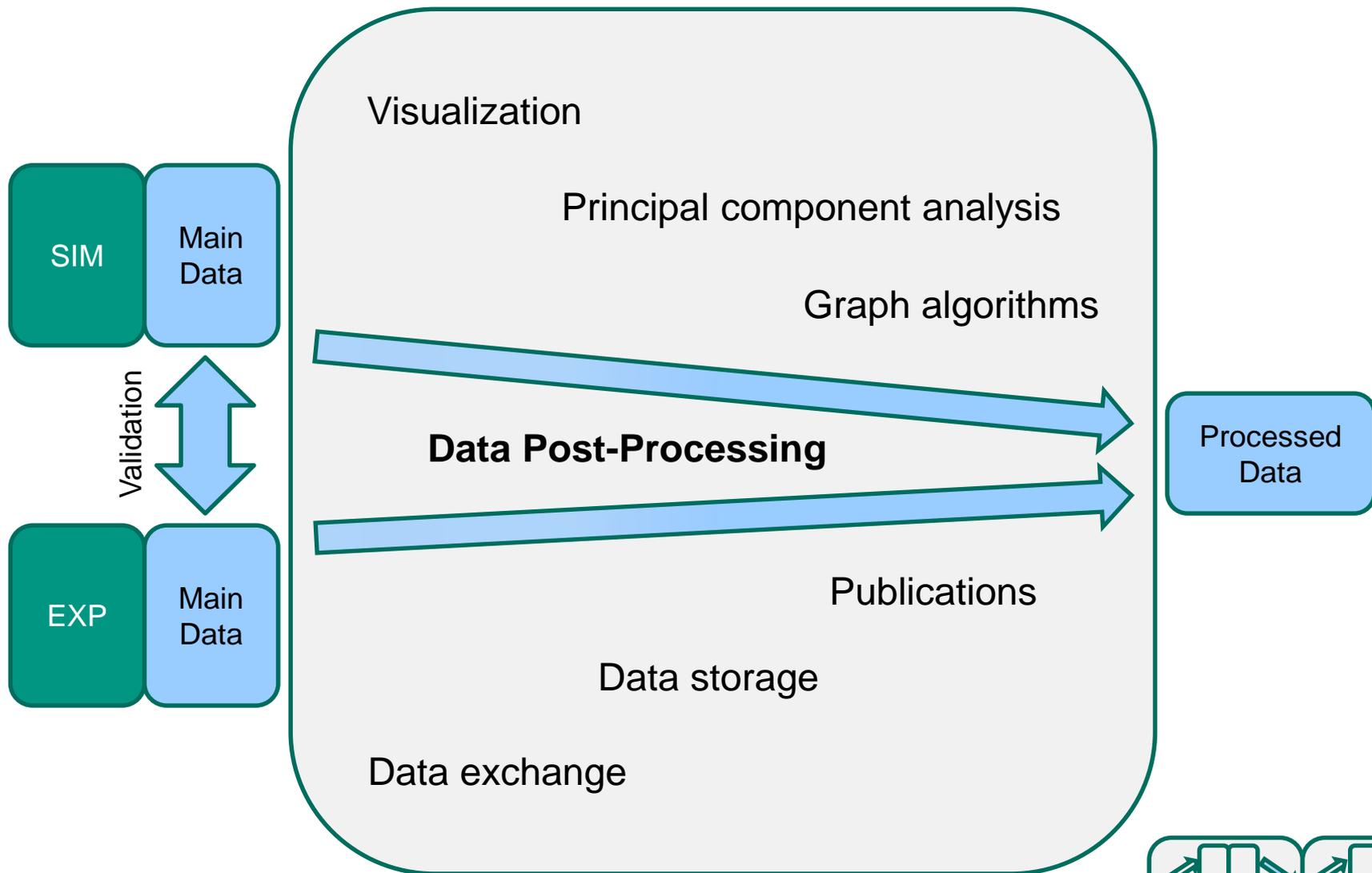
- chained brick-like structures
- split, merge and termination events in growing direction



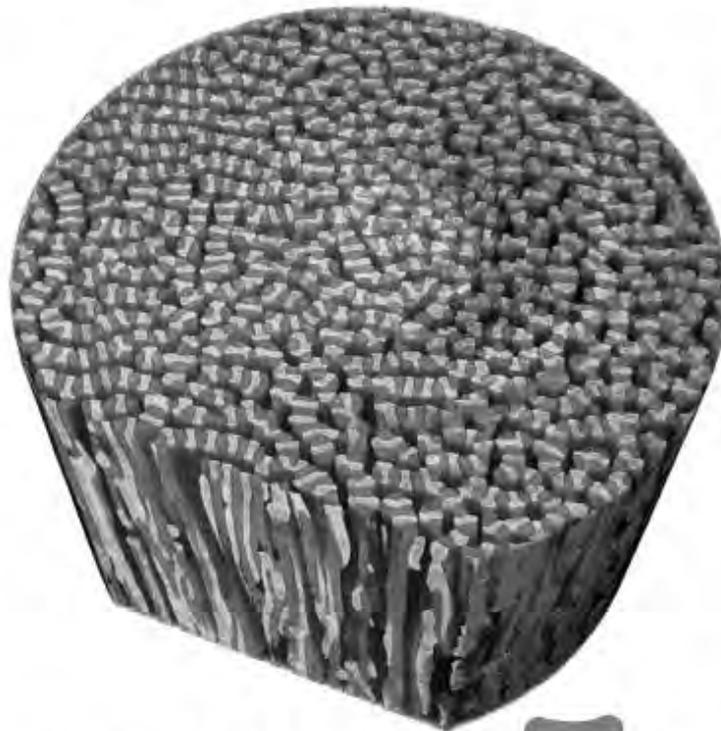
Main-Processing: Heat transfer in open cell metallic foams



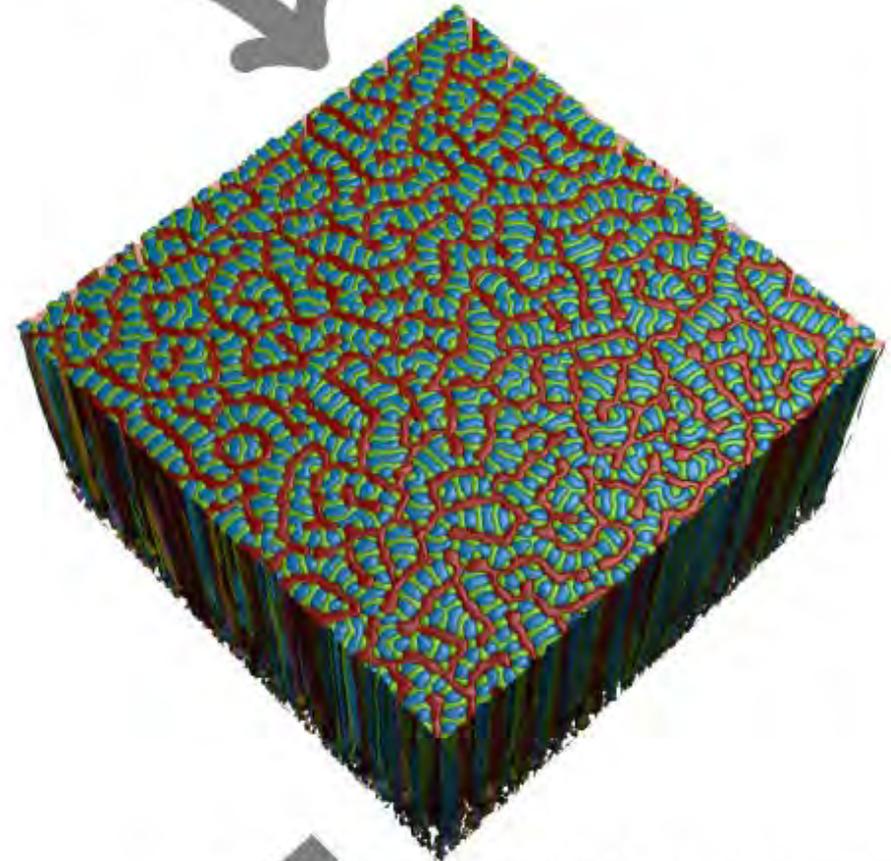
Data flow of Post-Processing



Data flow: Comparison Experiment - Simulation

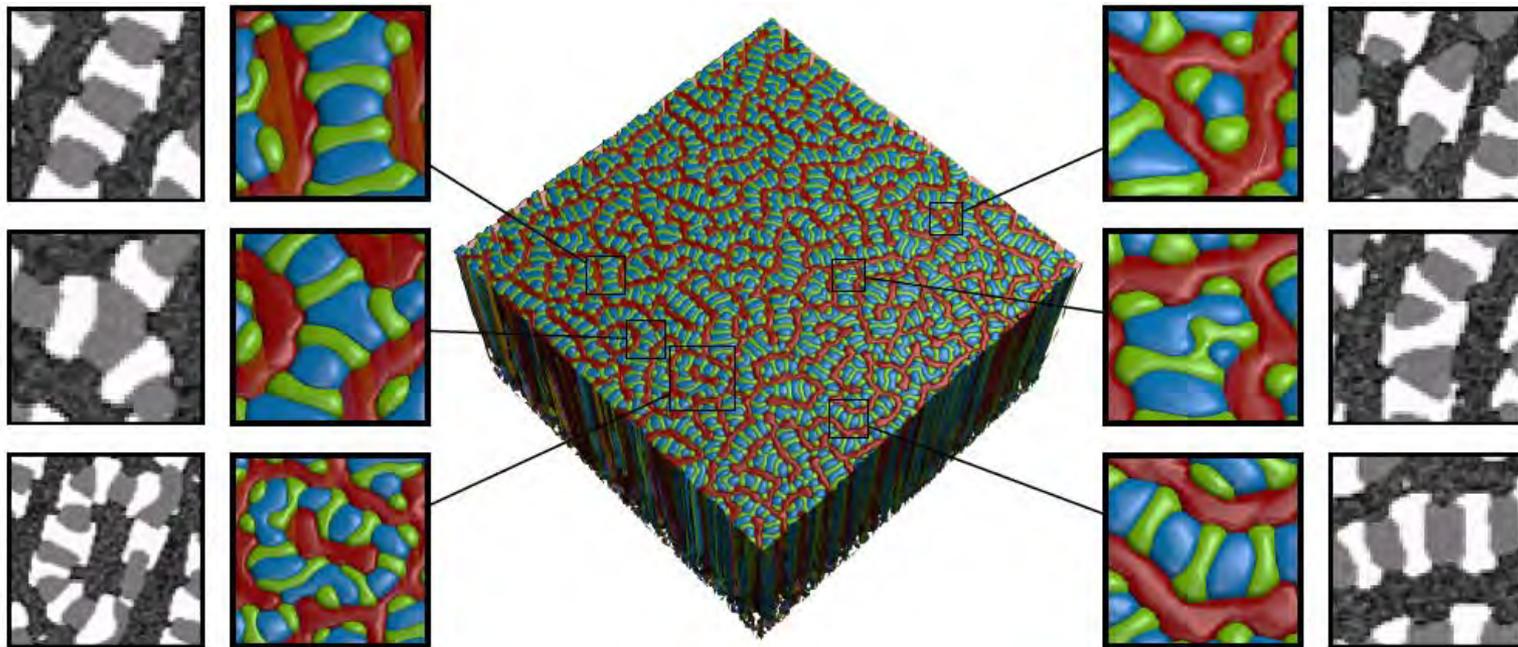


tomography of experimental Al-Ag-Cu structure of A. Dennstedt from DLR

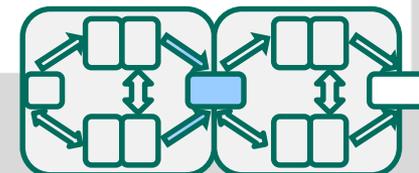


3D phase-field simulation of Al-Ag-Cu of $2420 \times 2420 \times 1474$ voxels on 84700 cores

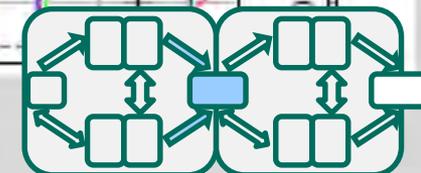
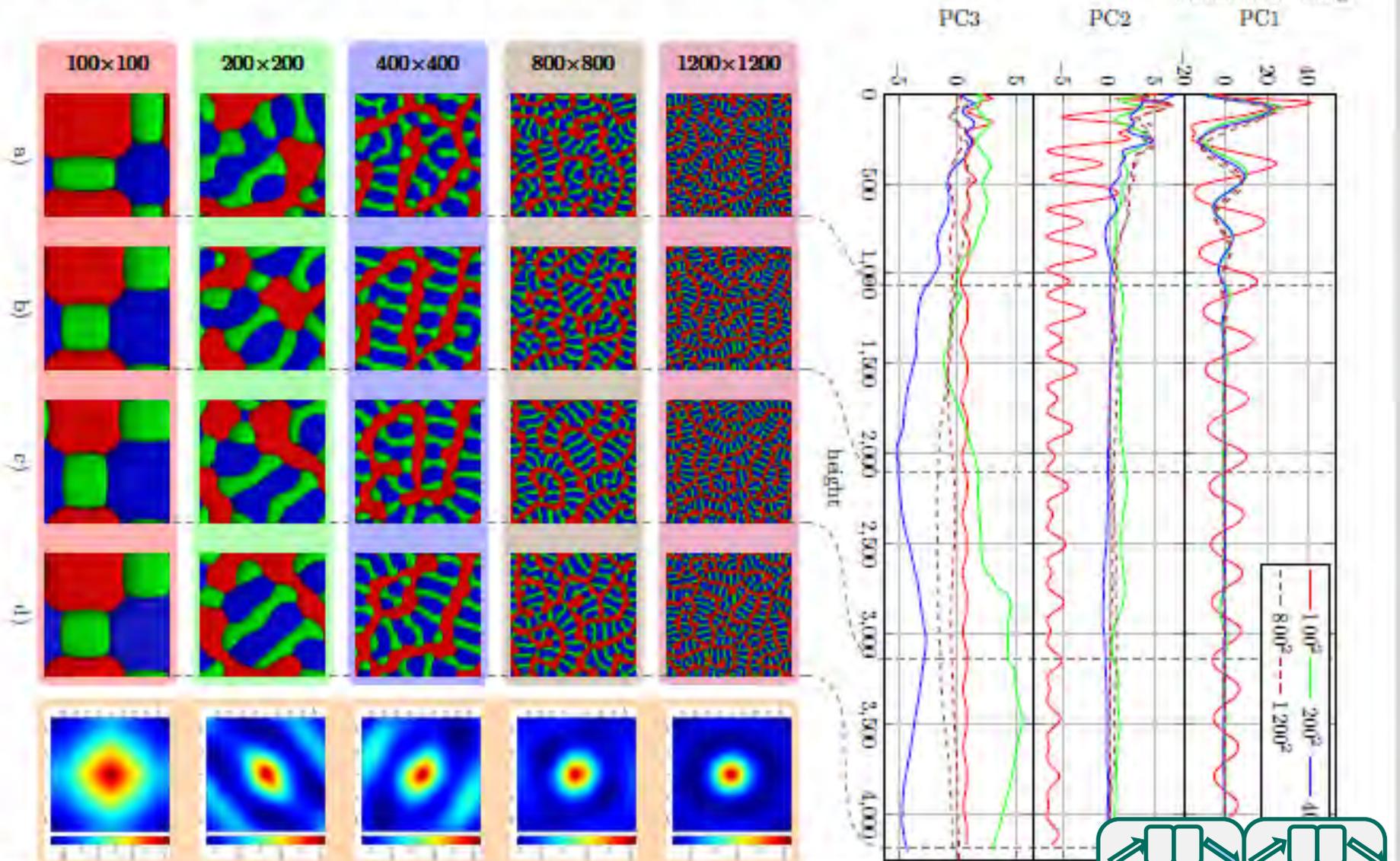
Microtomography and simulations of directional solidification in a ternary eutectic Al-Ag-Cu alloy



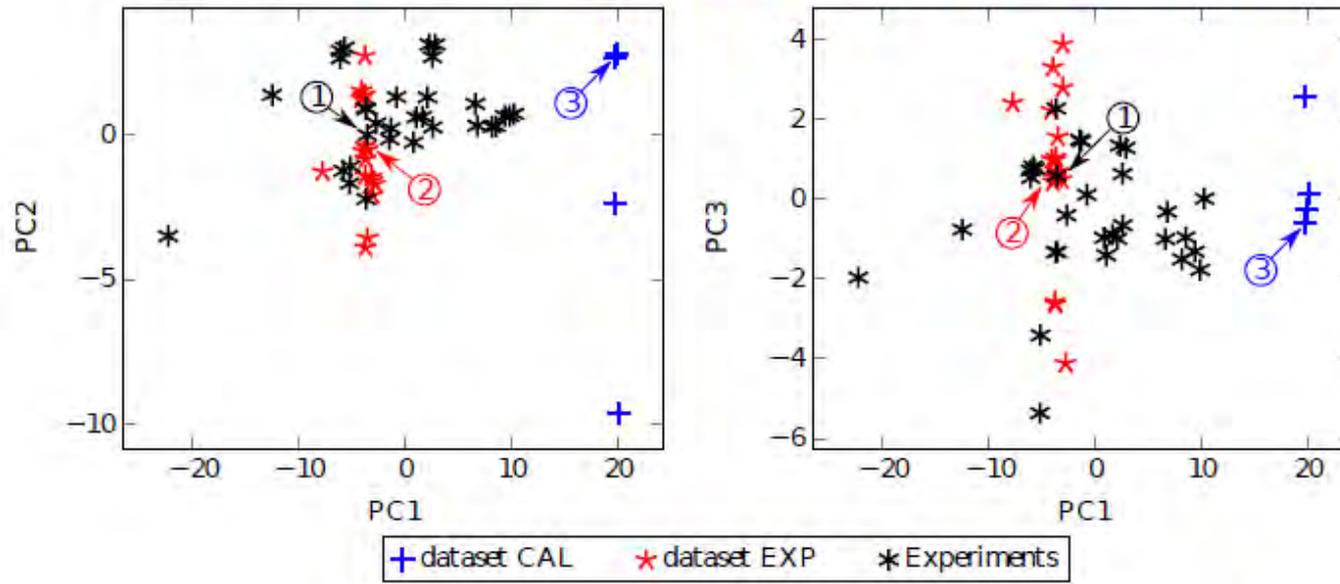
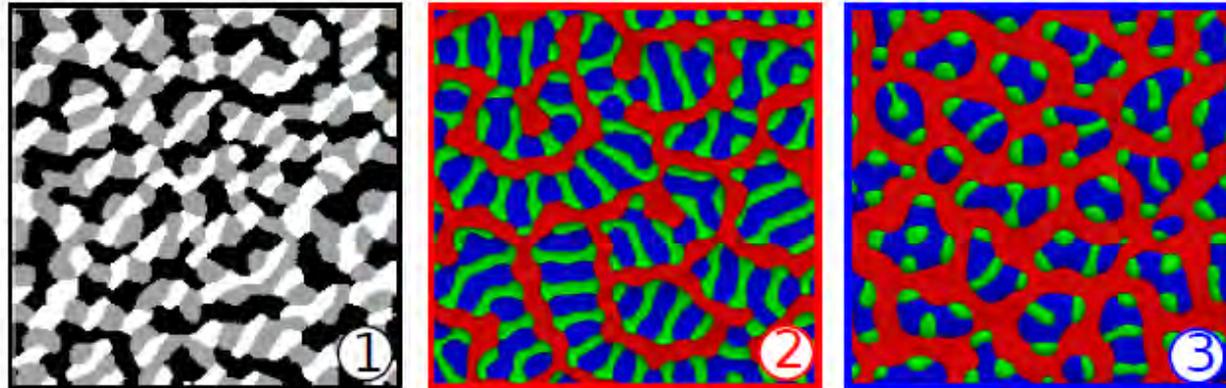
- Massiv Parallel Microstructure Simulation on high computer systems
- Pattern characterization, derivation of morphology diagrams
- Cooperation with A. Dennstedt, L. Ratke, DLR Cologne
- Cooperation with S. Kalidini, Georgia Tech., USA



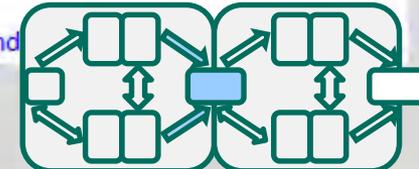
Data flow: Determination of RVE



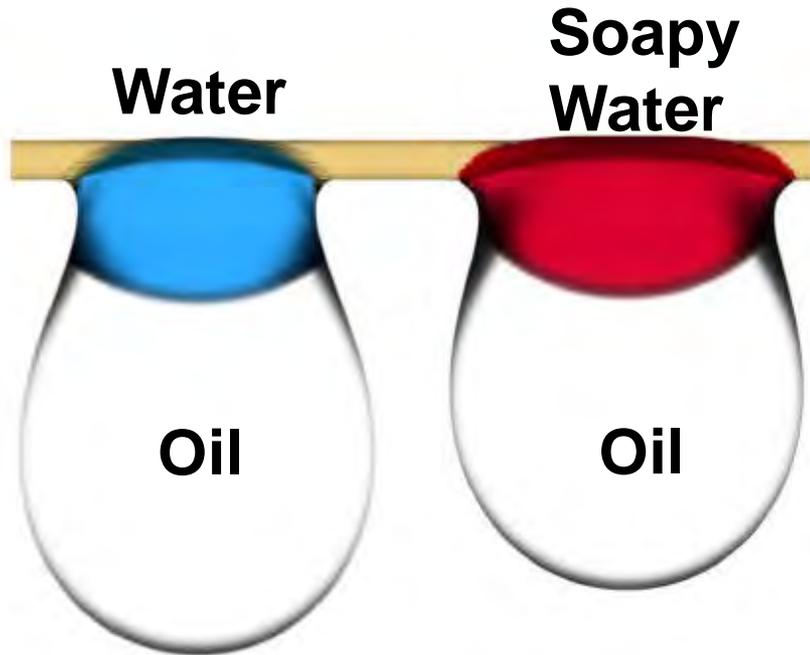
Data flow: Principal component analysis of experimental and simulated microstructures



Steinmetz, Yabansu, Hötzer, Jainta, Nestler and



Data flow: Comparison Experiment - Simulation

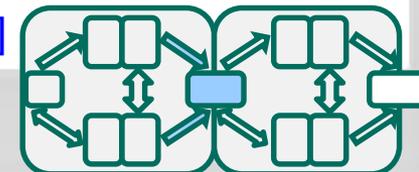


Simulation

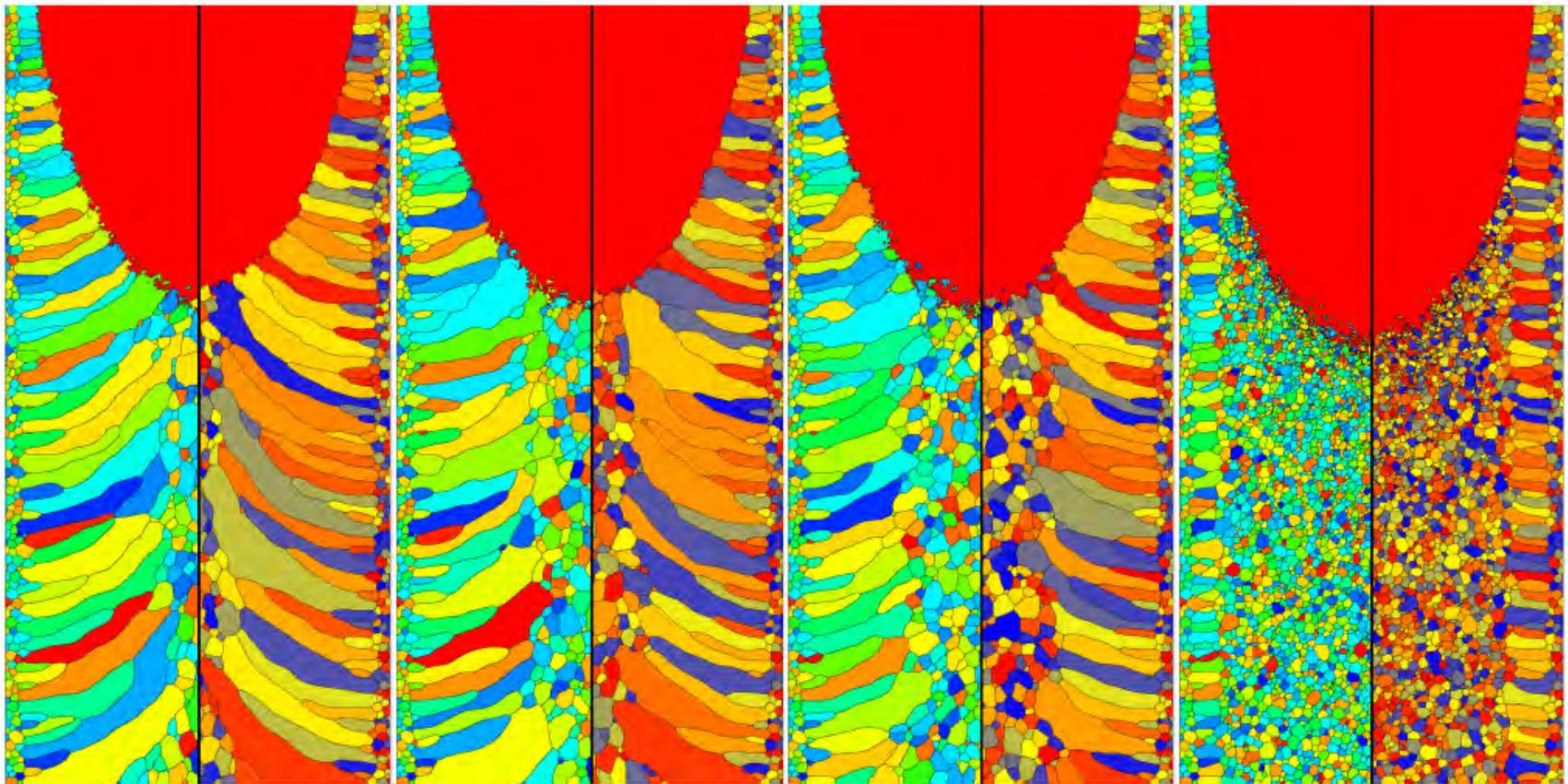
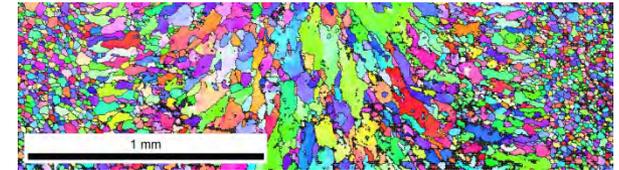


Experiment

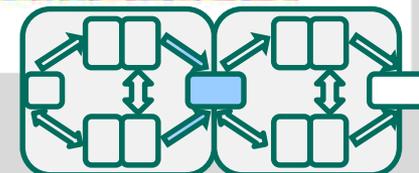
[F. Weyer, M. Ben Said, J. Hötzer, M. Berghoff, L. Dreesen, B. Nestler, N. Vandewalle, Compound Droplets on Fibers, Langmuir 31, Issue 28, ISSN: 07437463, DOI: 10.1021/acs.langmuir.5b01391. (2015) 7799-7805]



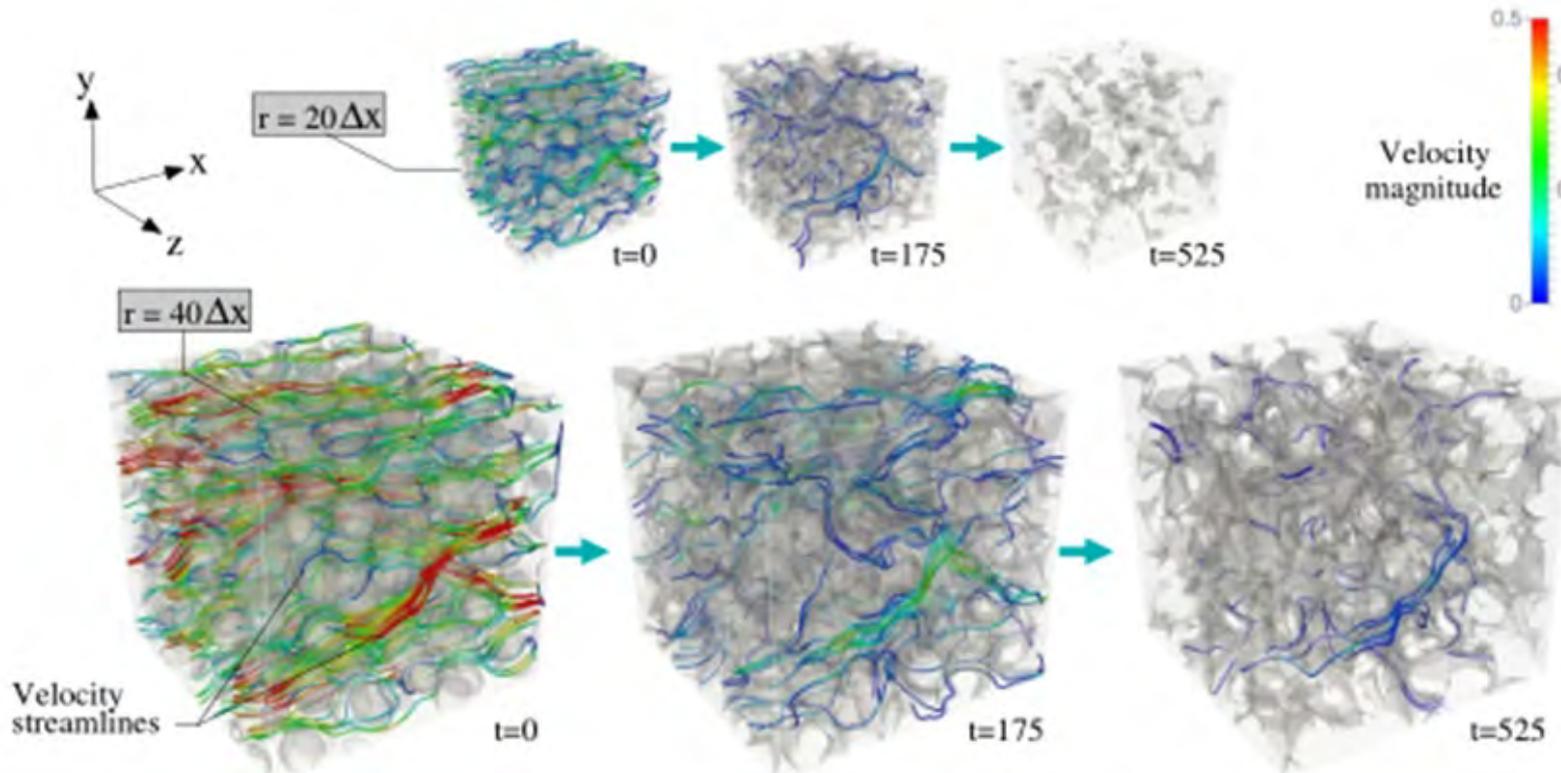
Grain structure formation in welding processes



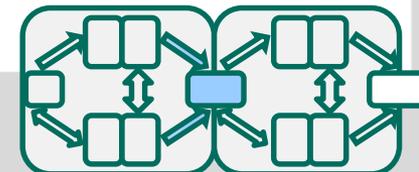
[O. Tschukin, Dissertation 2017]



- Velocity stream lines for different stages of cementation, time evolution of permeability, permeability-porosity relations for different grain sizes

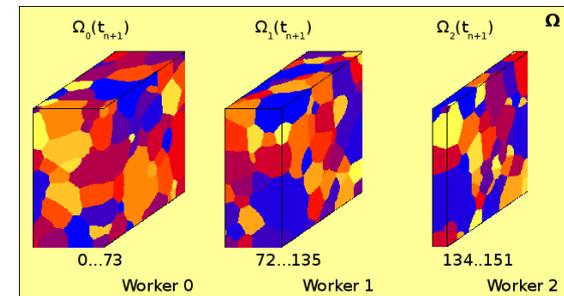


[N. Prajapati, M. Selzer, B. Nestler, *Geothermal Energy* 5, no. 1 (2017), N. Prajapati, K. Ankit, M. Selzer, B. Nestler, B. Busch, C. Hilgers, (2018) submitted]



Software solution – Pace3D (IAM-CMS)

- ◆ 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 parallelly 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
- ◆ Huge package of pre- and postprocessing methods



Documentation Handbook

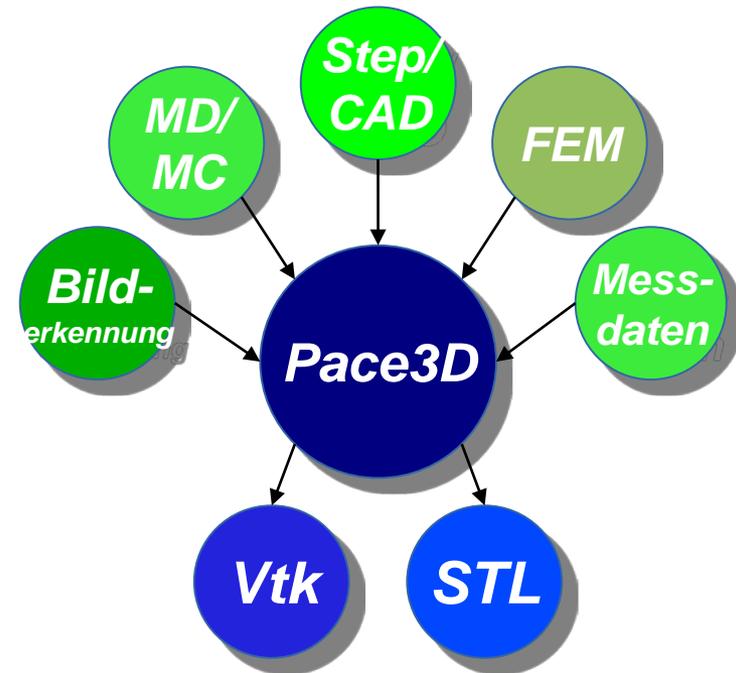
- Mehr als 600 Einstellmöglichkeiten
- Annotationsprache, die im Code Beschreibungen, Kommentare und physikalische Einheiten hinterlegt
- Generierung einer Benutzerdokumentation aus den Annotationen
- Typsichere Benutzeroberfläche
- Latex-Dokumentationskonzept zur Komposition einzelner Dokumente zu einem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



Activities in Committees and Workshops

- Mitglied des HLRS-Lenkungsausschusses (nationale Hochleistungsrechner)
- Mitwirkung bei der Erstellung eines Positionspapiers „Roadmap zu einer Digitalisierung der Materialwissenschaften“ in Zusammenarbeit mit DFG, DGM und Gesprächen mit dem BMBF
- Mitwirkung und Repräsentation der Digitalisierung in der Materialforschung für die NFDI – Nationale Forschungs-Daten-Infrastruktur
- Repräsentation bei dem BMBF Workshop „Material Digital – Schienenlegung und Weichenstellung für die Zugkraft der digitalisierten Materialforschung“
- Impulsbeitrag bei der BMBF-Materialkonferenz 4. bis 6. Juni 2018 in München
- Mitwirkung bei dem Workshop zum Forschungsdatenmanagement in den Ingenieurwissenschaften am 08. und 09. März 2018

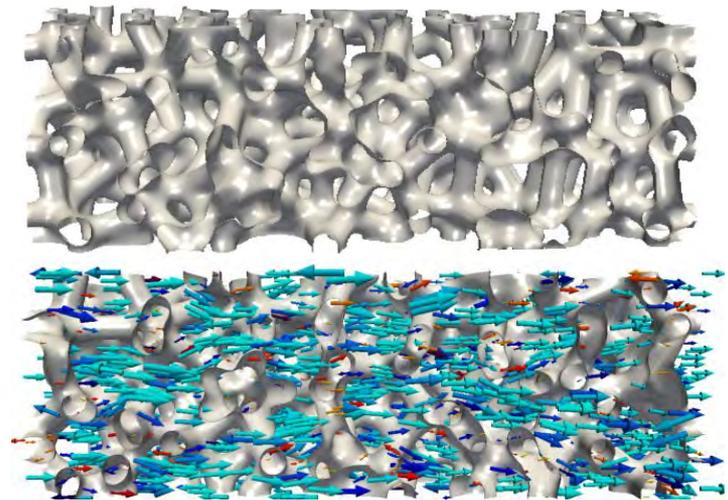
Awards

- doIT Software-Award 2004 and 2007, Stiftung Baden-Württemberg
- Gottfried-Wilhelm Leibniz Prize 2017, DFG

Third Party Funding

- Virt-Mat project, „Computational design of nanoporous structures for printed electronics”, Helmholtz funded
- DFG project “Sustainable Lifecycle Management for Scientific Software (SuLMaSS)” together with SCC, RDM and library, funded
- DFG Cluster of Excellence “AESC Algorithm Engineering for the Scalability Challenge”, in evaluation process
- DFG Cluster of Excellence “Energy Storage beyond Lithium”, in evaluation process
- DFG Transregio SFB TrimMat, Data management cross section, in evaluation process
- DFG Research Training Group MatCost, Data management cross section, in preparation
- DFG Research Training Group “Environmental Interface Studies”, Data management cross section, in preparation

Nanoporous structure and permeability:



Stability analysis of inkjets:



- P. Altschuh, Y. C. Yabansu, J. Hötzer, M. Selzer, **B. Nestler**, S. R. Kalidindi, Data science approaches for microstructure quantification and feature identification in porous membranes, *Journal of Membrane Science* 540, ISSN: 03767388, DOI: 10.1016/j.memsci.2017.06.020. (2017) 88-97
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