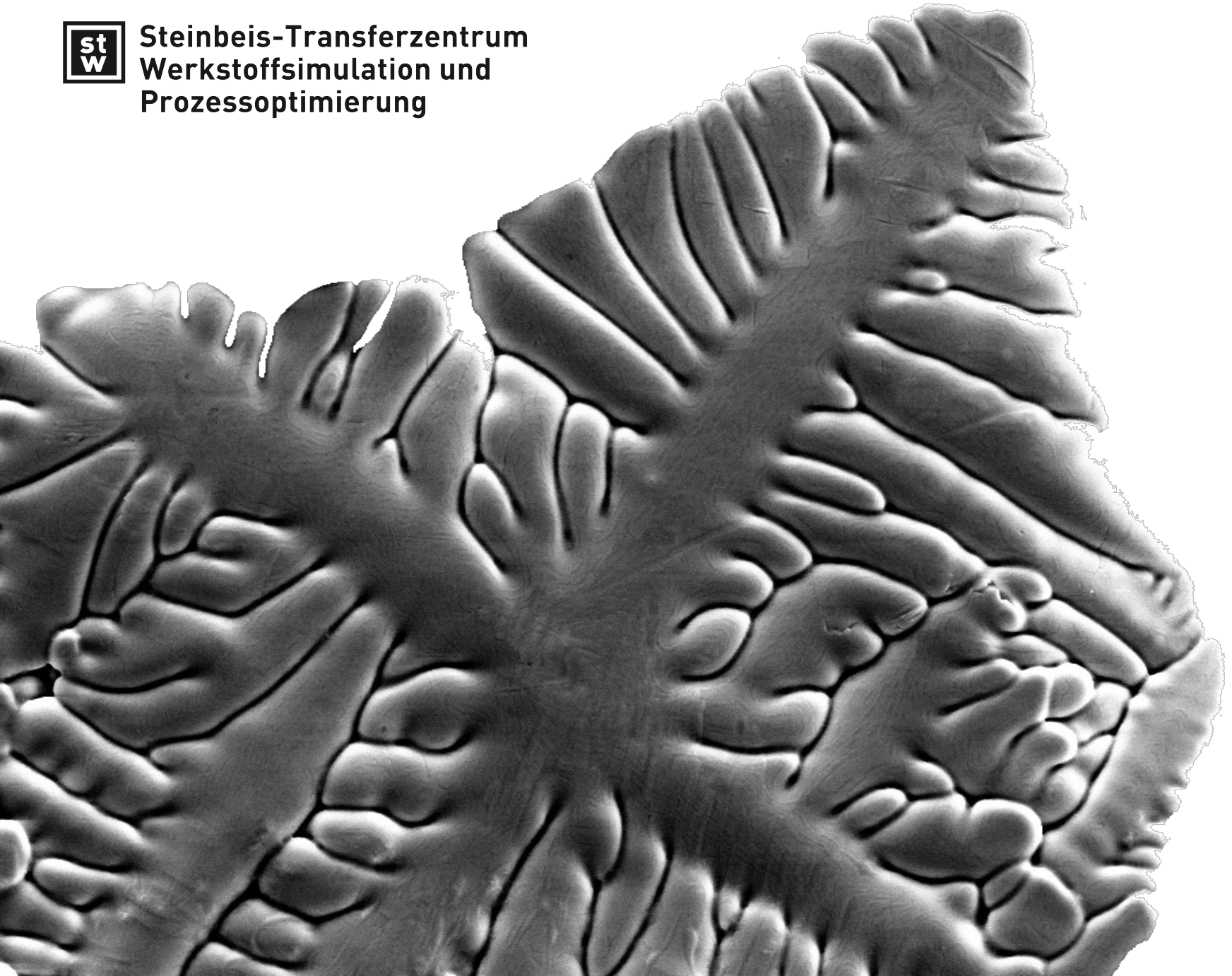




**Steinbeis-Transferzentrum
Werkstoffsimulation und
Prozessoptimierung**

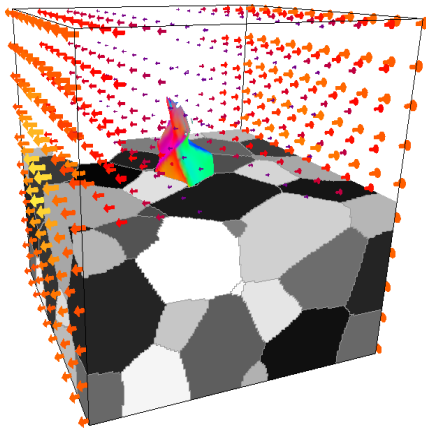


Visualisation methods and post-processing of volume data

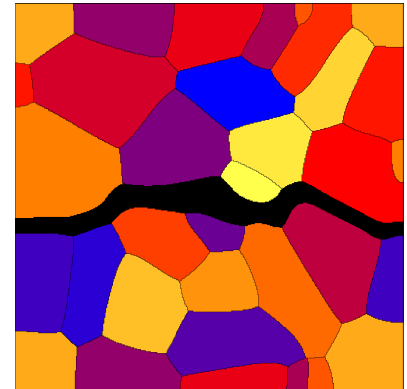
Michael Selzer

Steinbeis-Transferzentrum

Werkstoffsimulation und Prozessoptimierung



- ◆ Overview
- ✗ Scales
- ✗ Modelling
- ✗ Softwarepackage PACE3D
- ◆ Outlook

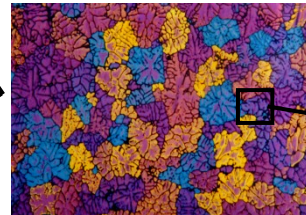


Processes on multiple scales

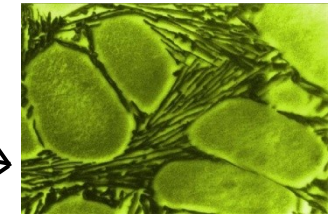
Experiment



macroscopic component

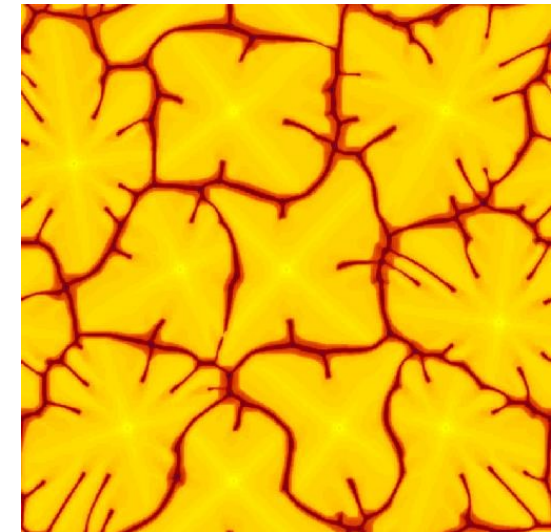
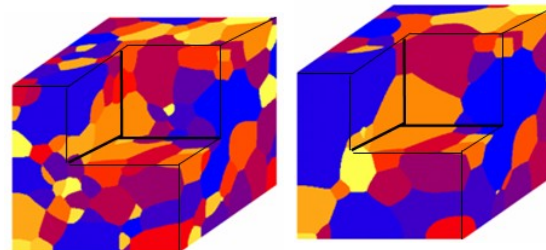
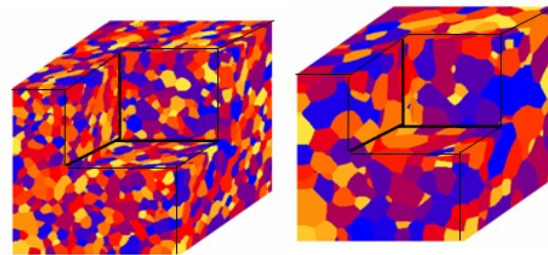
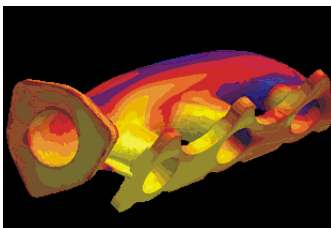
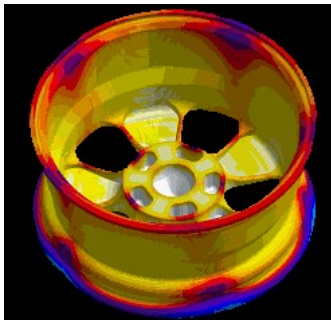


grain structure



solidification
microstructure

Simulation



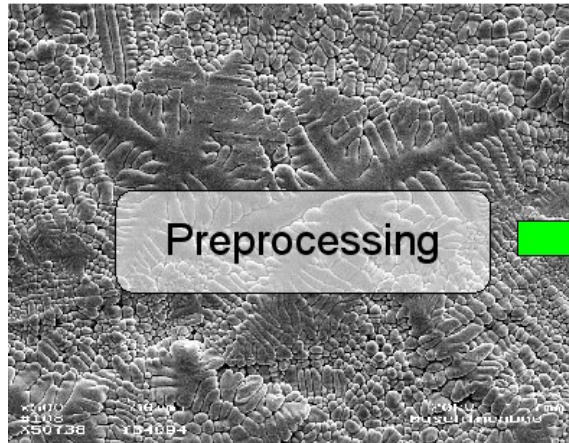
Workflow



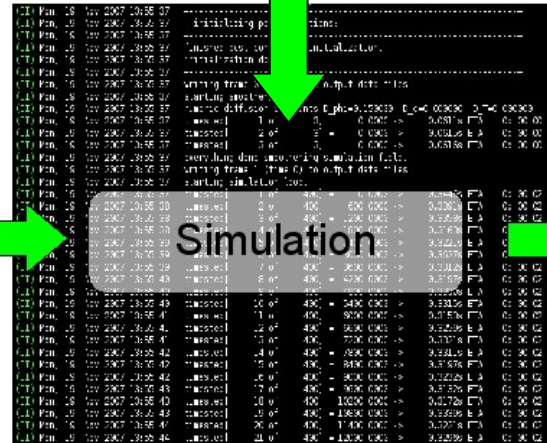
Model development

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

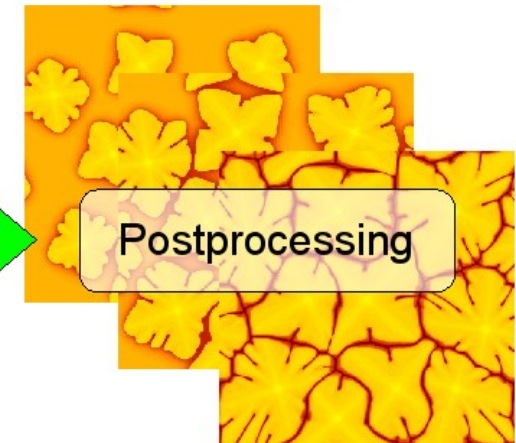
$$\frac{\partial \phi_\alpha}{\partial t} = \varepsilon \left(\nabla \cdot a_{\nabla \phi_\alpha} - a_{\phi_\alpha} \right) - \frac{1}{\varepsilon} w_{\phi_\alpha} - \frac{f_{\phi_\alpha}}{T} - \lambda$$



Preprocessing



Simulation



Postprocessing

- ✗ conversion of experimental data, e.g. from cross sections, EBSD
- ✗ software interface to connect atomistic simulations, e.g. MD
- ✗ coupling of thermodynamical data base, e.g. Calphad

- ✗ parallel implementation
- ✗ adaptive and fast algorithms
- ✗ modulare software design
- ✗ easy extendability

- ✗ available library of various methods for data evaluation and process analysis
- ✗ 3D visualization
- ✗ various graphical illustrations

Workflow



Model development

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Preprocessing



Simulation



Postprocessing

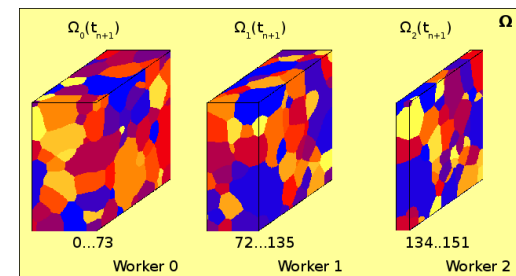
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PACE3D - Parallel Algorithms for Crystal Evolution

- ◆ Implementation in C, C++ for Linux
- ◆ the PACE3D - package contains modules for the solution of various applications:
 - ✗ phase-field models for microstructure formations in multicomponent and multiphase materials
 - ✗ descriptions for inert particles and volume preserved phases
 - ✗ CFD solvers for modelling fluid flow processes based on the Navier-Stokes equations and on the Lattice-Boltzmann method
 - ✗ elasticity and magnetism
- ◆ simulations can be run sequentially or parallelly using MPI on high performance computers
- ◆ the discretization works with staggered grids
- ◆ performance-optimization of the software is achieved by adaptive meshes, computing time and memory saving algorithms, dynamical domain decomposition and data compression
- ◆ the software has a modular structure with a library of different model formulations
- ◆ the PACE3D - package contains pre- and postprocessing methods



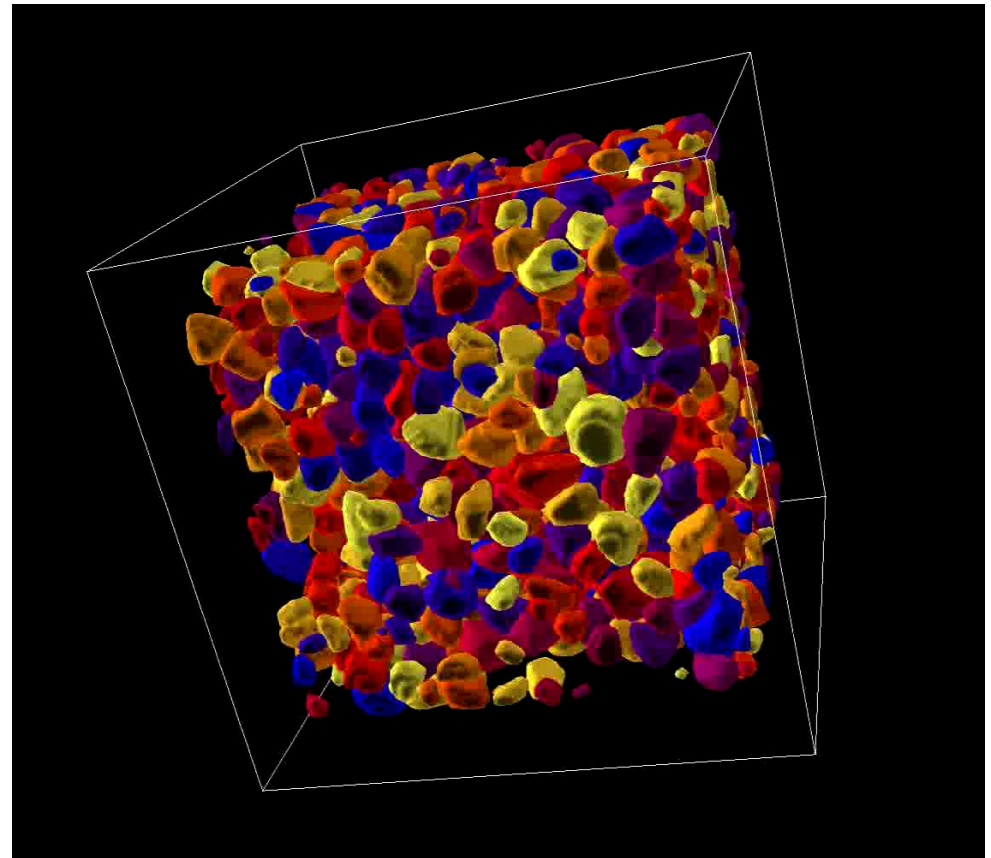
Shrinkage of powder particles during a sintering process

Simulation configuration:

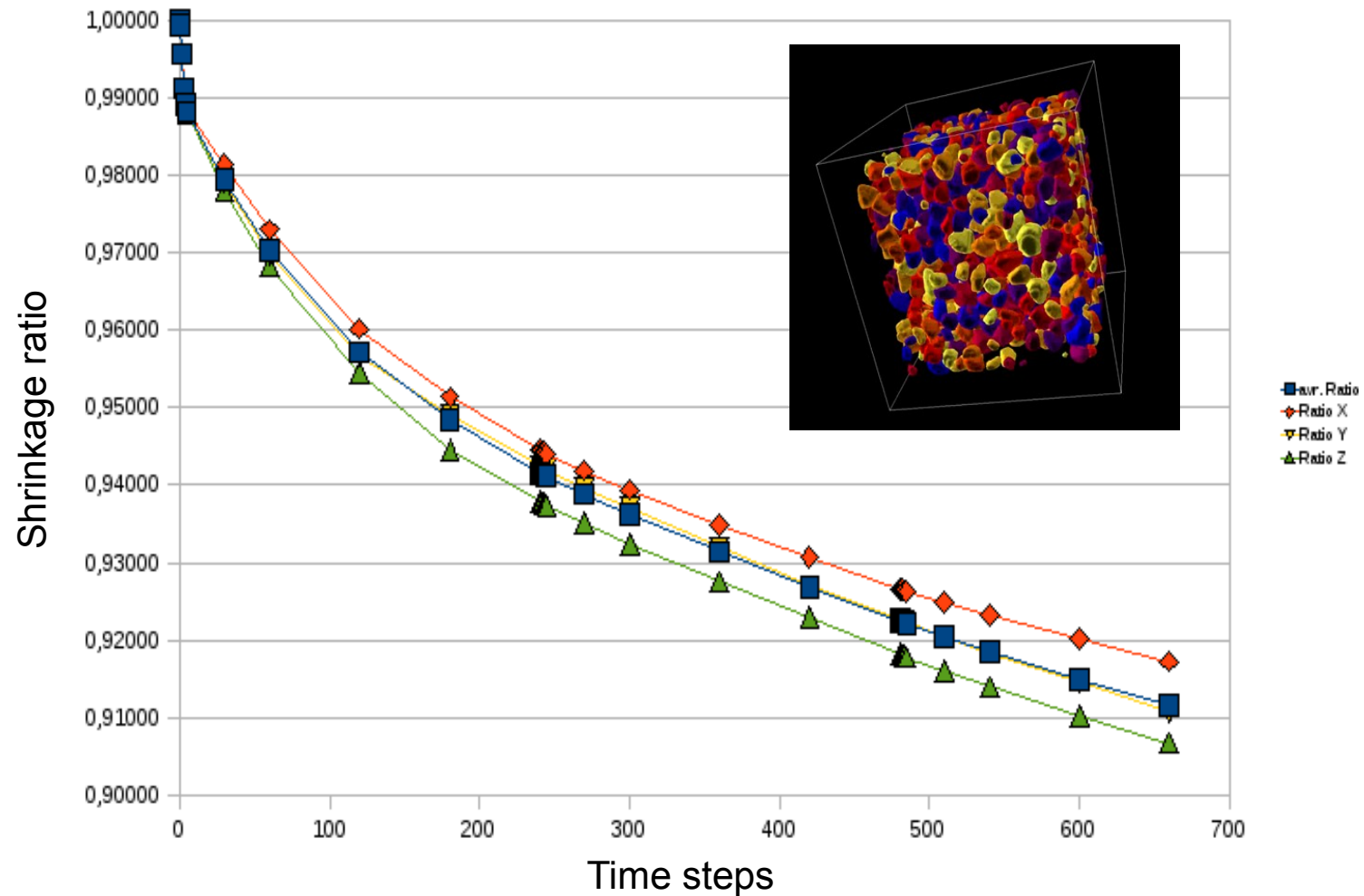
- 600^3 cells
- 1200 particles
- random number of edges and orientations for anisotropic surfaces of the powder particles
- volume constraints for each particle to compute initial structure
- ratio of gas and particle volumes from experiments (IKM, Hoffmann)

Simulation run:

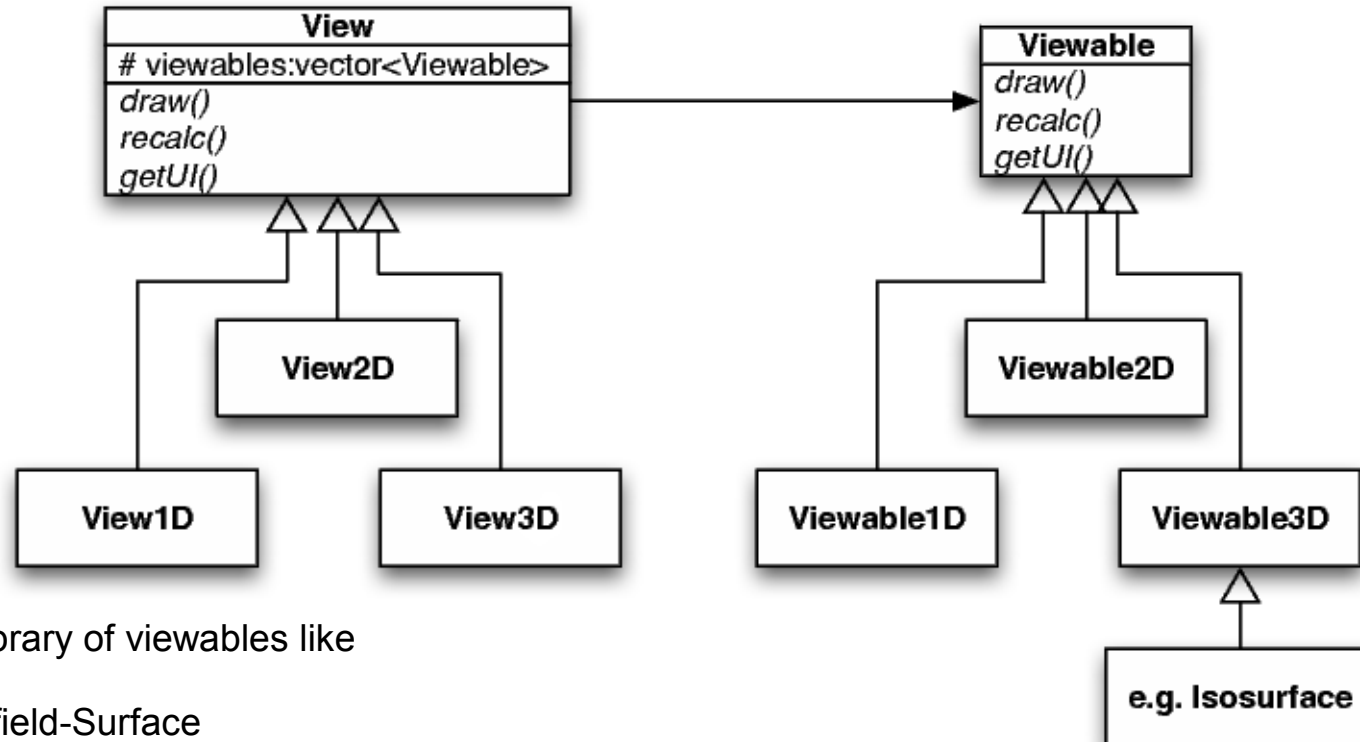
- gas phase is volume preserved
- computation of coarsening
- evaluation of shrinkage rate / porosity



Shrinkage rate of powder particles



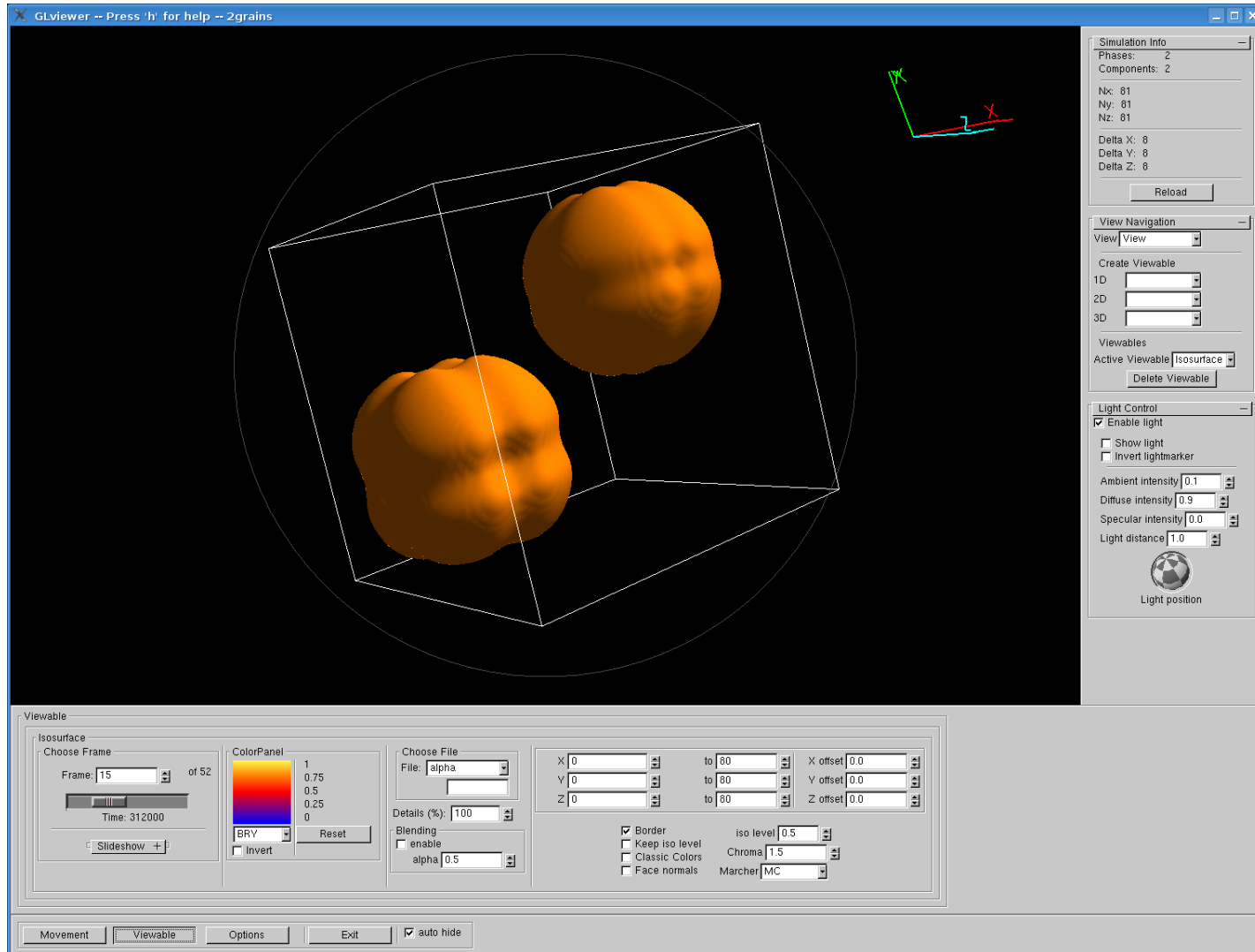
GLViewer – Brief architecture



Hugh library of viewables like

- Cube
- Phasefield-Surface
- Streamlines
- Heightmap
- ...

Visualization of simulation data - Workstation



Visualization of simulation data - CAVE



Business Model

- ✗ Pre- and Postprocessing of volume data
- ✗ Simulation of various physical properties on the mesoscopic scale including
 - fluid flow
 - phase transformation
 - elastic deformation

- ✗ Multiscale modelling: Meso - Macro
 - coupling of macroscopic boundary conditions with mesoscopic computations
 - derivation of microstructure - property correlations depending on the process conditions

- ✗ Application of methods to other material systems such as ceramics, biomimetic / biological systems and polymers
- ✗ Model extension to include further physical fields, e.g. plasticity

Visions

- ✗ development of methods for scale-, process step and material system bridging modelling and simulation
- ✗ process chains in manufacturing
- ✗ professionalization of the software for a flexible industrial use in various applications