The Intersection of Simulation and Tomography

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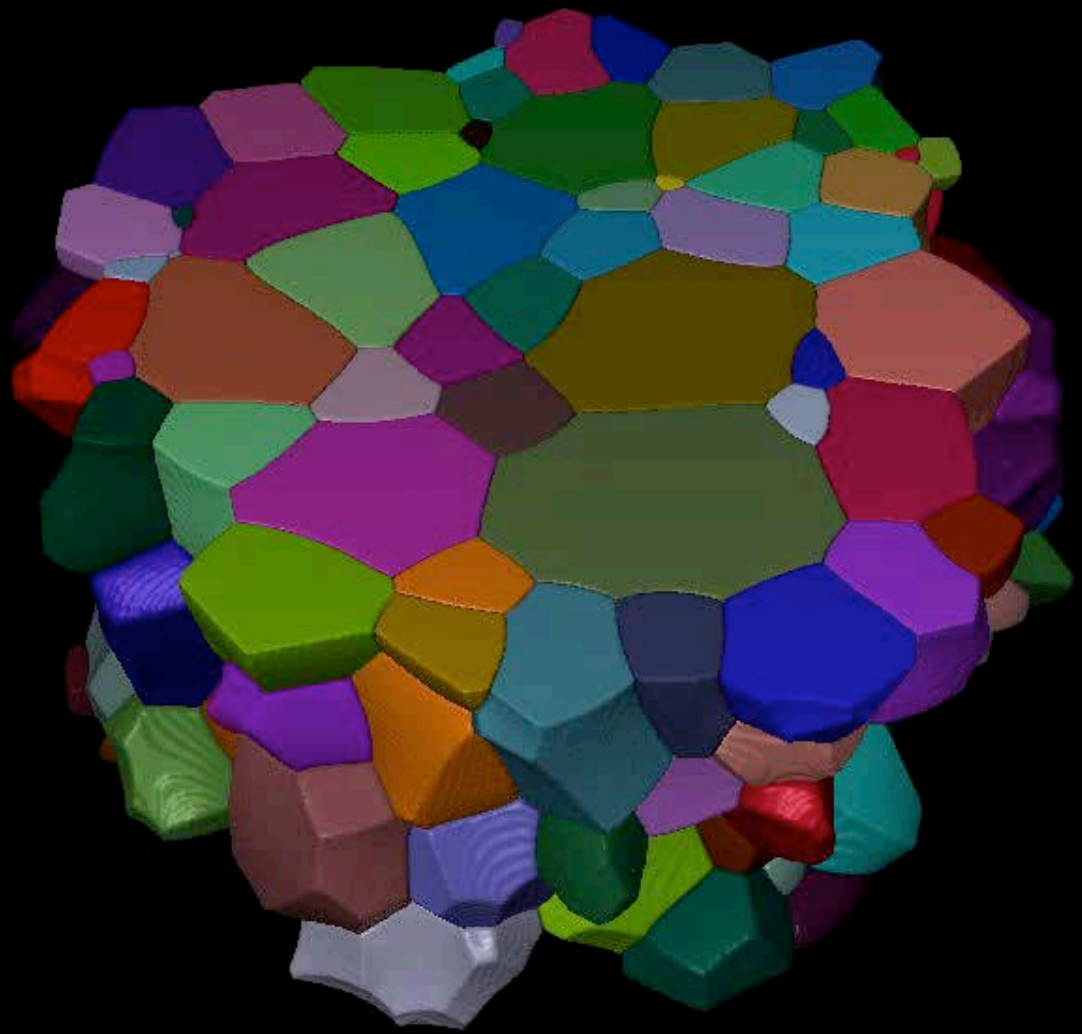
Outline

- Examples linking simulation and tomography
  - Grain growth
  - Solidification
- Why is this important?



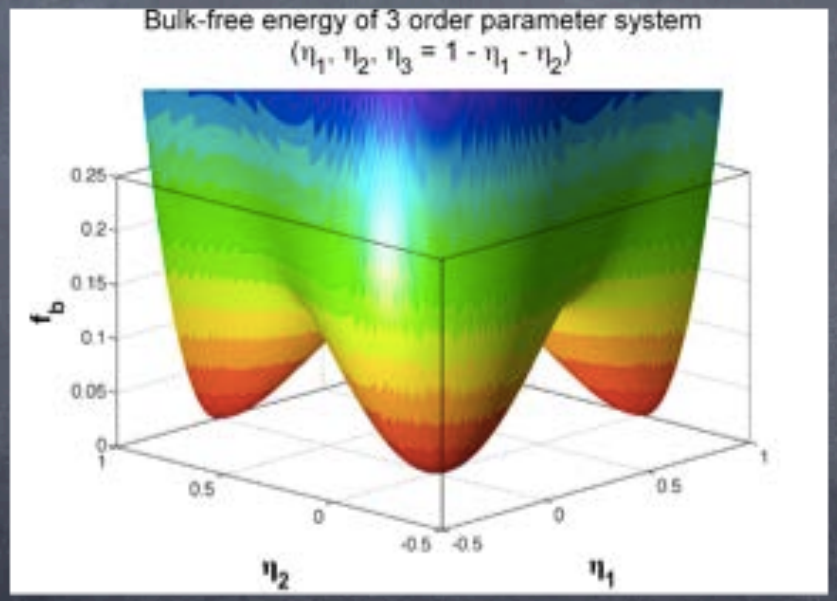
$V = -MH$

Trijunctions 120 deg

Phase Field Method for Isotropic Grain Growth

Dynamics: Energy must always decrease

$$\frac{\partial \eta_q}{\partial t} = -M\left(\frac{\partial f_b}{\partial \eta_q} + K\nabla^2\eta_q\right) \quad \text{for} \quad q = 1\ldots N$$



S.M. Allen and J.W. Cahn, Acta Materiala 1979, L.Q Chen and W. Yang, Phys. Rev.B, 1994.

Phase Field Method for Grain Growth

Advantages:

- No need to track interfaces (diffuse interface)
- Can follow grain boundary evolution through topological transitions, e.g. face removal and addition

Disadvantages:

- Diffuse interface is much thicker than real grain boundary thicknesses
- However, $V=-MH$ can be obtained in the limit $\delta H \ll 1$

δ

Comparison Between Simulation and Experiment

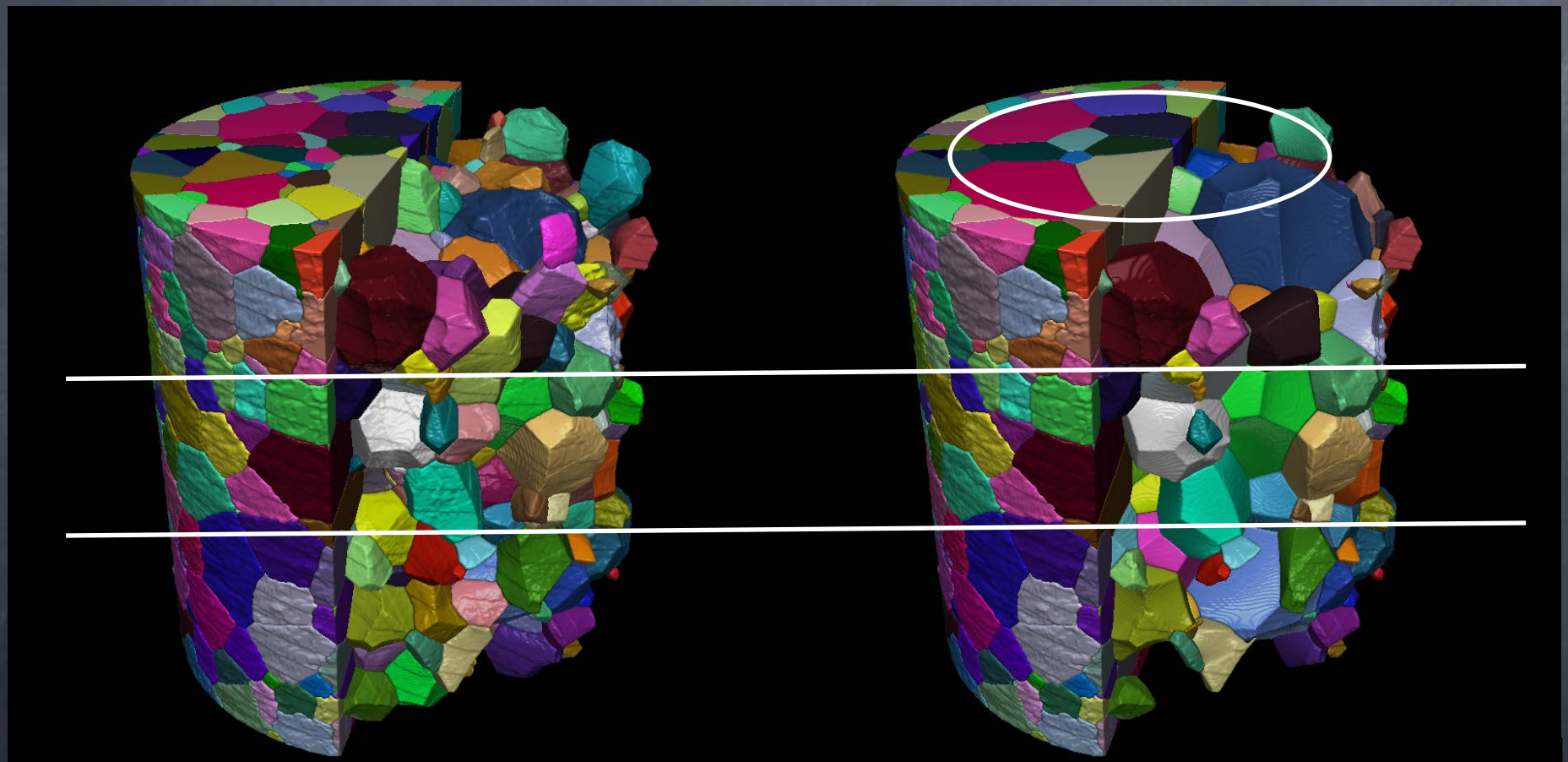
- Always done by comparing statistically averaged quantities: e.g. Grain size distribution, average grain size, average number of faces per grain...

- We adopt a different approach: Compare the morphologies and grain sizes of individual grains

Does a phase field simulation predict the correct grain topology and morphology?

Approach

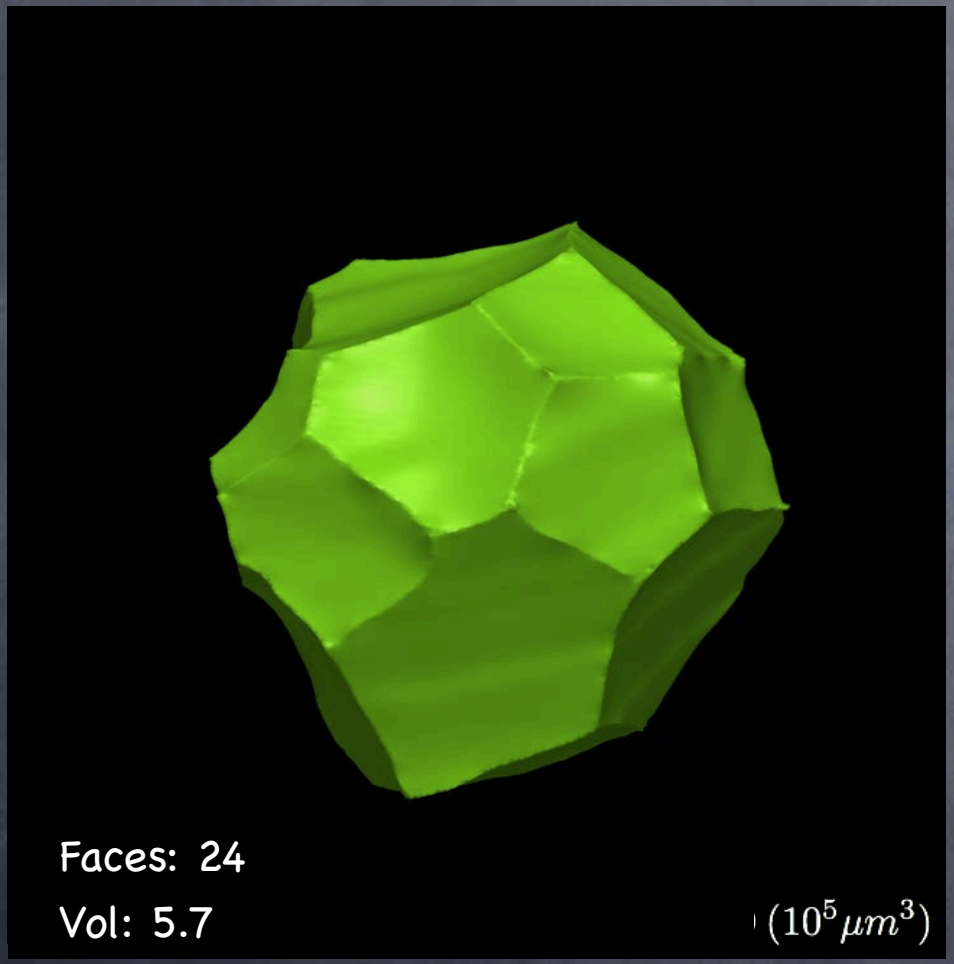
Use experimentally measured grain network in Ti-21S as an initial condition in a phase field model of model of grain growth



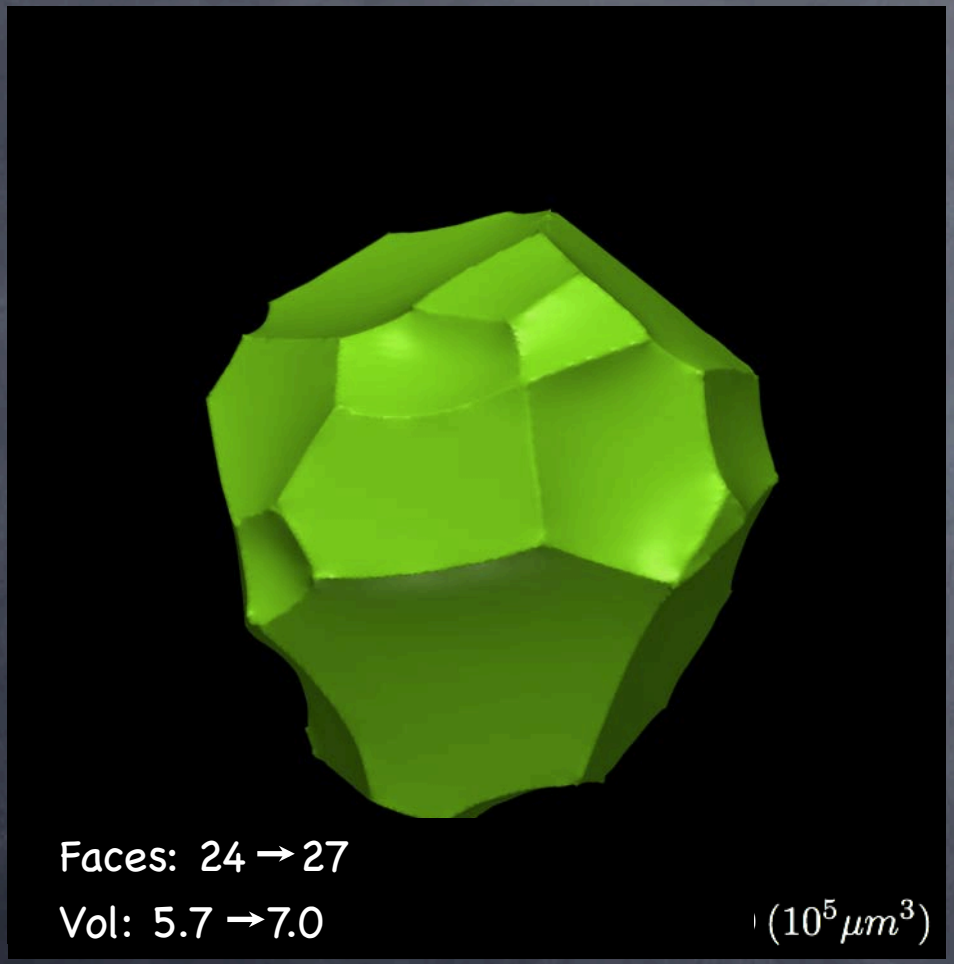
Goal: compare the morphology of individual grains

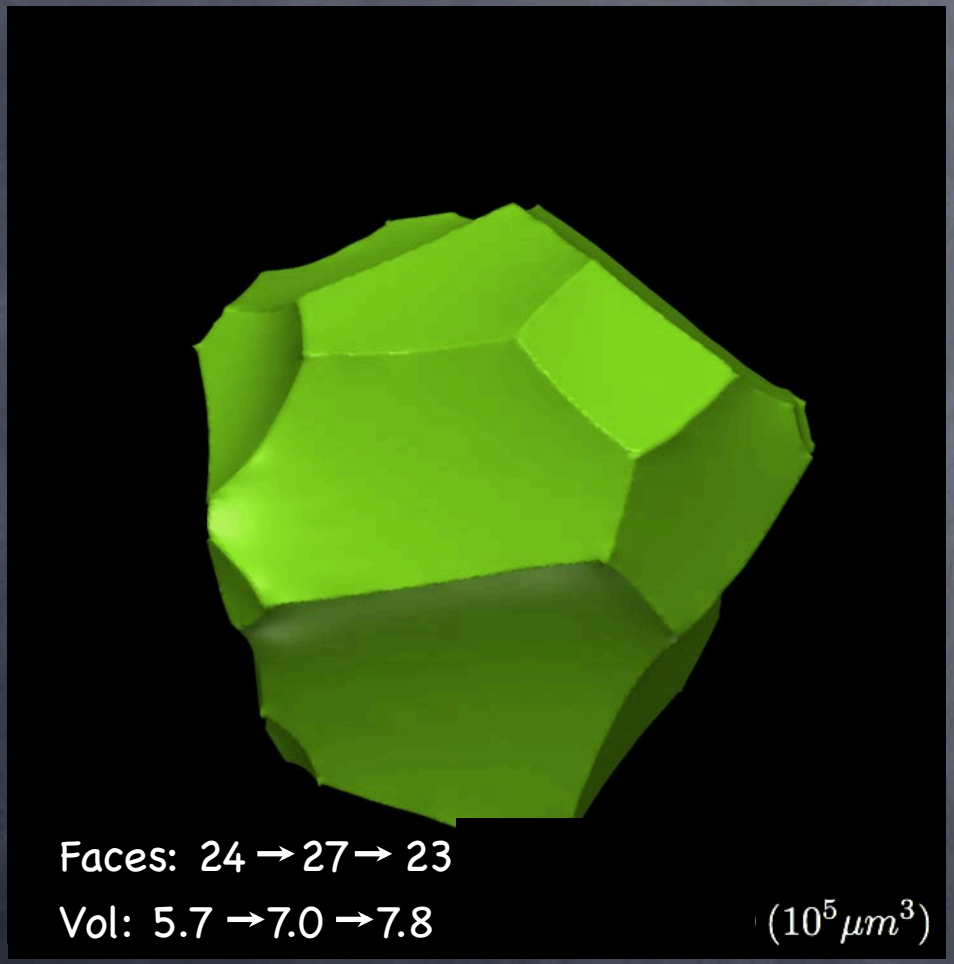
Experimental time 1

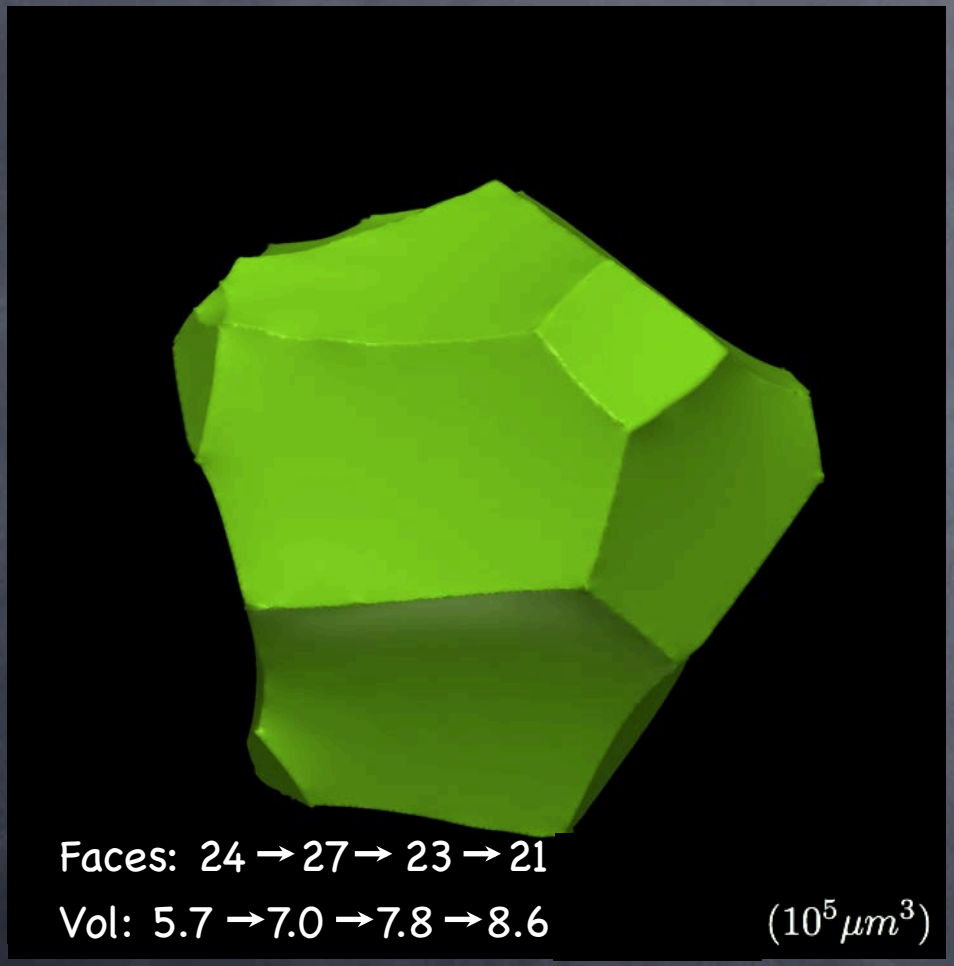
Simulation time 2

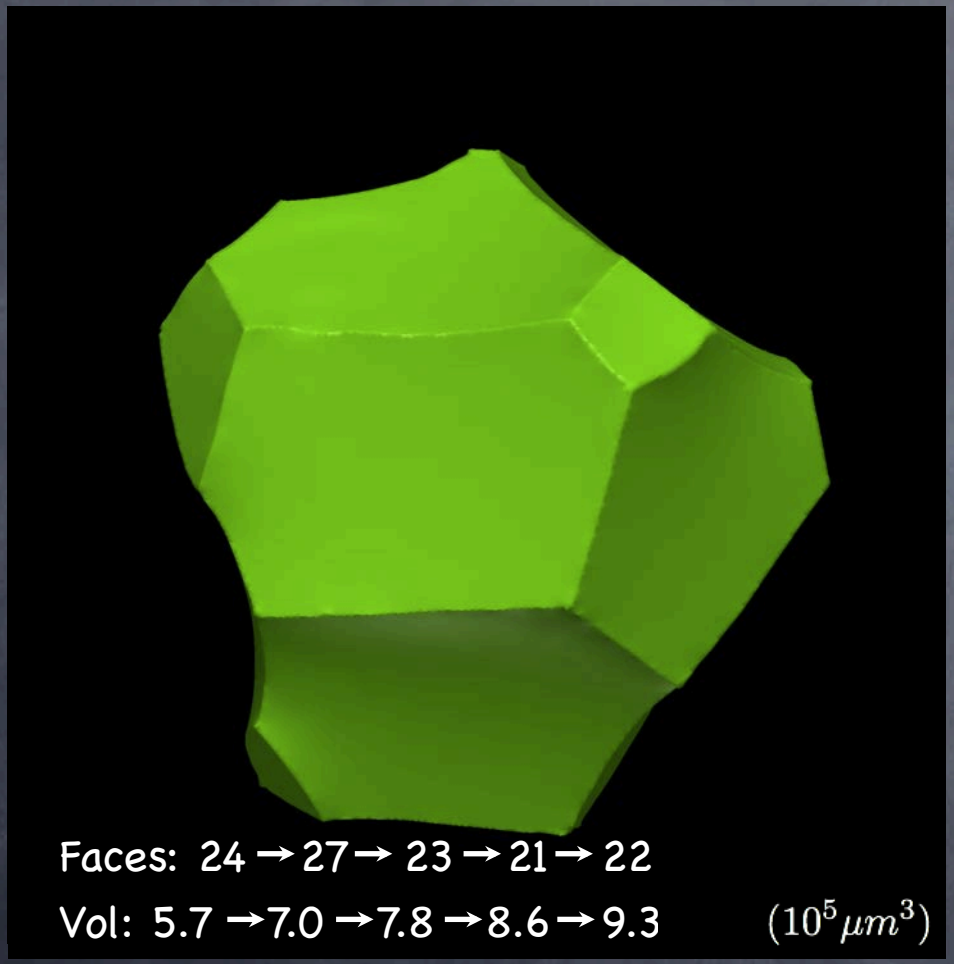


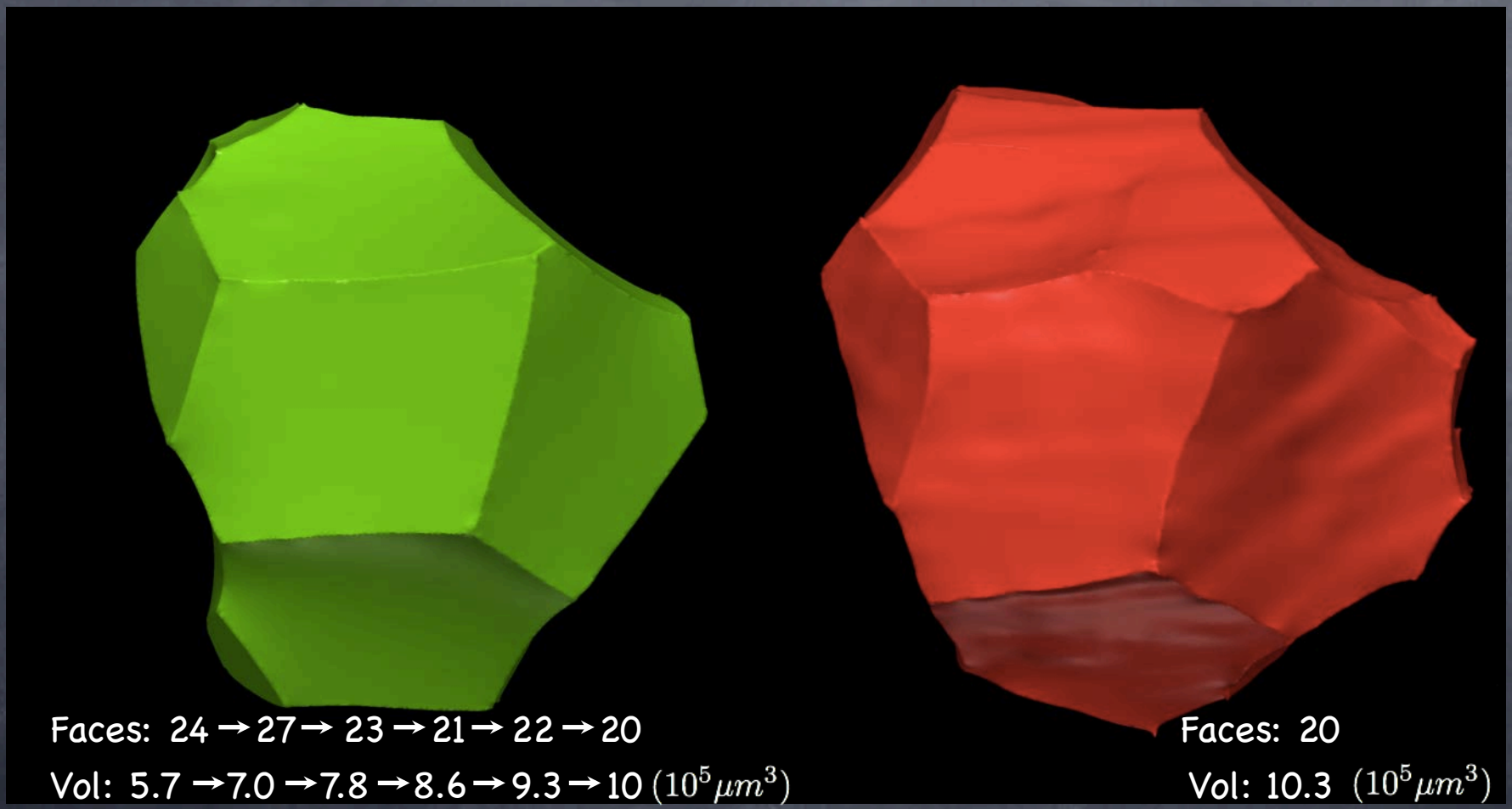
Experimental time 1


Faces: 24 → 27
Vol: 5.7 → 7.0
$(10^5 \mu m^3)$


Faces: 24 → 27 → 23
Vol: 5.7 → 7.0 → 7.8
$(10^5 \mu m^3)$


Faces: 24 → 27 → 23 → 21
Vol: 5.7 → 7.0 → 7.8 → 8.6
$(10^5 \mu m^3)$


Faces: 24 → 27 → 23 → 21 → 22
Vol: 5.7 → 7.0 → 7.8 → 8.6 → 9.3
$(10^5 \mu m^3)$

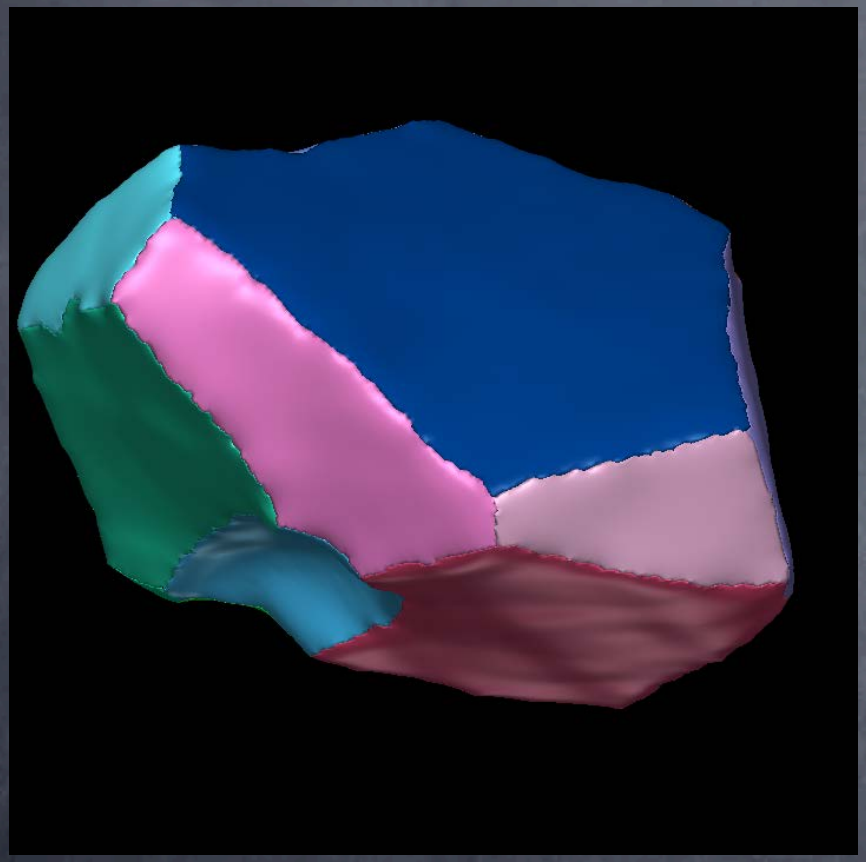


Isotropic simulation time 2 Experiment time 2

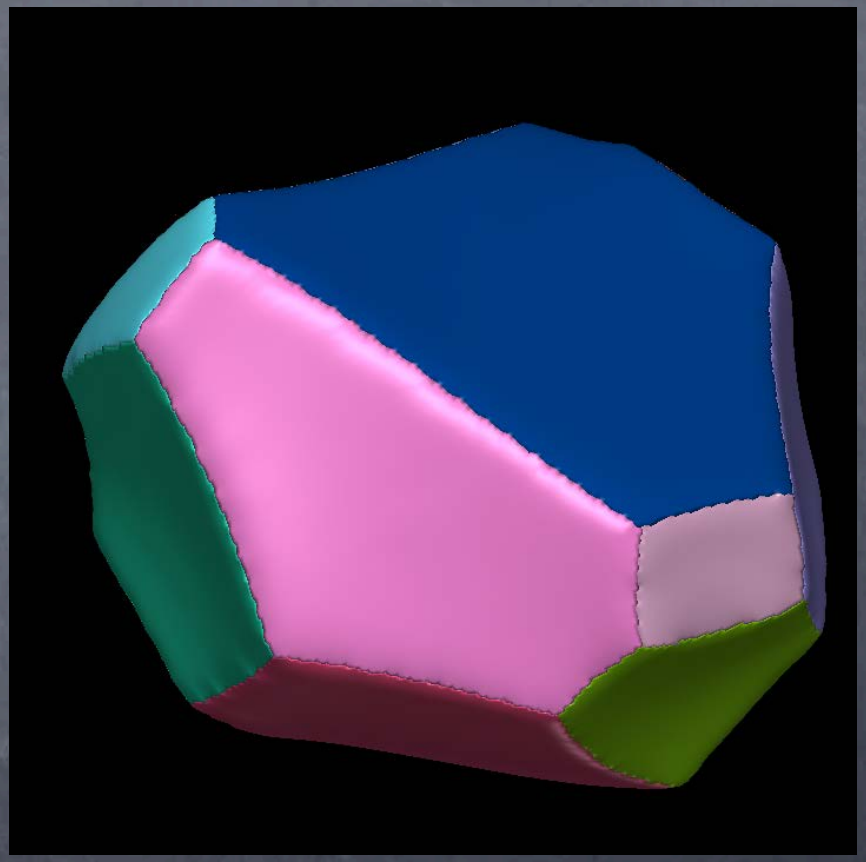
No scaling or rotation between simulation and experiment

The phase field method can correctly determine topological singularities and the velocity of boundaries

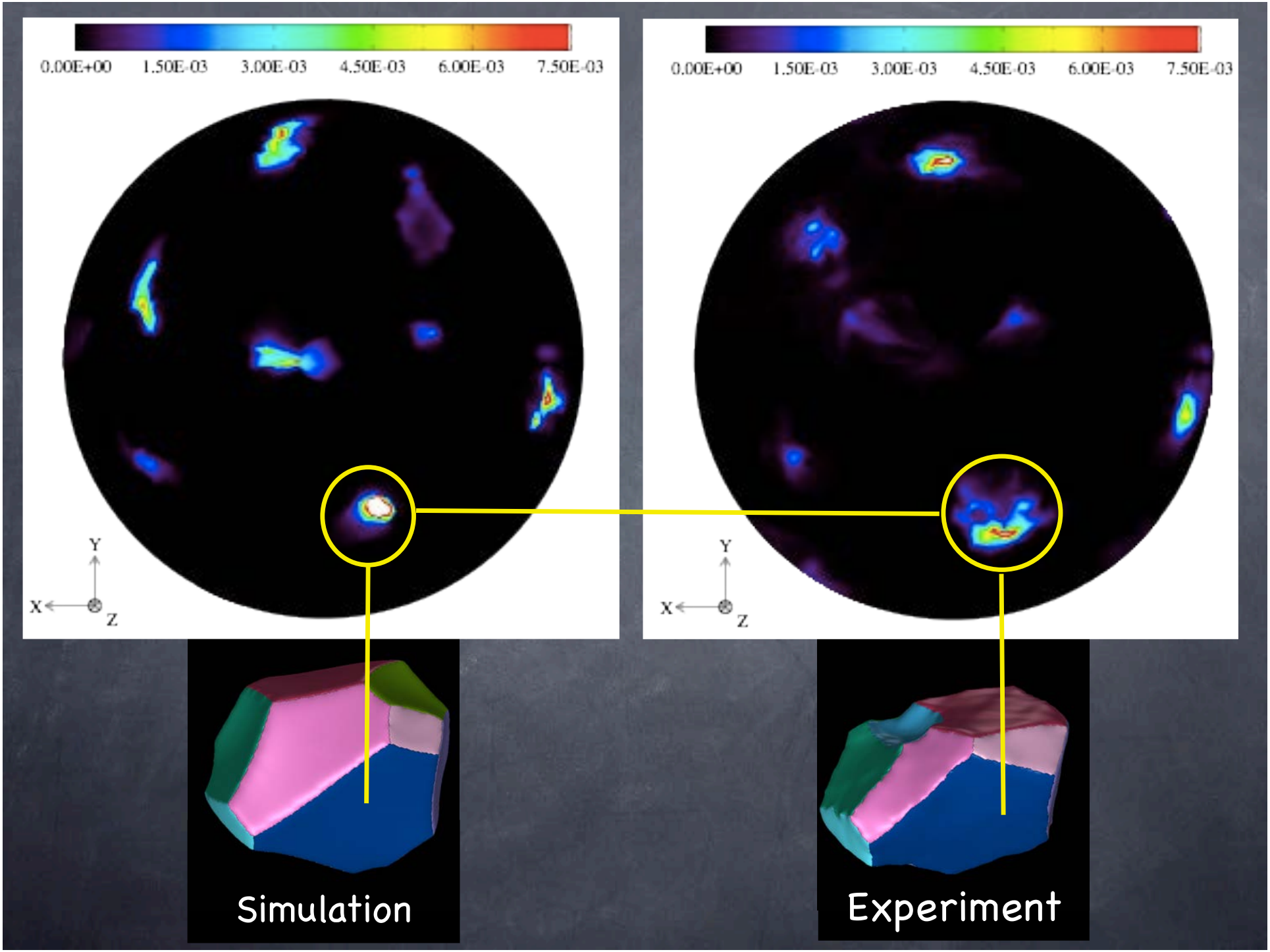
Another example of good agreement



Experiment time 2



Simulation time 2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Z
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6.00E-03
7.50E-03
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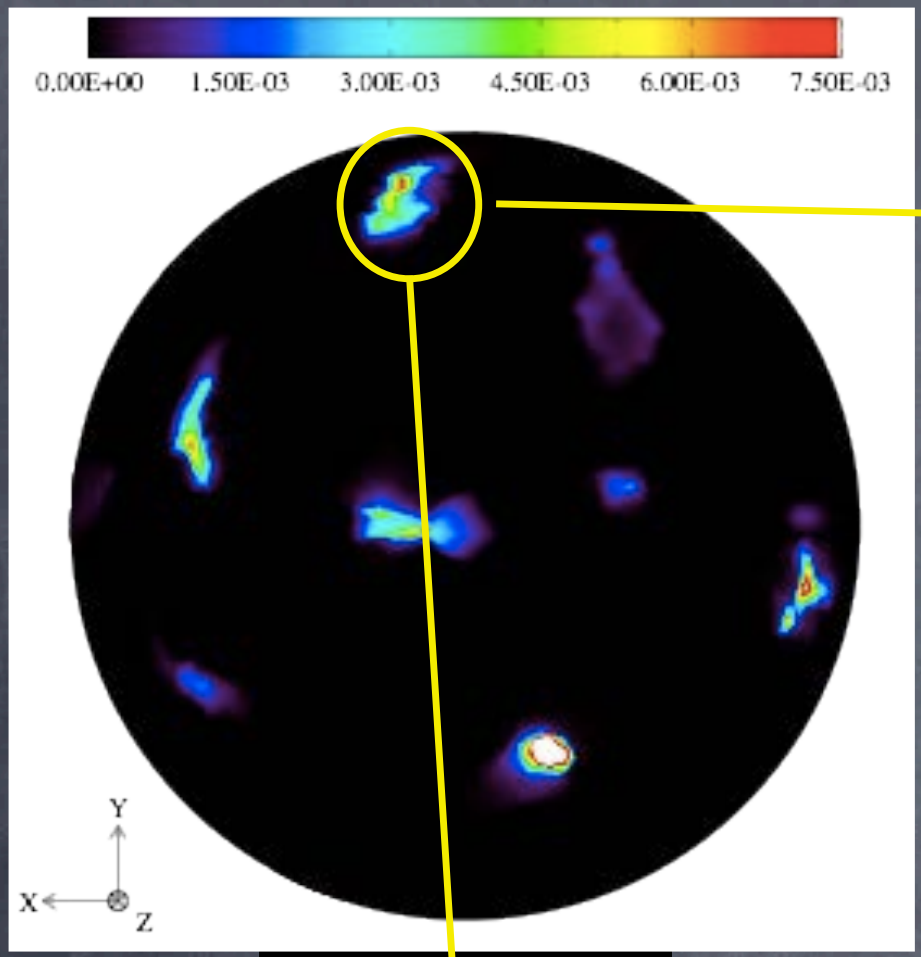
Simulation
Experiment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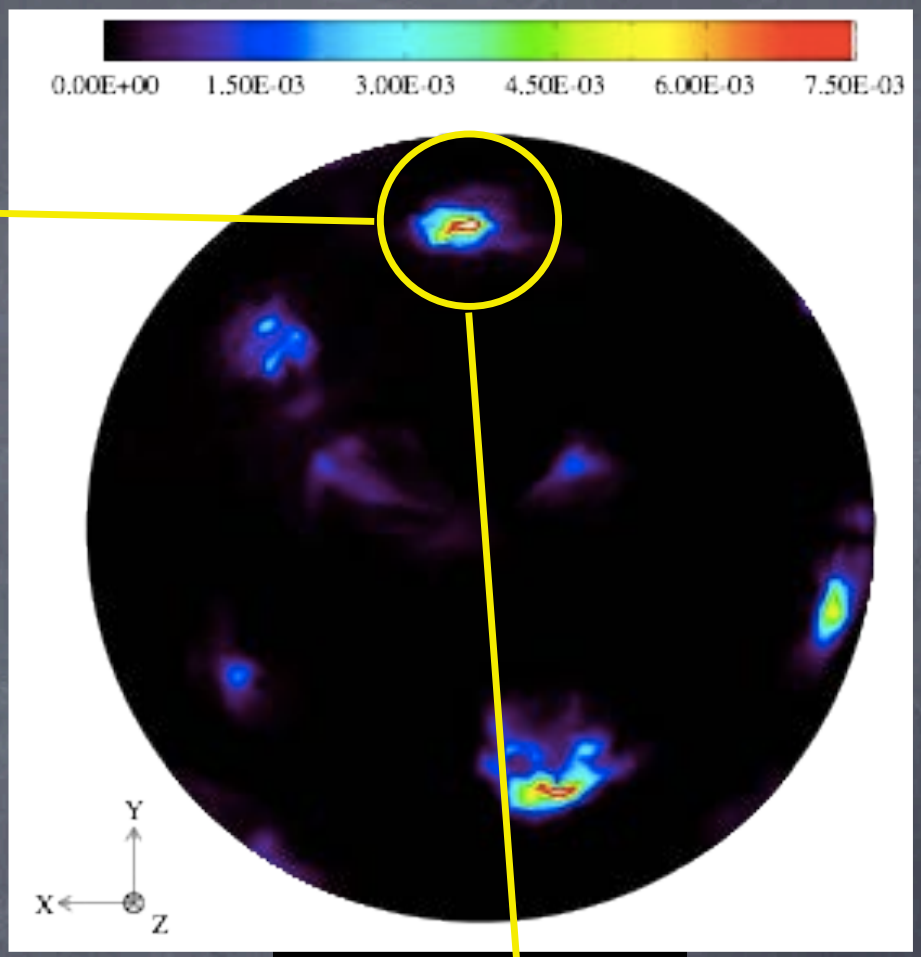
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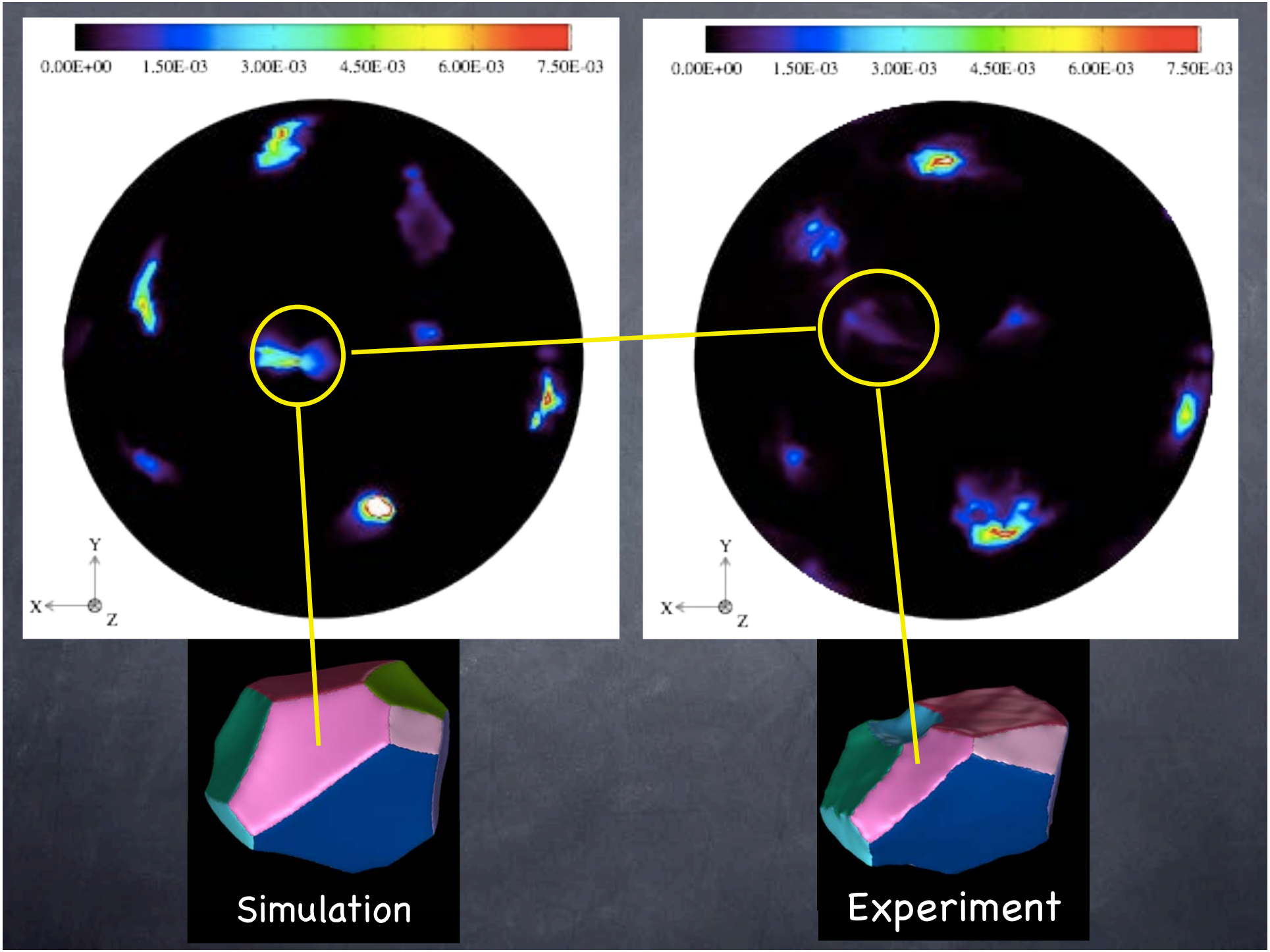
Simulation

Experiment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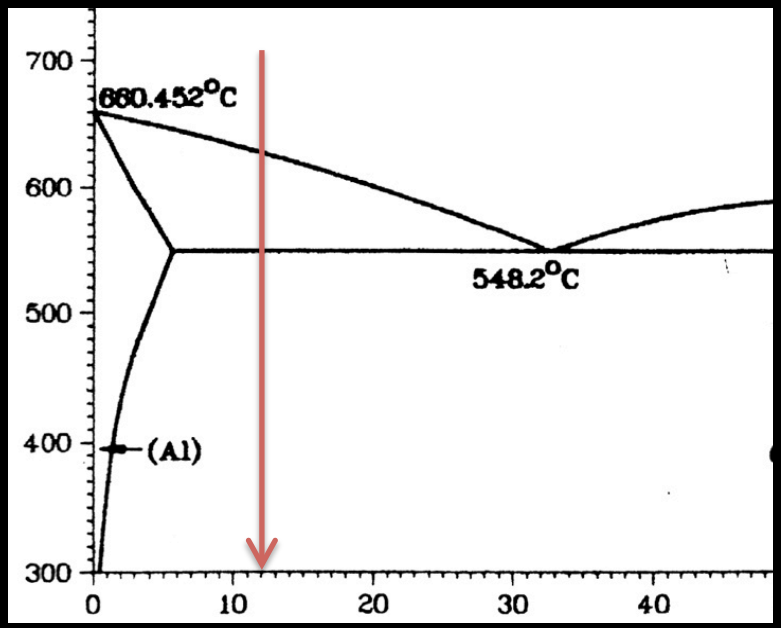
Simulation
Experiment

X-ray CT experimental details

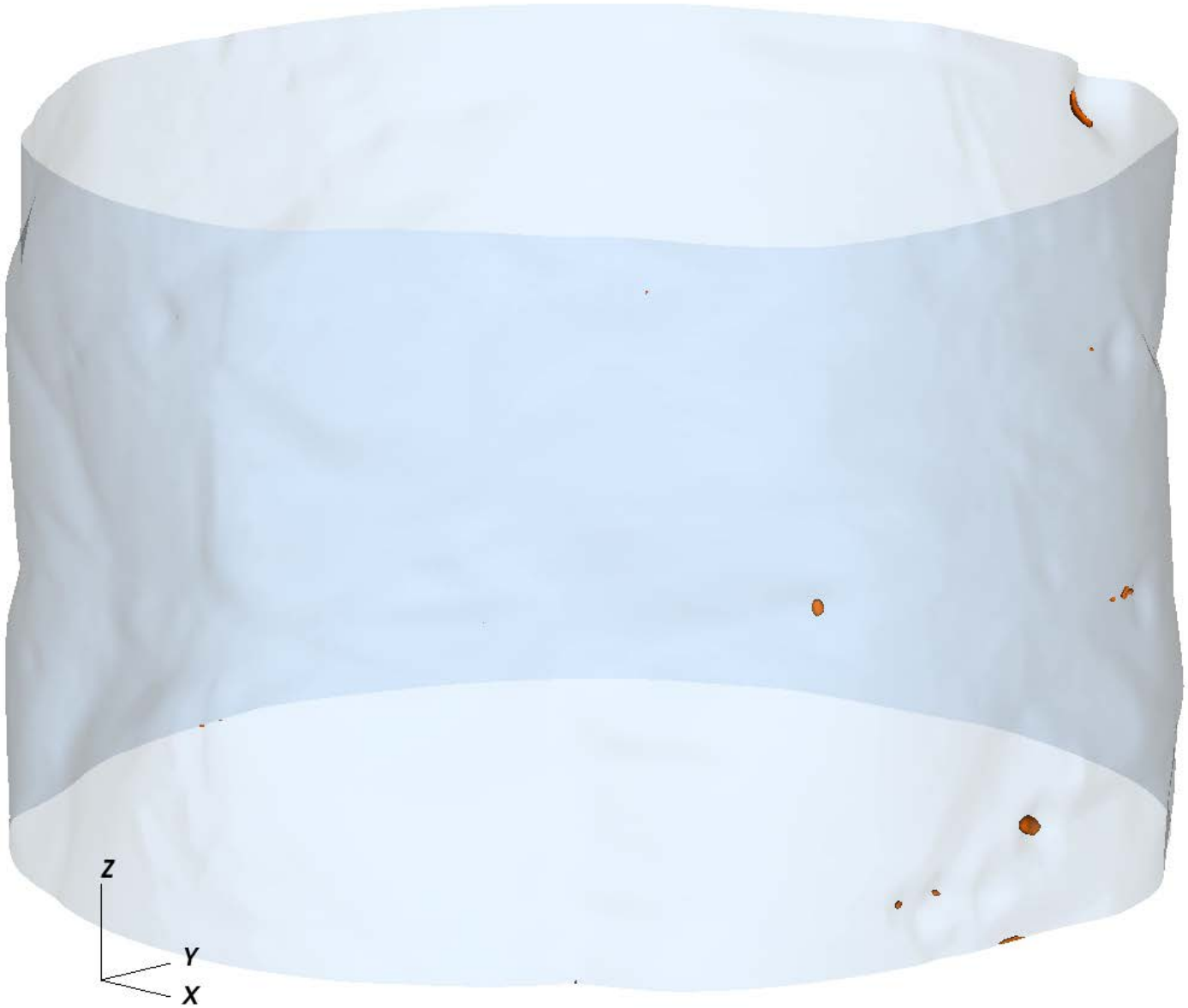
- Voxel sizes of 0.65 μm^3
- 2048 X 2048 X 1000 voxel datasets
- Camera records 70 frames a second
- Absorption contrast
- Tomography at the APS, 2BM beamline
- Altered the software at 2BM to allow for TIMBIR
- Using TIMBIR: 1.6 seconds between each 3D reconstruction (recent experiments 0.25 seconds)
- A factor of 16 faster than the standard approach
- 1 TB per experiment

Dendritic Growth

- Al-24wt%Cu
- Cooled from the liquid ~ 1 C/min: sample is isothermal
- 1mm diameter x 5mm tall samples
- 1 revolution per second: negligible centrifugal forces
- Segmentation using a 3D level set approach that minimizes noise within the phases and gives a signed distance function*



*Gibbs and Voorhees, Integrated Mat. and Manuf. Proc. **3** (2014)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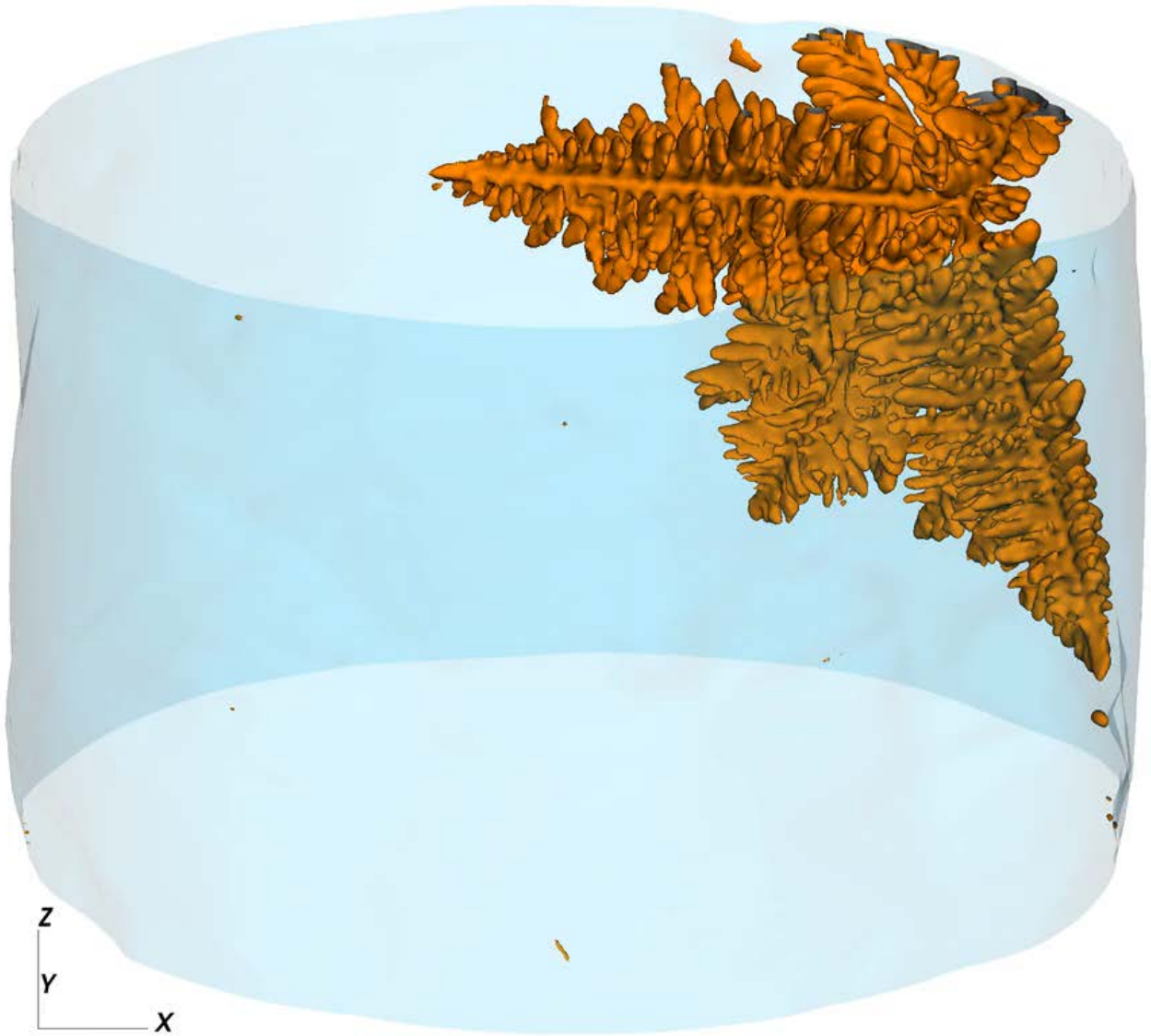
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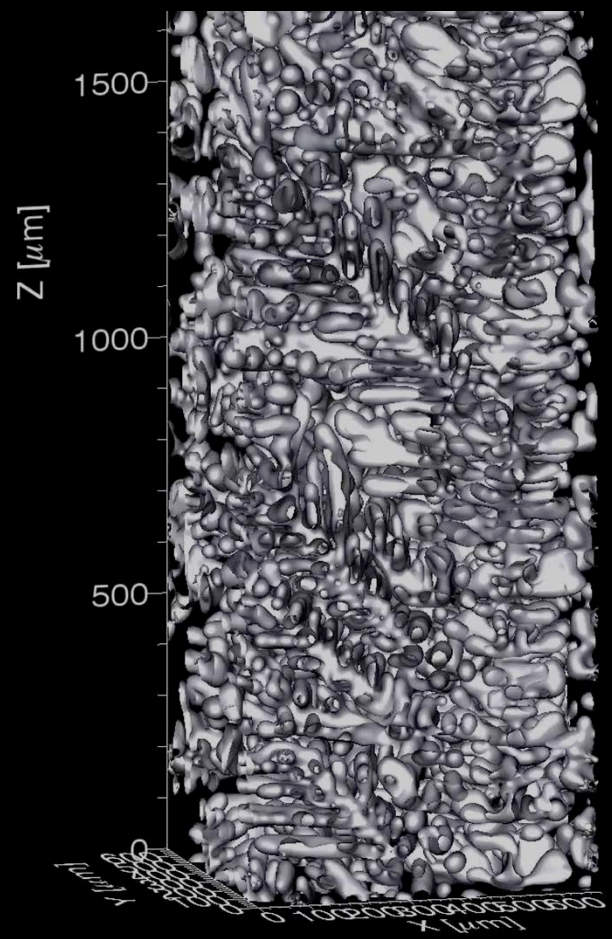
Evolution Following Solidification



Dendritic solid-liquid mixture

Dendritic solid-liquid mixtures

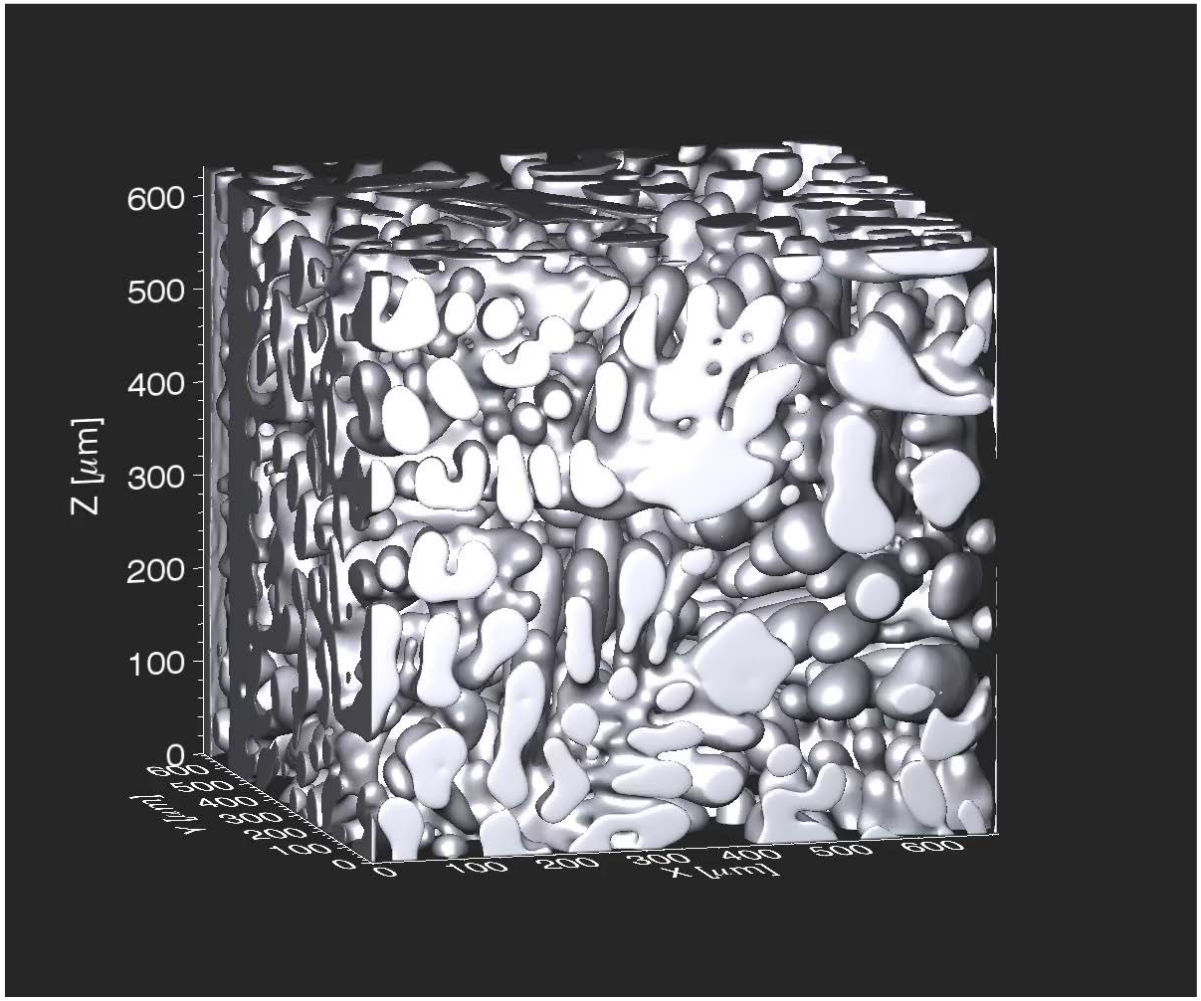
Diffusion

$$\nabla^2 C = 0$$

At the interface:

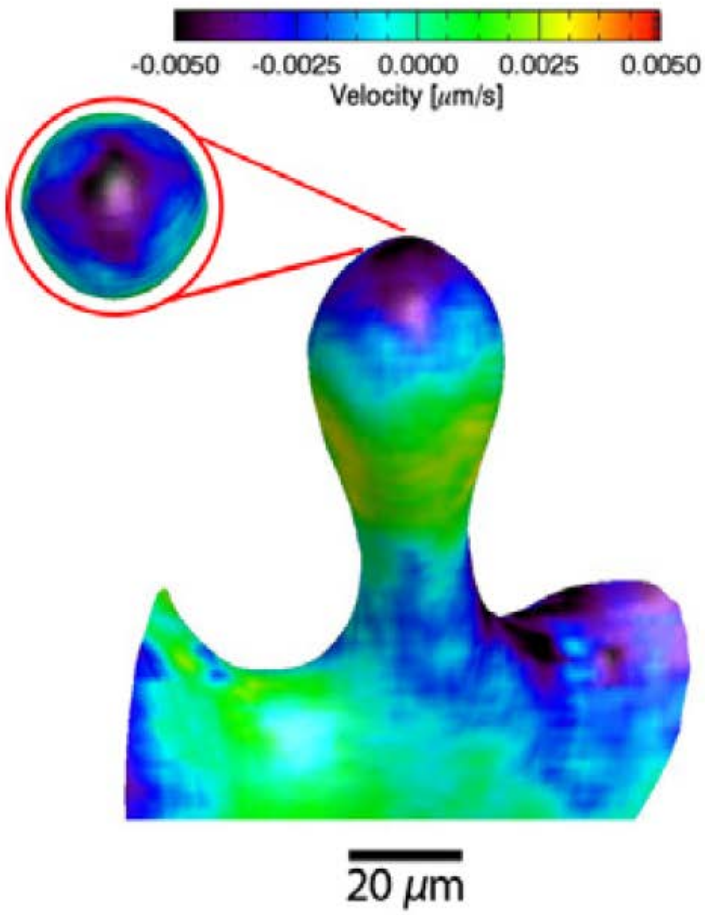
$$C_I = C_\infty + l_c H$$

$$[\![C]\!] V = -D \nabla C \cdot \mathbf{n}$$

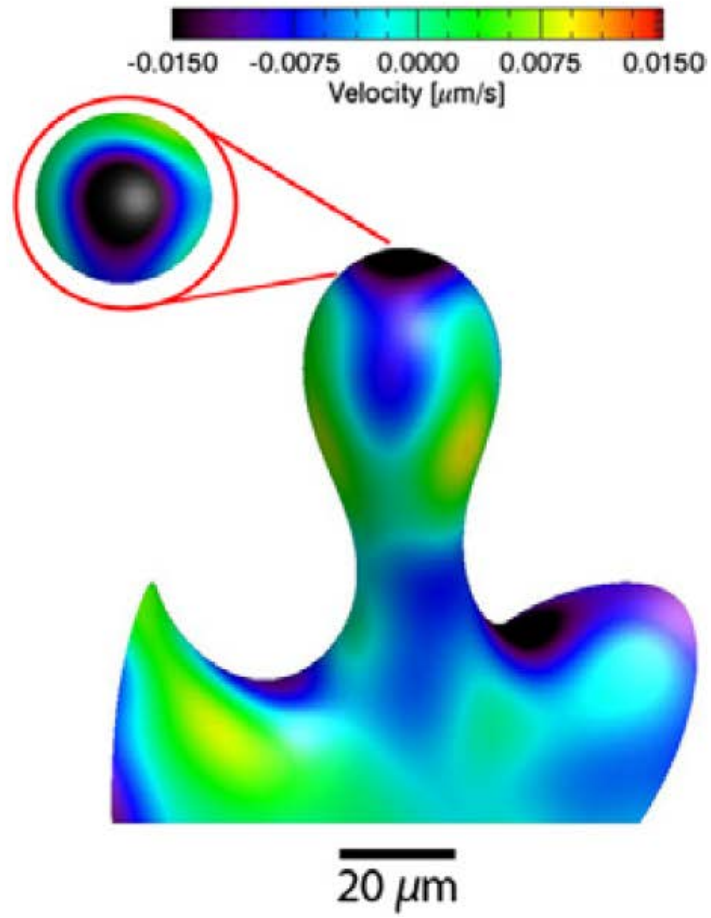


Connection with Simulation

- Using a phase field method and a portion of the structure:

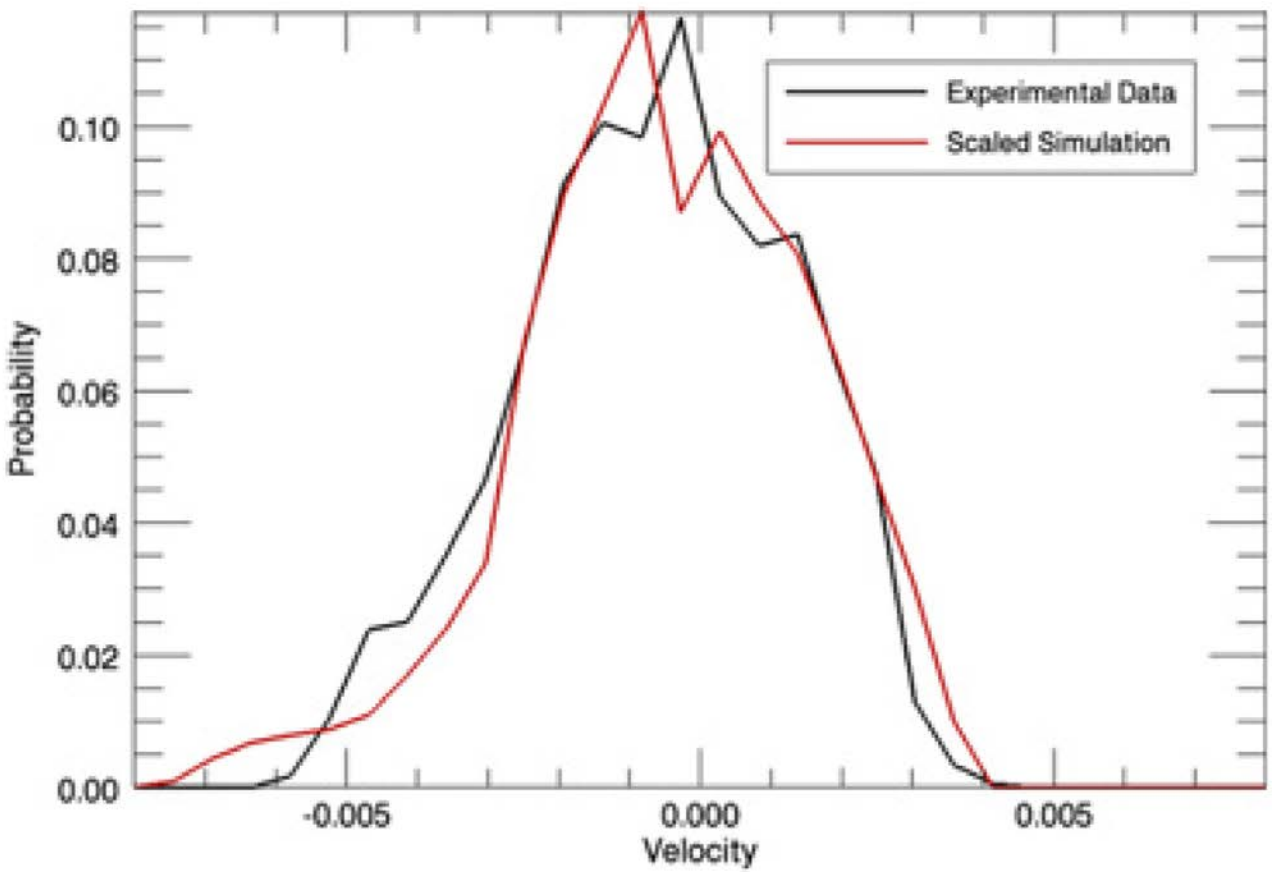


Experiment



Simulation

Quantitative comparison



Conclusion: Simulation and experiment

Which Thermophysical Parameter ?

- Interfacial energy measurement is reliable
- Liquid diffusion coefficients are extremely difficult to measure due to convection
- This leads to enhanced diffusion coefficients
- This is consistent with simulation predicting velocities that are too high
- ur experiments were isothermal there was little convection
- Conclusion: the diffusion coefficient in the literature is a factor of 3 too high

The Connection

- Problem: unknown thermophysical parameters, huge data sets, poorly understood physics
- Solution: run the simulation and the experiment simultaneously
  - Only record data when there is a disagreement or something interesting happening: *Intelligent data reduction*
  - Compare the simulation and experiment: determine materials parameters
- Facilitating this approach:
  - Combine high performance computing and synchrotron experiments
  - Enhanced data connections
  - Real time data analysis algorithms