Coarsening in Liquid Foams: A Hybrid Simulation-Experimental Technique

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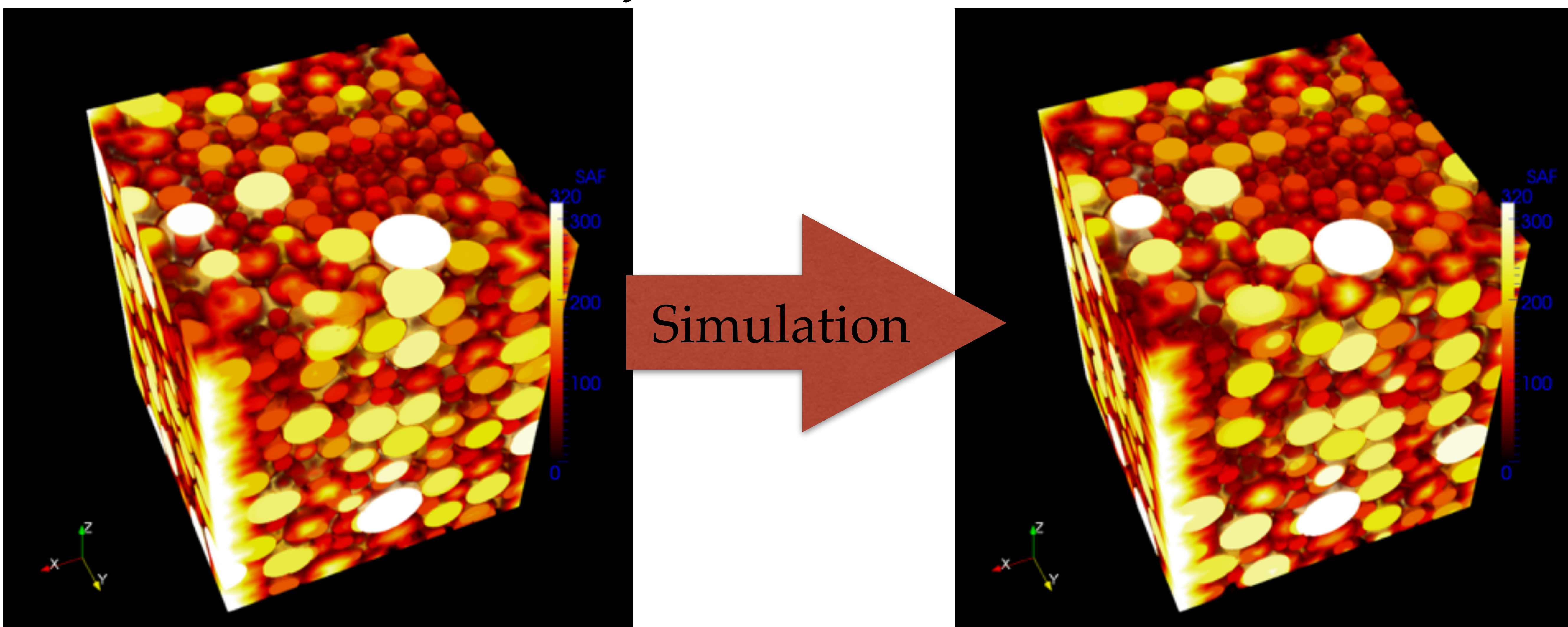
Outline

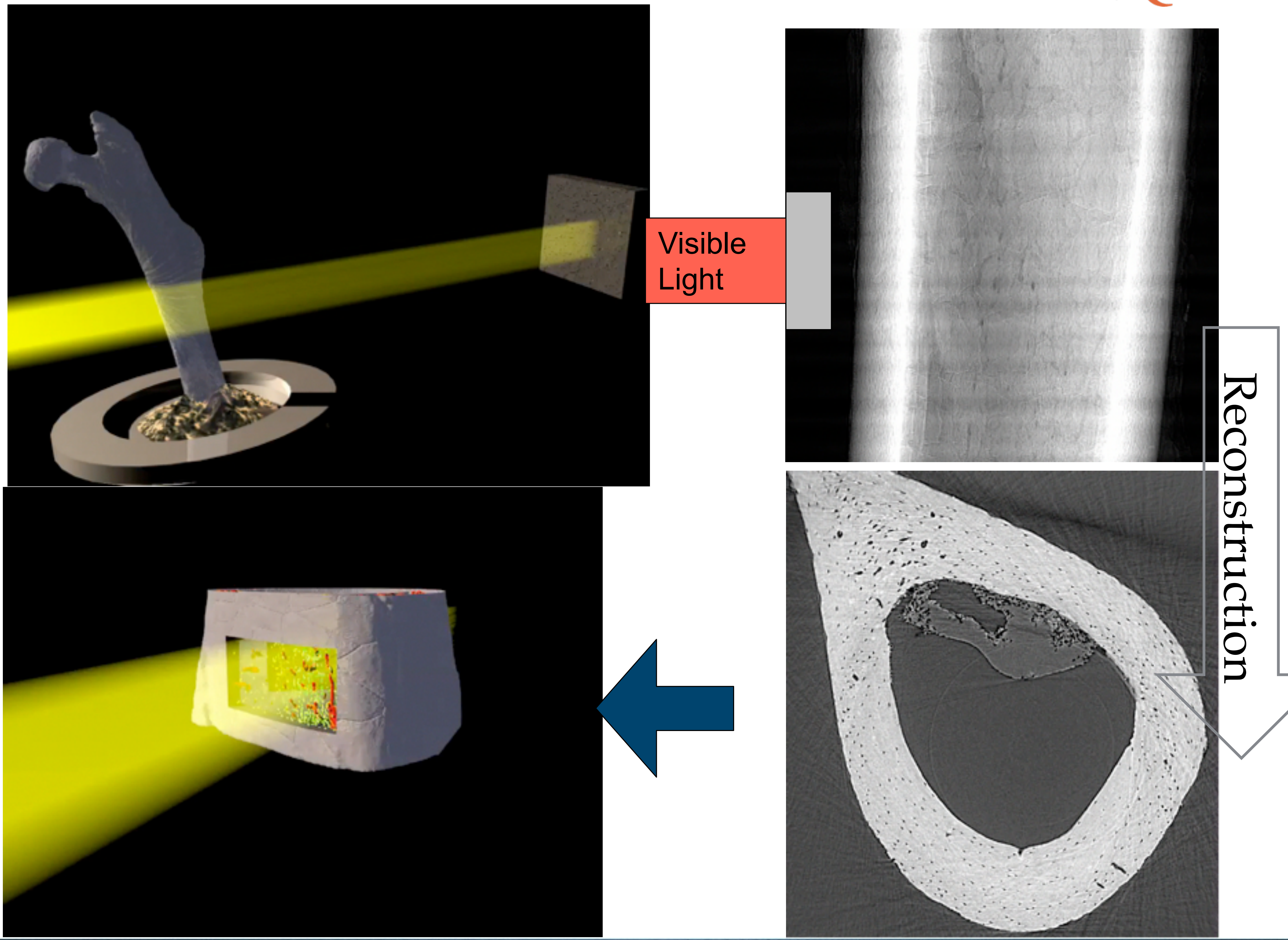
- Motivation
- Experimental Approach
  - Synchrotron-based X-ray Tomographic Microscopy
- Simulation Approach
  - Cellular Potts Method
- Combining Approaches
  - Improving Labeling
  - Simulating Coarsening
- Challenges
- Future Directions

Motivation

- Experiments are constantly improving
  - But they will never tell the whole story
  - Many events happen too quickly to see
- Simulations allow everything to be controlled
  - But they have ‘no’ connection with reality.
  - Can validate statistically

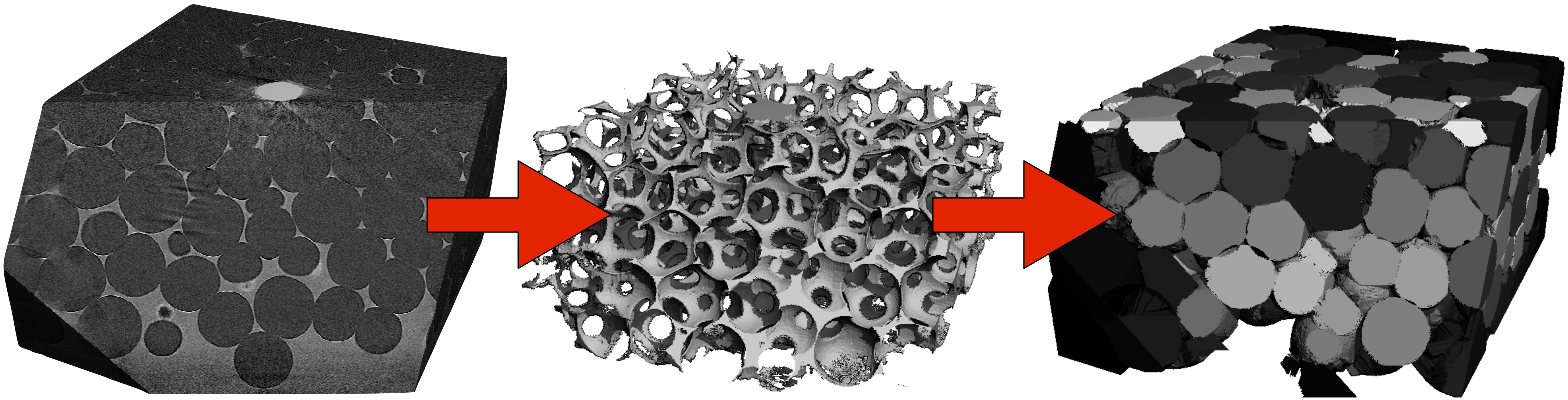


Synchrotron-based X-Ray Computed Tomography



Experimental Data

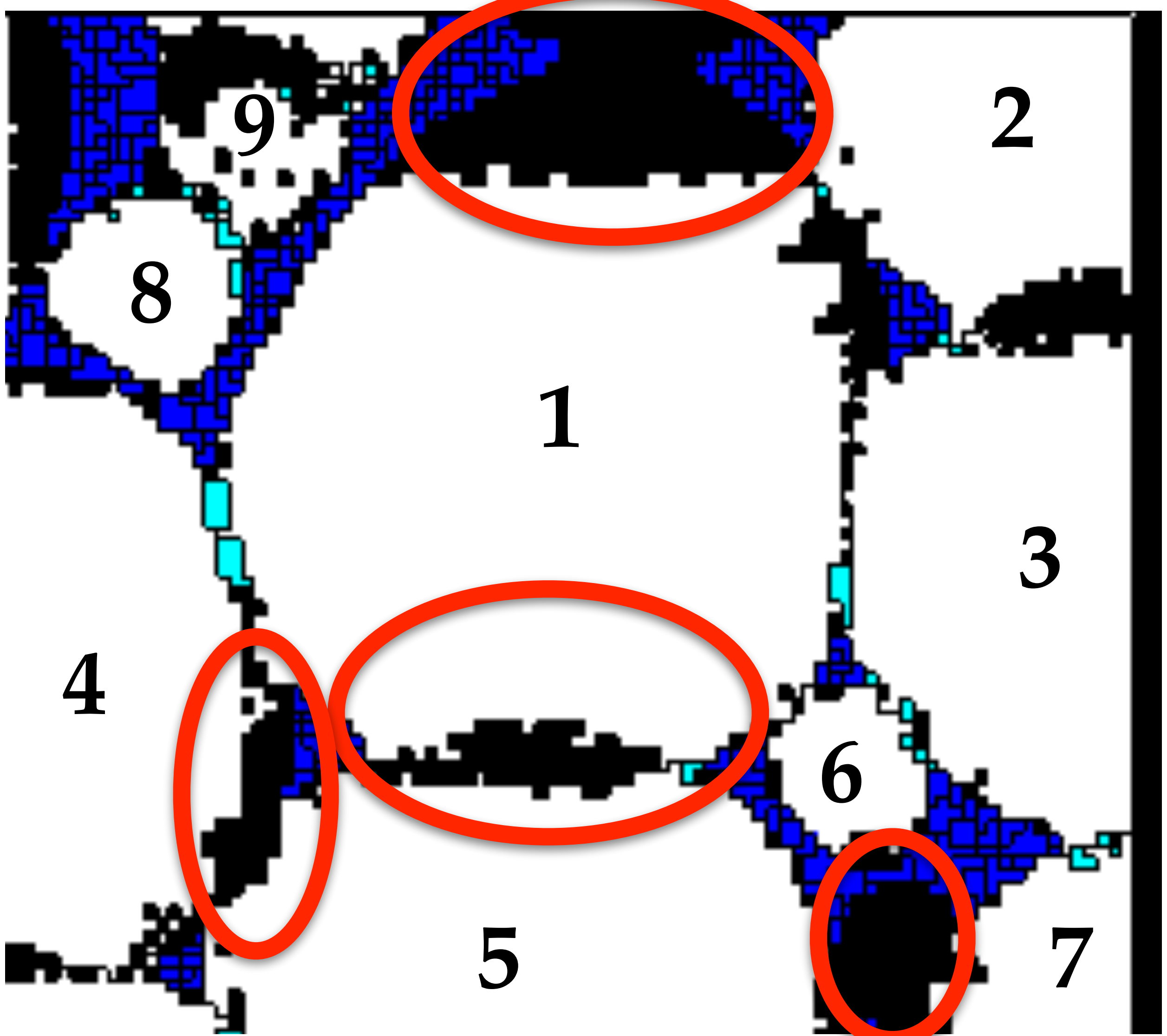
- Water in Plateau borders absorb light
- Air does not
- Films are too thin to be identified
- Segment plateau borders
- Label bubbles using distances from nearest Plateau border

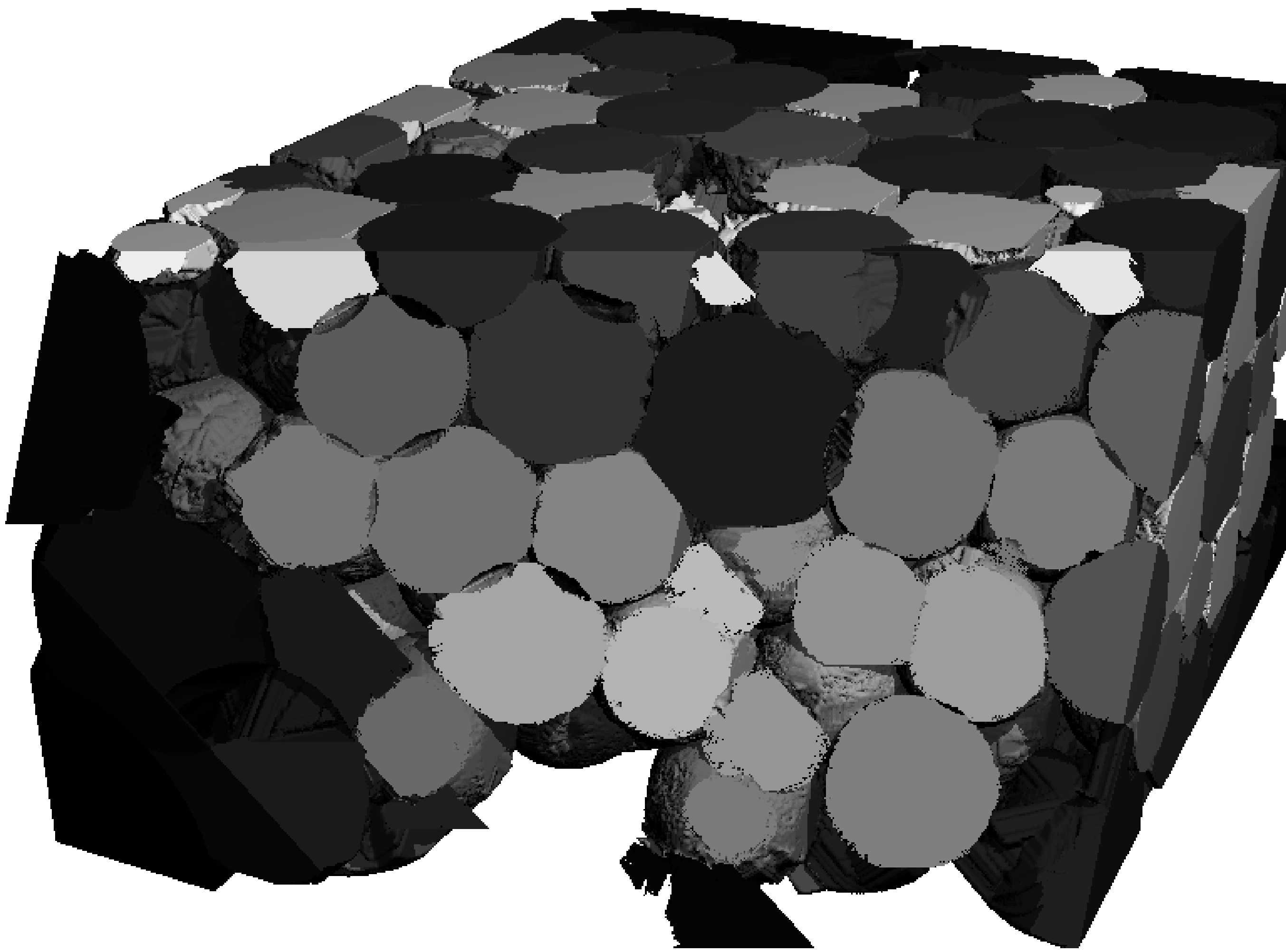


Mader K, Mokso R, Raufaste C. Quantitative 3D Characterization of Cellular Materials: Segmentation and Morphology of Foam. Colloids and Surfaces A (2012)

Experimental Data

- Bubble labels are clearly identified
- Interfaces (films, faces) are less clear
- Image processing rules are not a good guide for calculating these faces
- Need more complicated rules





Cellular Potts Model

- Lattice-based approach (2D or 3D)
- Simulates Domains
  - Similar form the same bubbles
  - Difference have contact energy
- Hamiltonian equation to govern states
  - Surface tension
  - Conservation of mass
  - Ideal gas behavior
  - Any other preconditions (external forces, etc)

Air, 2	Air, 1	Air, 1	Air, 2
Air, 1	Air, 2	Air, 2	Air, 1
Air, 1	Air, 2	Air, 1	Air, 2
Air, 1	Air, 2	Air, 2	Air, 1

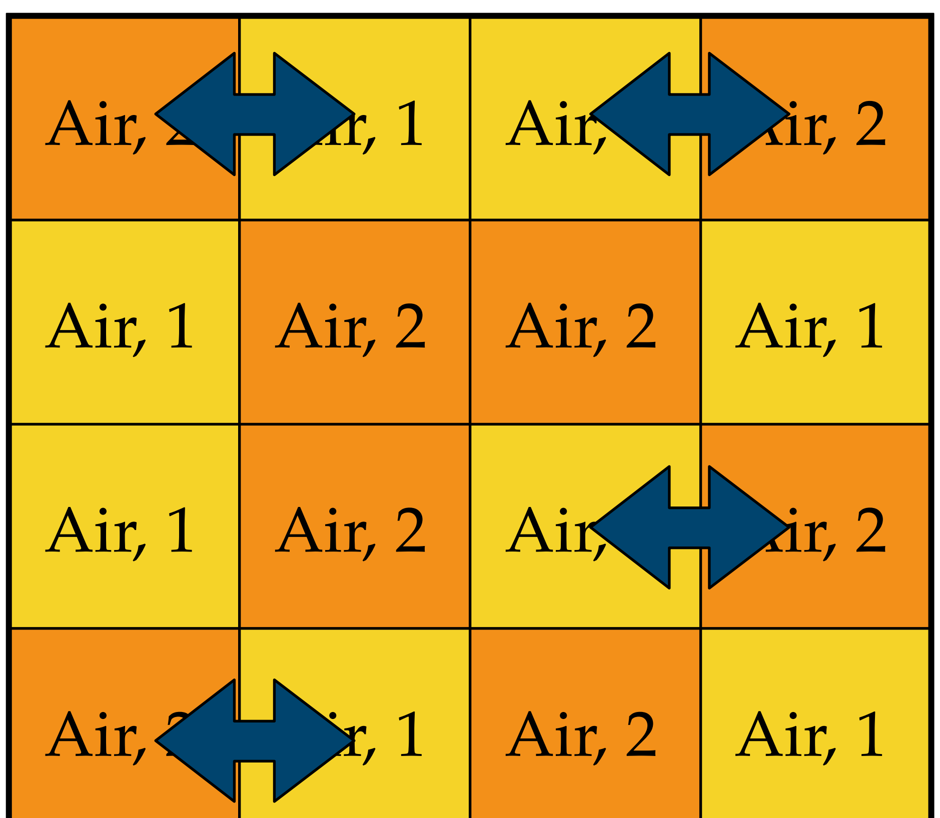
$$E = \frac{1}{2} \sum_{i} \sum_{\langle j \rangle_i} J[1 - \delta(S_i - S_j)],$$

Thomas, G., de Almeida, R., & Graner, F. (2006). Coarsening of three-dimensional grains in crystals, or bubbles in dry foams, tends towards a universal, statistically scale-invariant regime. Physical Review E, 74(2), 021407. doi:10.1103/PhysRevE.74.021407

Monte Carlo Steps - Time

- States changes as part of random-process based on energy and temperature (Boltzmann)
- Locally minimize effective energy
  - Contact energy depending on cell types
- High temperature -> Fast changes but less stable
- Low temperature -> Slow changes, can get stuck in local minimum

Initial Condition (t=0)



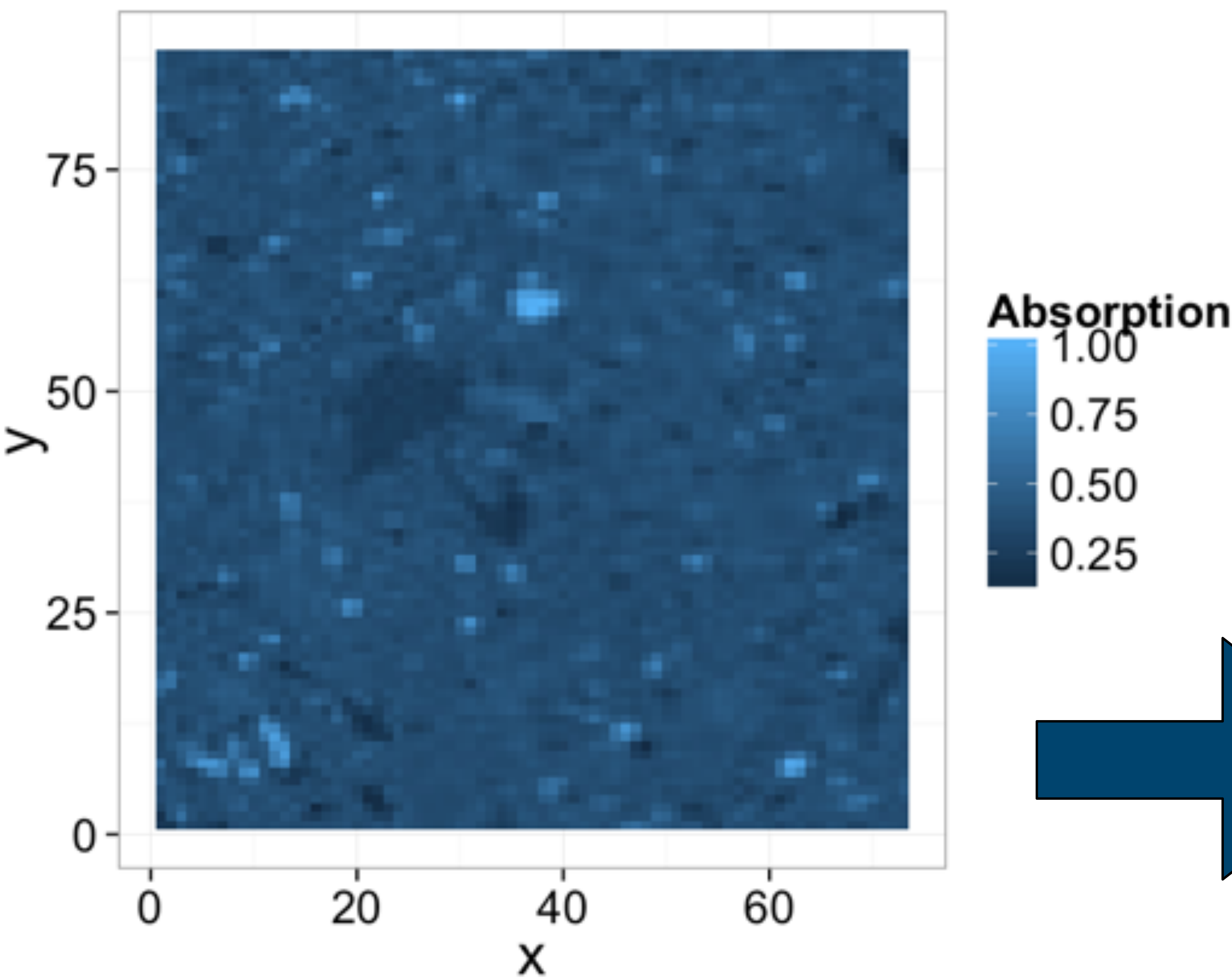
Next State (t=1)

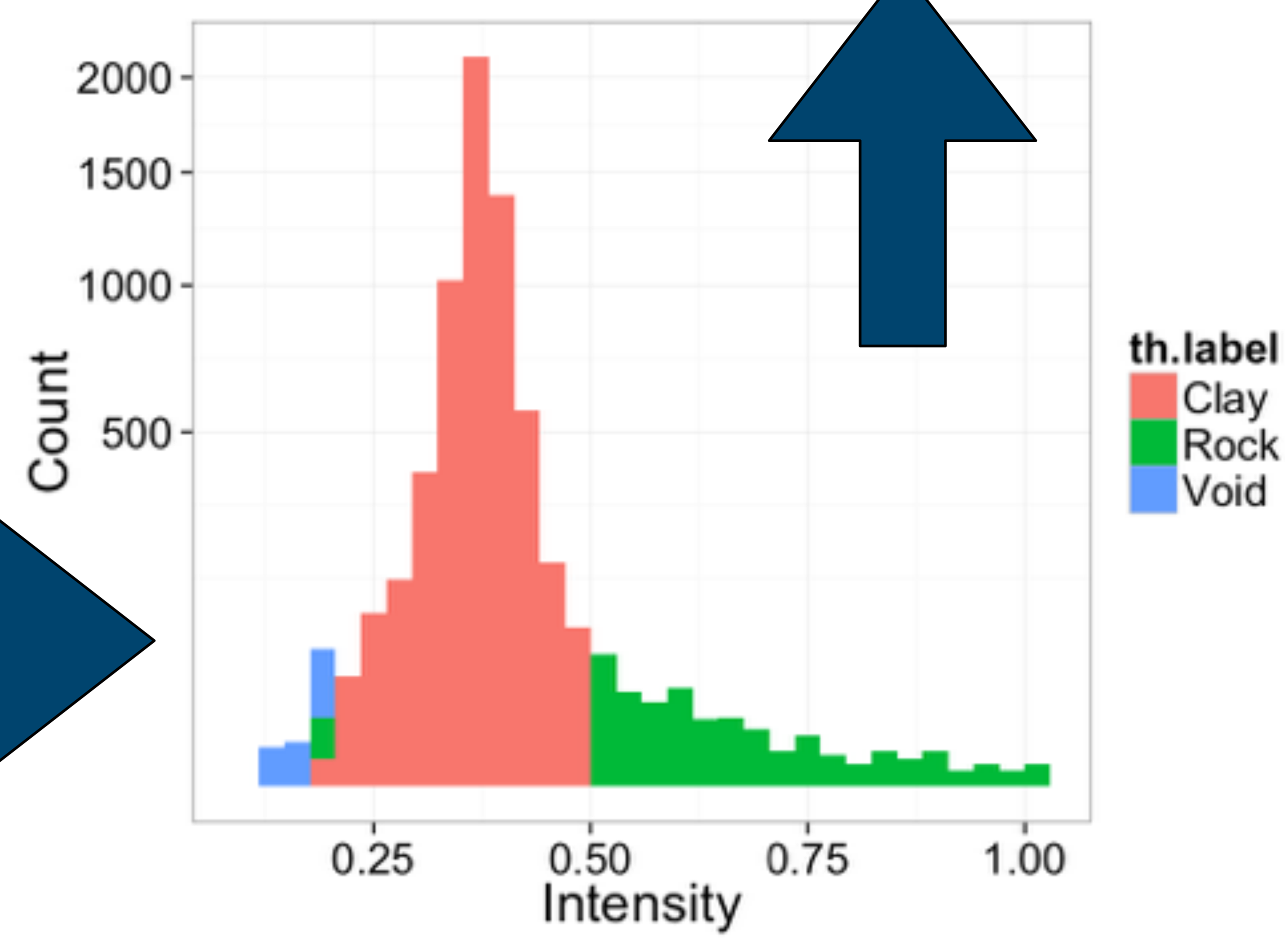
Air, 1	Air, 2	Air, 2	Air, 1
Air, 1	Air, 2	Air, 2	Air, 1
Air, 1	Air, 2	Air, 2	Air, 1
Air, 1	Air, 2	Air, 2	Air, 1

Multiple Phases

- Can handle multiple phases
- Requires interaction coefficients for different phases
- Absorption (or phase) contrast in images can be mapped to materials

Rock	Clay	Clay	Void
Clay	Void	Void	Clay
Rock	Rock	Rock	Void
Rock	Void	Clay	Fat

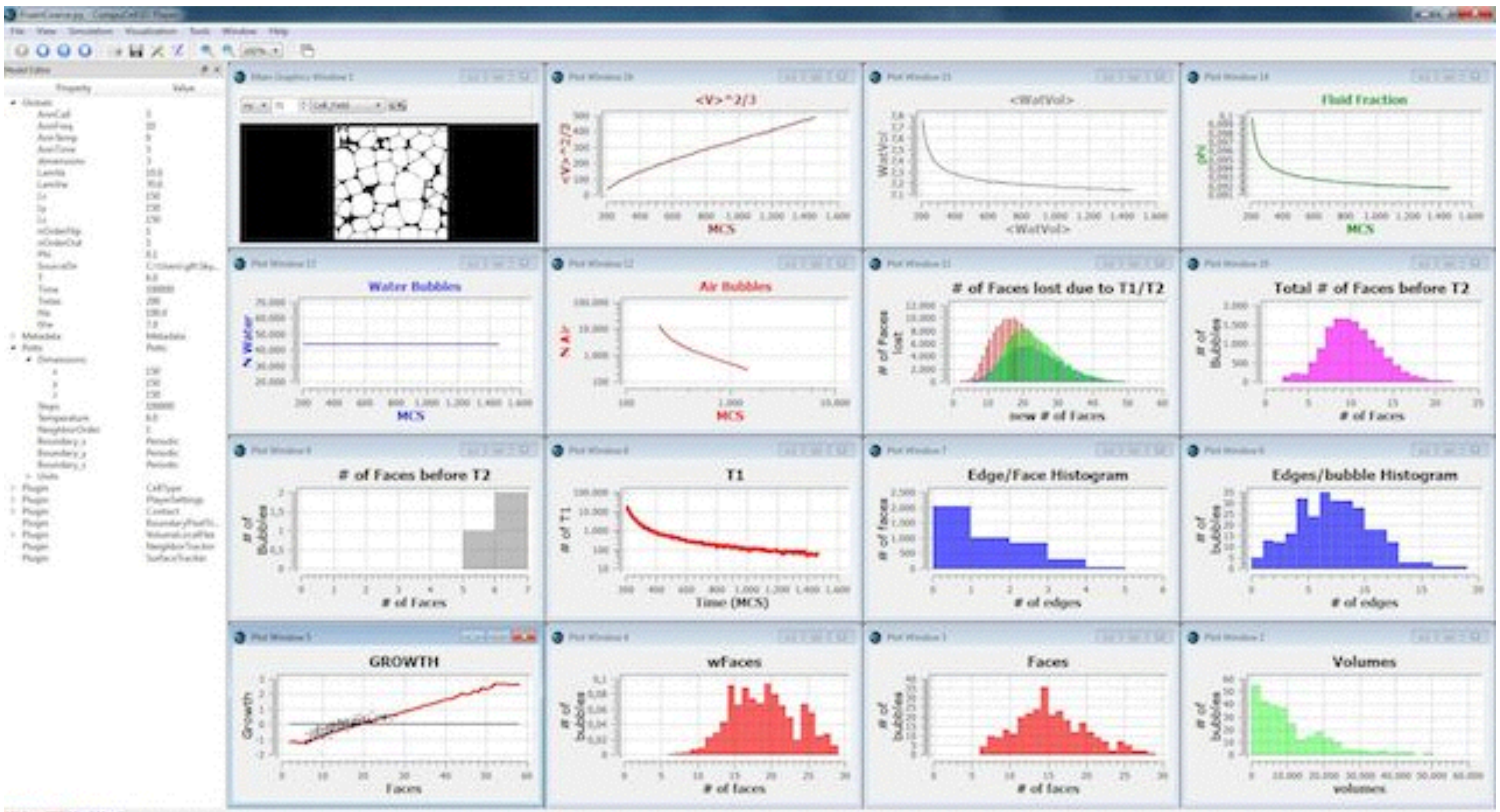




CompuCell3D: Flexible GUI for Cellular Potts

- Open Source
- Control parameters with scripts
- Run simulations in parallel
- Usable on Cloud computing resources: Amazon AWS tested

- 32 core machine, 60GB RAM, 640GB for $3 / hour (cheaper than PhD students)
- 1564 Cuda Cores with 8 cores for $0.77 / hour

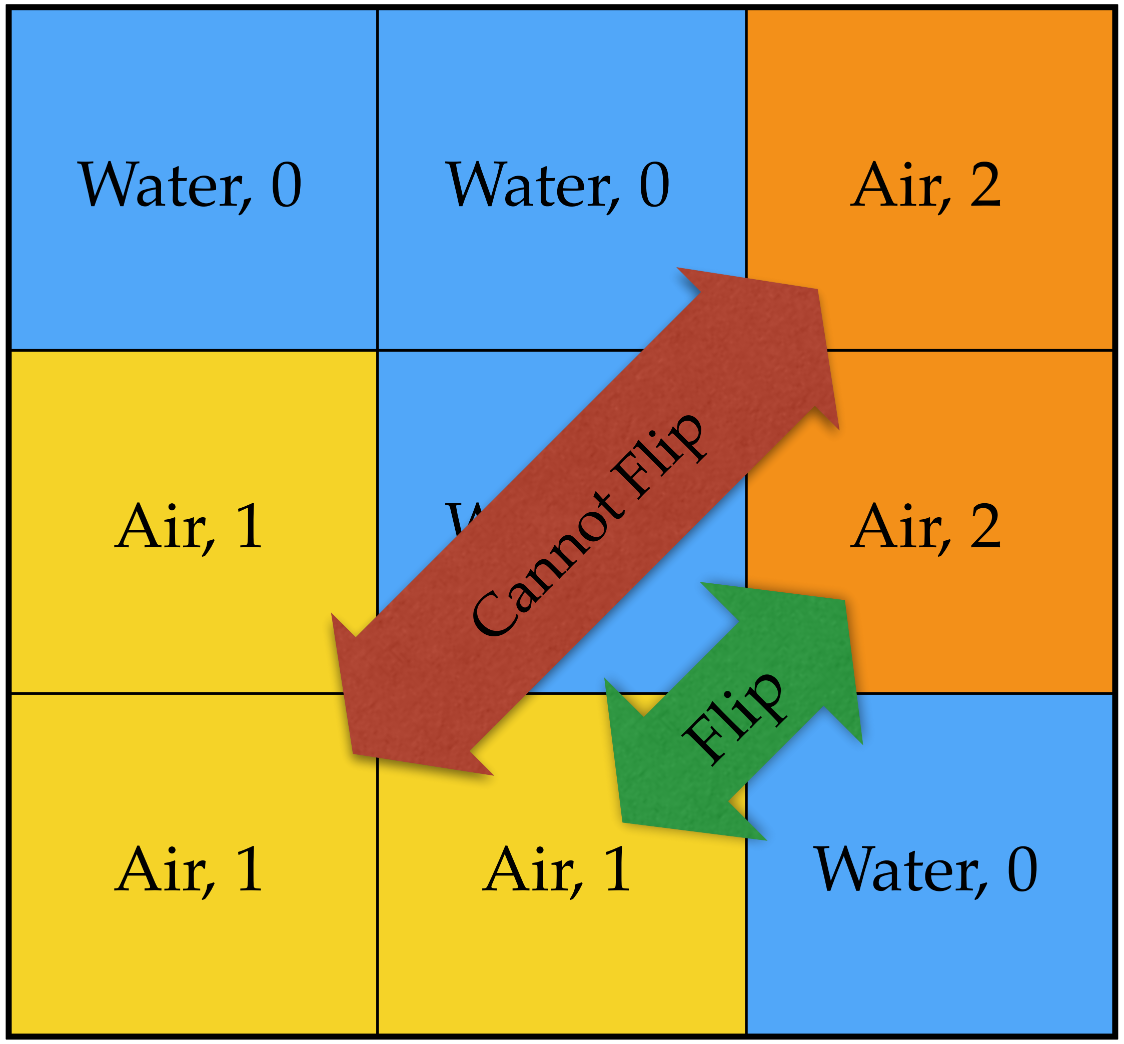


- http://compucell3d.com/

Multi-Scale Modeling of Tissues Using CompuCell3D – M. Swat, Gilberto L. Thomas, Julio M. Belmonte, A. Shirinifard, D.Hmeljak, J. A. Glazier, Computational Methods in Cell Biology, Methods in Cell Biology 110: 325-366 (2012)

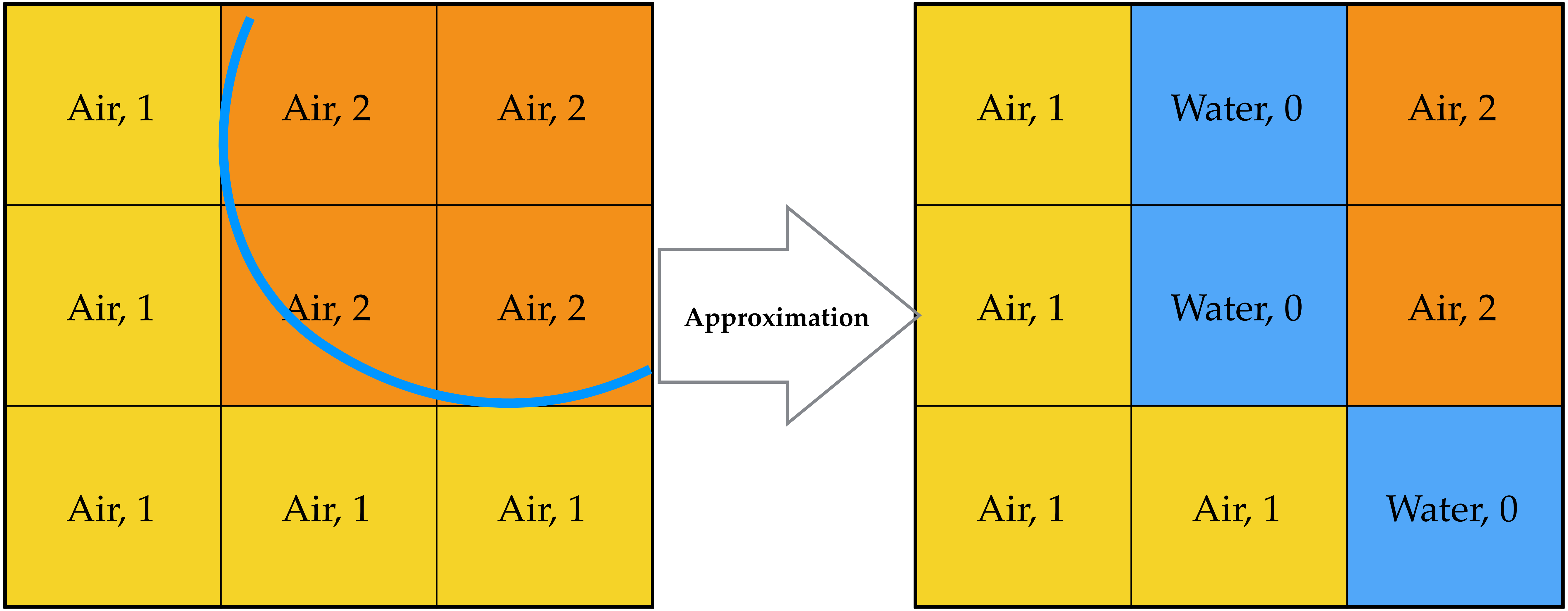
Wetter Foams

- Initial model has no water
- Water added as incompressible phase
- Limits diffusion and flipping
- Voxel can either be entirely water or entirely air



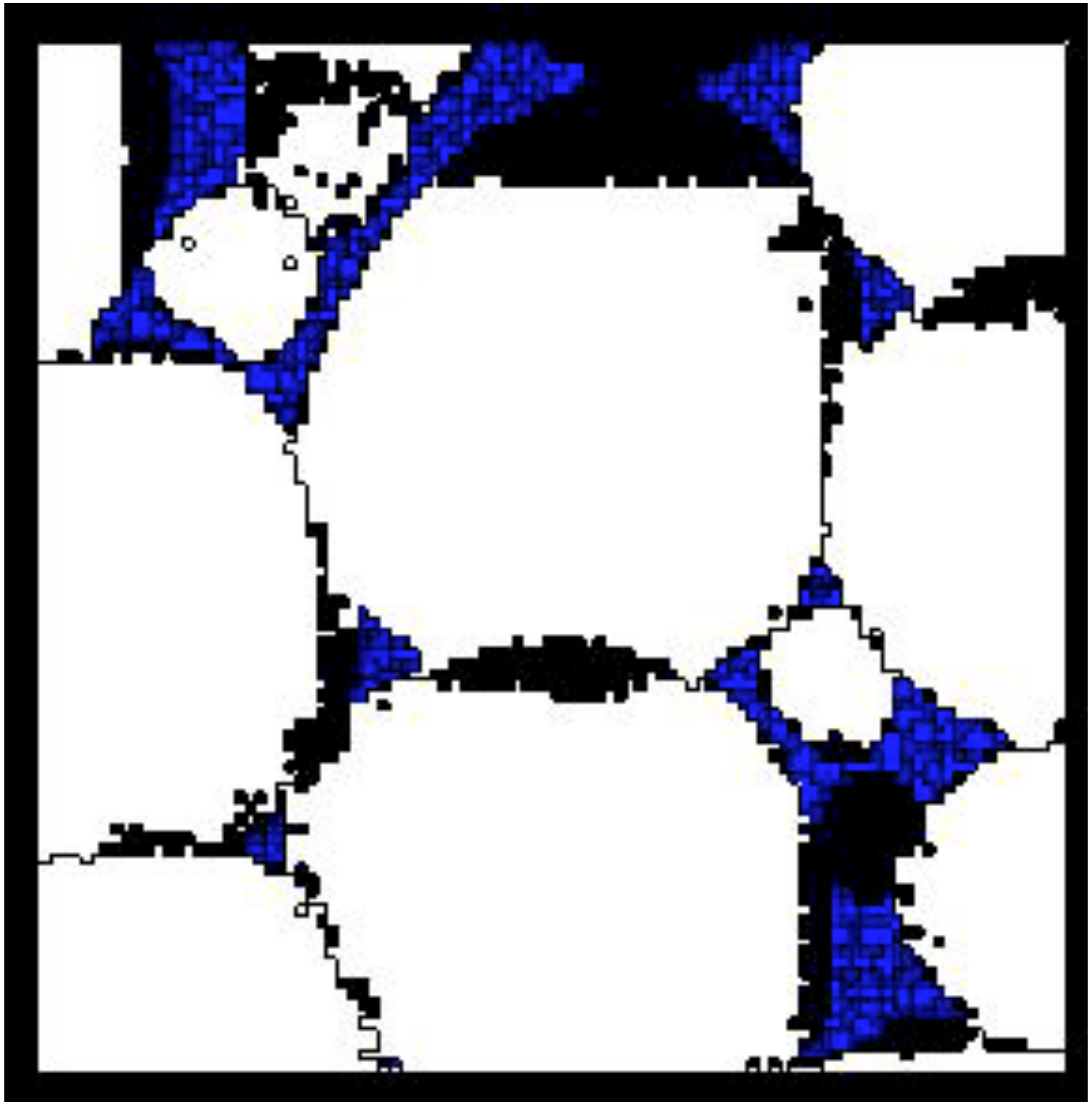
Films

- Voxels are a poor approximation for interfaces
- Voxel size = 3μm, Bubble Diameter = 60μm
- Film thickness < 300nm
- Proper interfaces for films would require at least 1000x finer simulations



From Experiments to Simulations

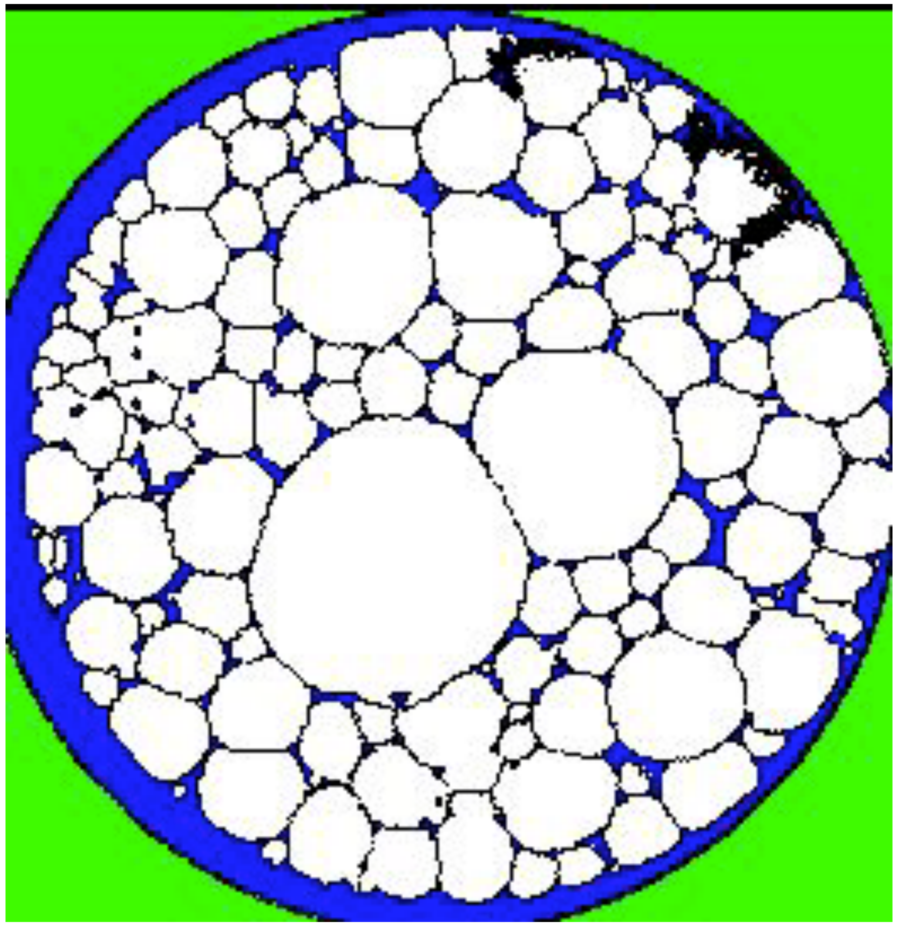
- Labeling underfills bubbles
- Cellular Potts is a smarter way for filling than tessellation or distance maps



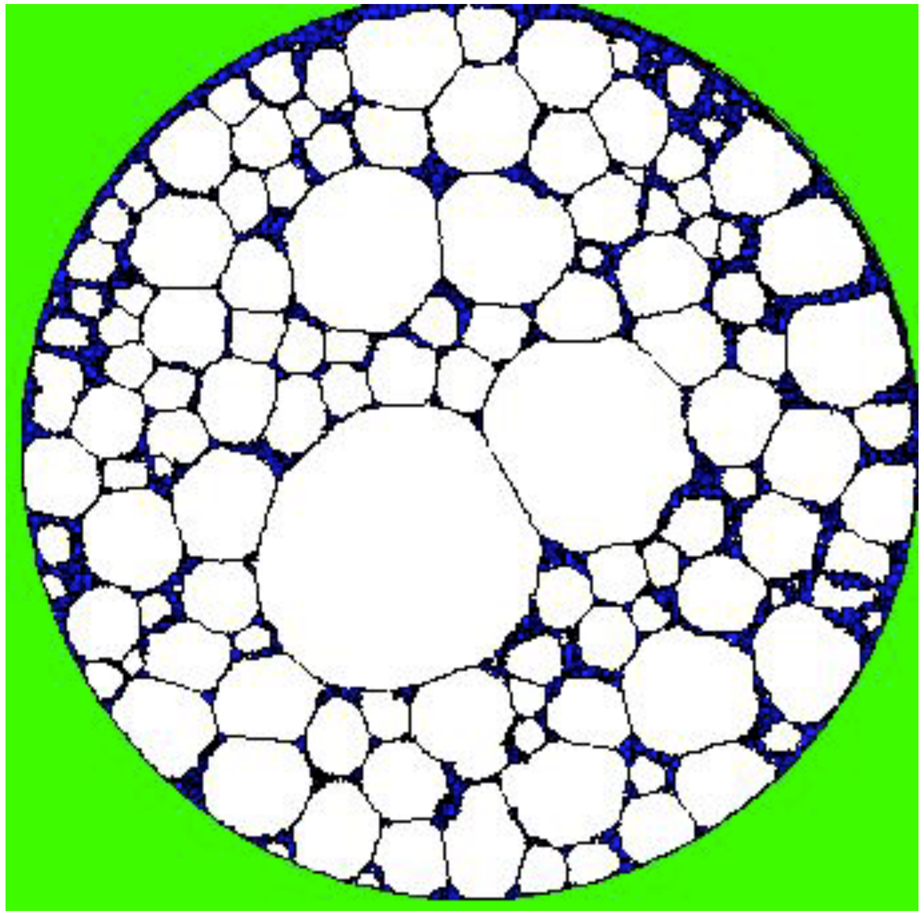
Large, Sensitive Parameter Space

- Time step size
- Frequency and length of annealing
- Interactions between all materials
  - Water -> Air
  - Air -> Air
  - Container -> Water
  - Container -> Air

$\propto \texttt{materials}^2$



Unstable Simulation



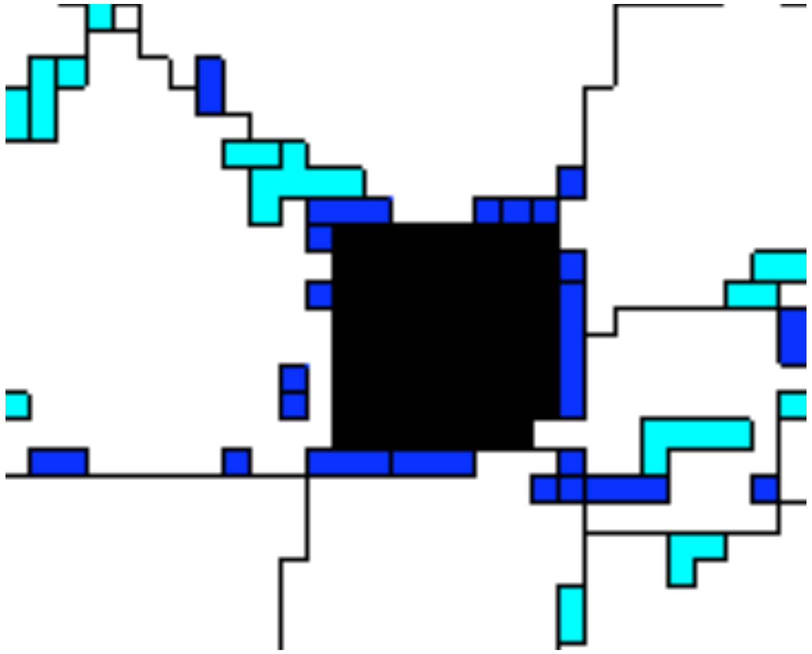
Stable Simulation

From Experiments to Simulations

- Same lattice space : Voxels in images are voxels in the simulation
- Phase (air or water) already known
- Bubble identify and exact boundaries are not
- Small water volumes (less than a voxel) are invisible but important for foam structure and simulation stability

Labeled Experimental Data

CompuCell3D with 'Fixed water' and 'Random free water'



After 160 time steps (relaxation)

From Experiments to Simulations

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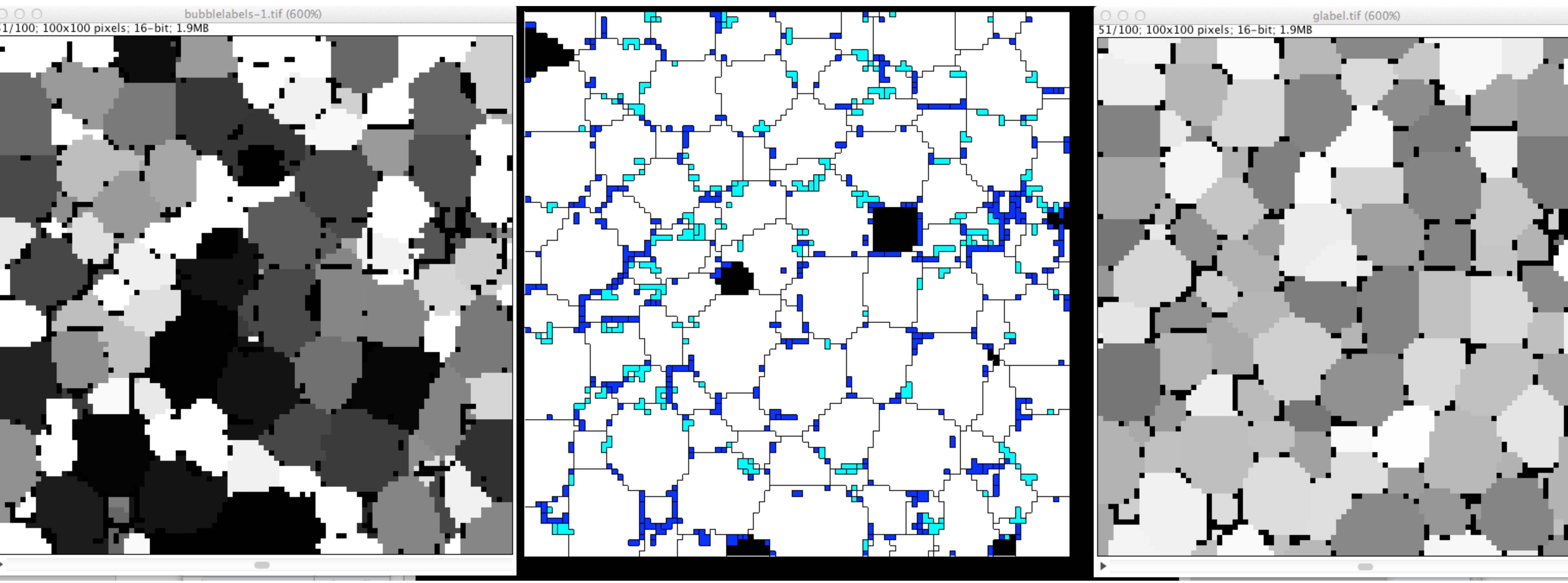
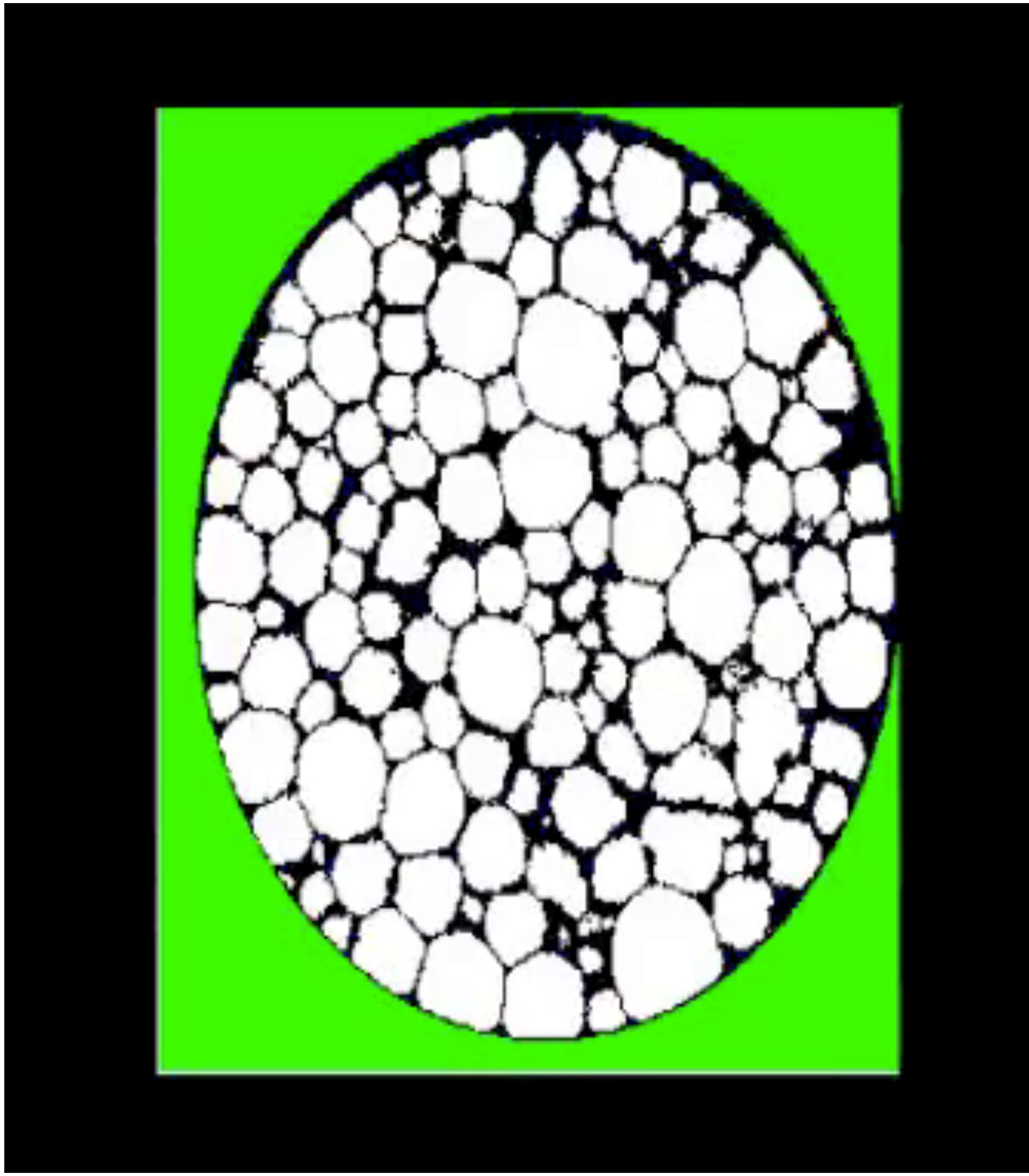


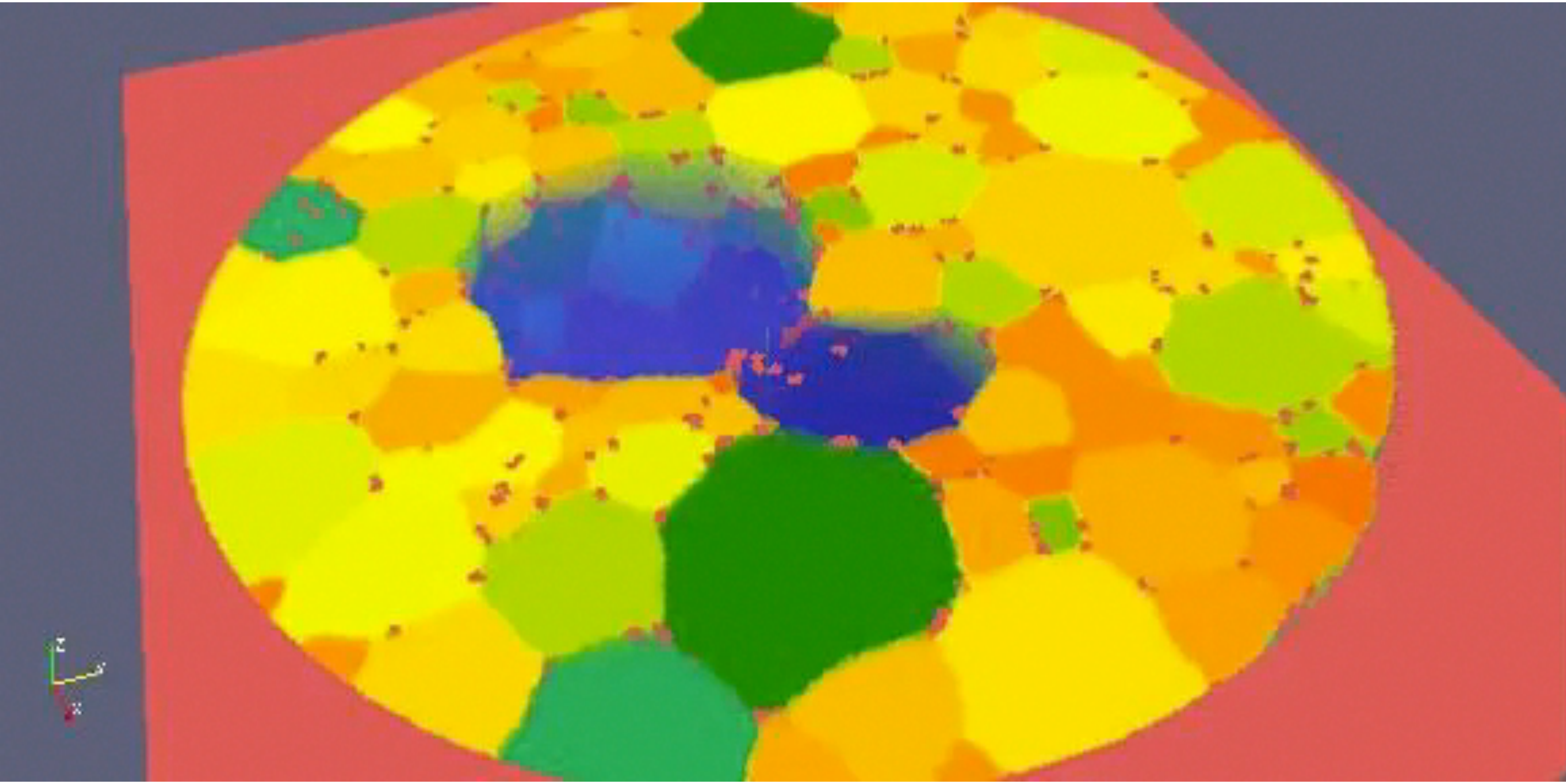
Coarsening Simulations

- With the right combination of parameters / interactions can simulate coarsening
- Starting point is an experimental measurement of foam
- Water and air are allowed move freely



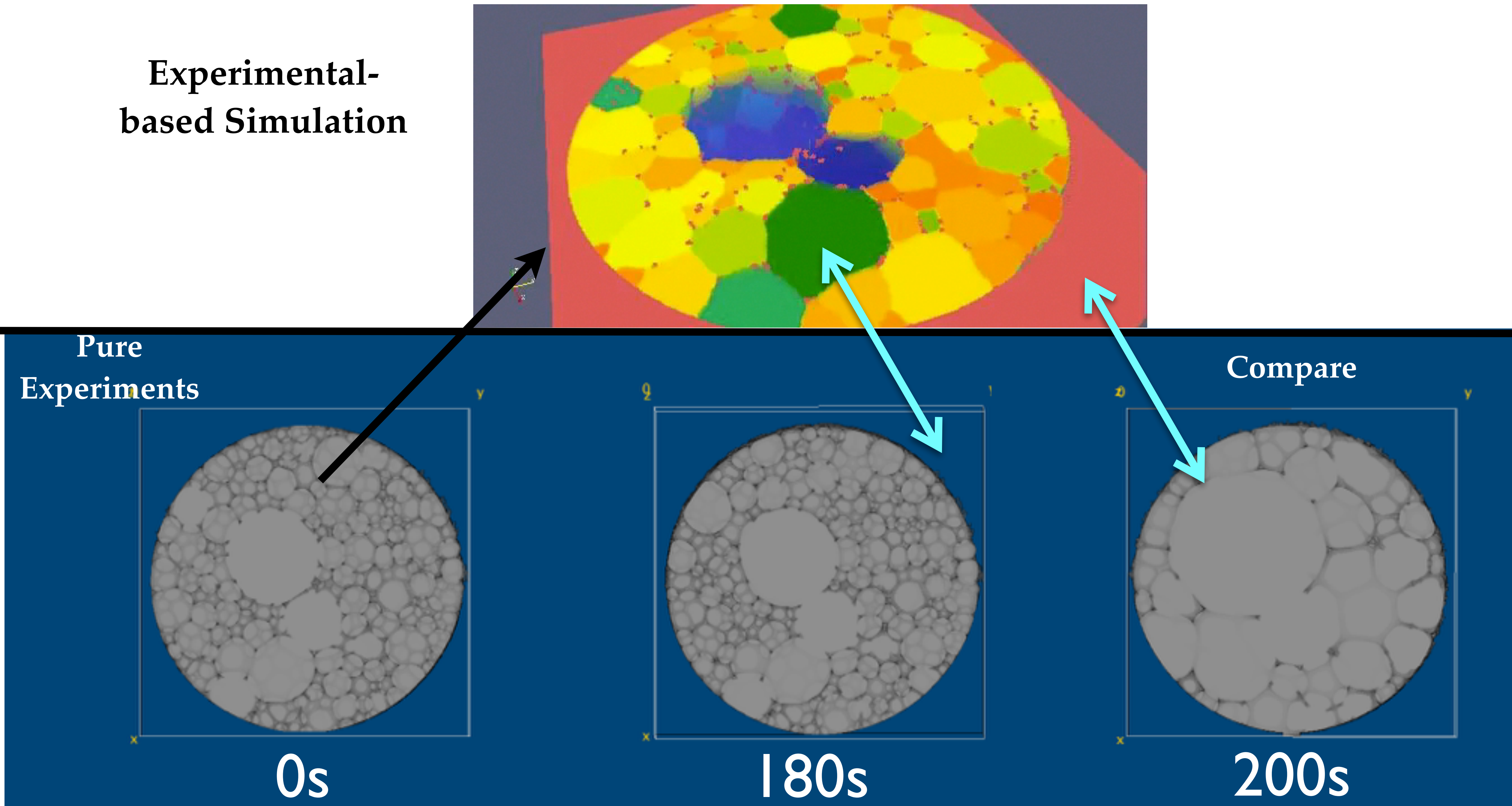
3D Coarsening

- Once bubbles are identified correctly and free-water distributed
- Run a coarsening experiment
  - Allow all phases to move freely



Matching Experiments with Reality

- Tune parameters and volume fraction until water distribution and bubble size distribution match



Conclusions

- Cellular Potts is a good fit for 3D imaging modalities
- CPM can show a number of important behaviors like coarsening and topological rearrangements
- With minimal parameter tweaking and free water adding, labeled synchrotron data can be stably incorporated into CPM simulations
- Reasonable looking coarsening can be simulated using experimental data as a starting point

Challenges

- **Approach**
  - Simulations are computationally and memory intensive to run, even on small systems (300x300x300), big systems are almost unimaginable:
    - standard tomography: 14 Gigavoxels (>500 times larger)
      - >56 gigabytes of memory
    - with proper films: 14 Teravoxels (>500K times larger)
      - >56 terabytes of memory
  - Films are not well approximated by voxels
- **Analysis**
  - Sweeping parameter space is very time consuming
  - Stability is difficult to predict, many combinations are unstable
- **Comparison**
  - Real volume fraction vs simulated volume fraction
  - Simulations must be made wetter to maintain stability
  - Time steps (pixel copy attempts) to seconds?

Outlook

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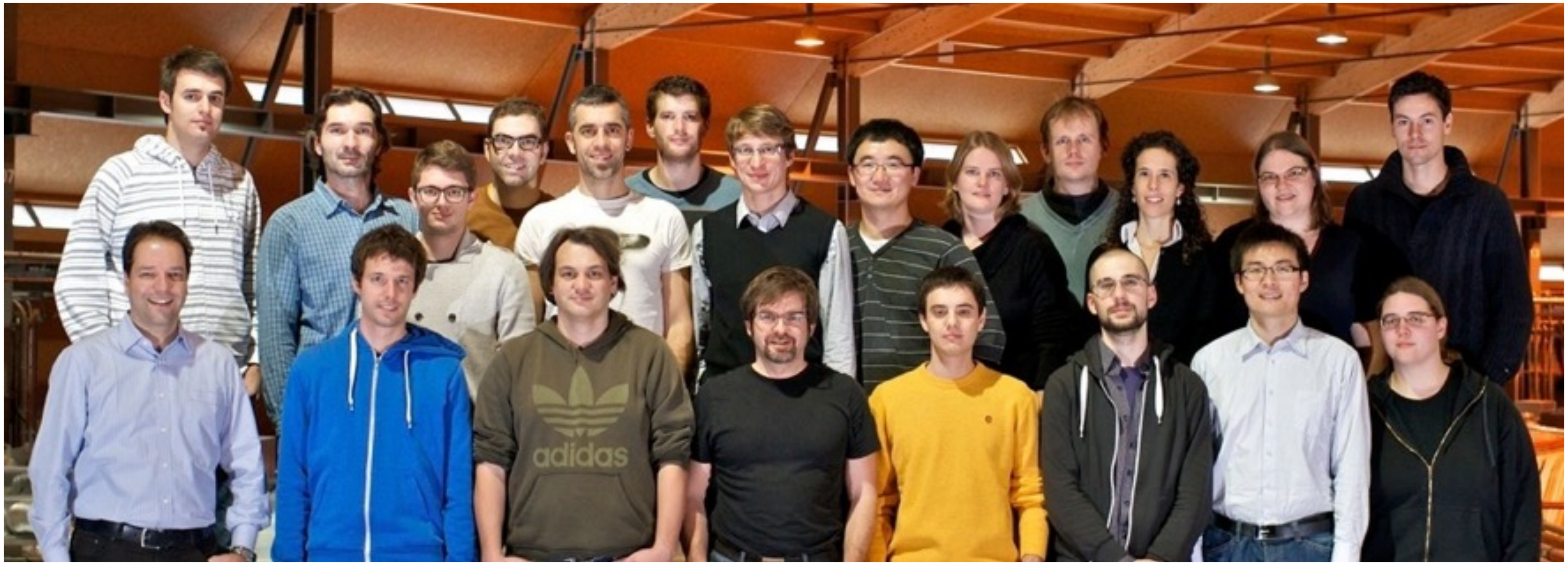
- **General**
  - Developing robust approach for parameter selection (theory, material science, etc?)
  - Looking at rheology experiments (flow through a constriction, around an obstacle)
  - Understanding the limits of simulation methods
  - One click simulations (integrating image analysis with simulation in one easy GUI)
- **Liquid Foam**
  - Combining results with surface based approaches (Surface Evolver)
  - Adding interface rules as constraints (constant curvature?)
- **Beyond**
  - Analyzing other multiphase systems (coarsening in snow and ice-cream)
  - Biological cellular systems (osteocyte cells in bone)

Acknowledgements

- IT Department at PSI
- Thank you for your attention



TOMCAT Team (11/12)

Collaborations

- Other systems to investigate
- Learn more about image analysis:
  - http://kmader.github.io/Quantitative-Big-Imaging-Course/
- Get starting yourself
  - https://gist.github.com/kmader/2b40b7f74bbd7a250634
  - http://bit.ly/1oAWyGs