Homology of Complicated and Random Evolving Patterns

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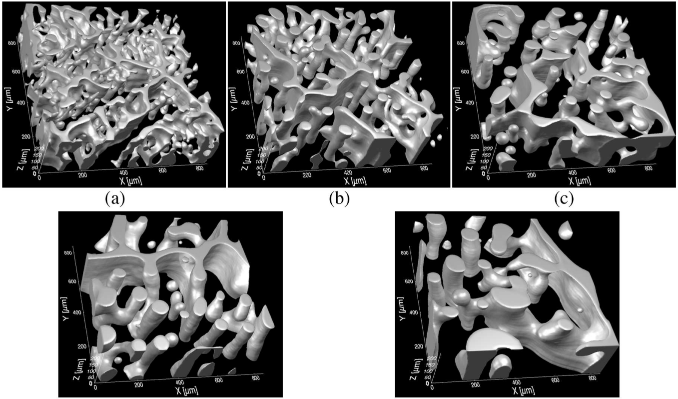
Complicated Patterns in Materials

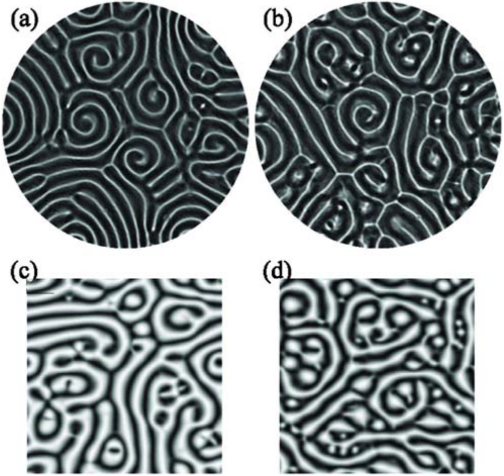
Complicated irregular patterns can be observed throughout the applied sciences, for example in materials science.
Can mathematical tools provide a reasonable quantitative measurement?



(a) (b) (c)
(d) (e)

Complicated Patterns in Fluids

Certain fluids experiments and simulations exhibit spiral defect chaos. How can one assess the correctness of the simulations?

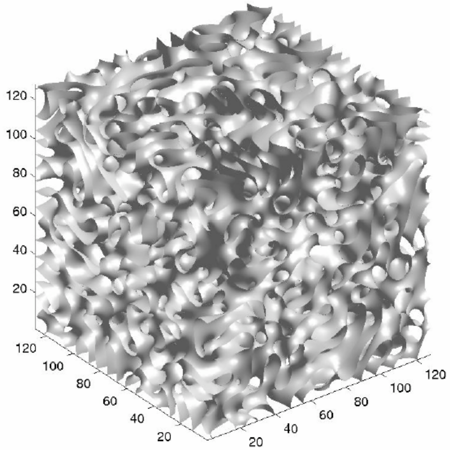


Experiment

Simulation

Three-Dimensional Cahn-Hilliard Example

Even for relatively small three-dimensional microstructures the Betti numbers have to be determined computationally:



This isosurface has Betti numbers
$\beta_0 = 1$,
$\beta_1 = 1701$,
$\beta_2 = 0$.

Computed using the CHomP software.

Models for Phase Separation

Quenching of homogeneous binary or multi-component alloys may lead to phase separation generating complicated microstructures. The resulting patterns are generally a transient phenomenon and evolve with time.

A variety of phenomenological models for such processes have been proposed over the years, including:

- Cahn & Hilliard (1958), Cook (1970), Langer (1971): The classical Cahn-Hilliard model and its stochastic extension

$$\boxed{u_t = -\Delta(\varepsilon^2 \Delta u + f(u)) + \sigma \cdot \xi}$$

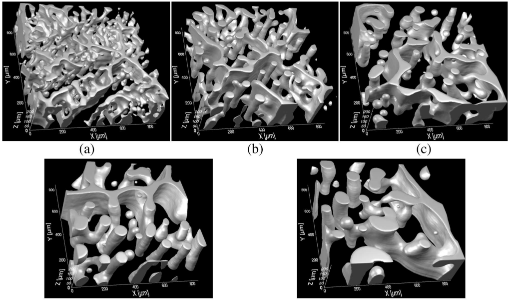
- Novick-Cohen (1988): Inclusion of frictional inter-phase forces leads to the viscous Cahn-Hilliard model

$$\boxed{\beta \cdot u_t - (1-\beta) \cdot \varepsilon^2 \Delta u_t = -\Delta(\varepsilon^2 \Delta u + f(u))}$$

Quantitative Model Assessment

- How realistic are these phenomenological models?
- Do they reproduce the microstructures accurately?
- Is a meaningful quantitative assessment possible?

Due to the irregularity and high complexity of the involved microstructures, computational homology is an obvious choice.



(a) (b) (c) (d) (e)

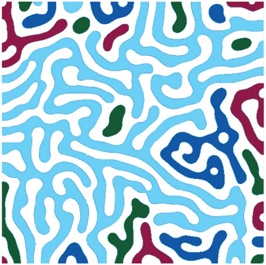
(Courtesy of P. Voorhees, Northwestern University.)

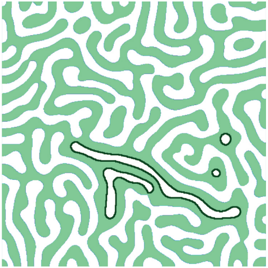
Homological Analysis of Microstructures

Gameiro, Mischaikow, W. (Acta Materialia, 2005):

For total mass μ, consider the Betti numbers β_0 and β_1 of the sets

$$\boxed{X^{\pm}(t) = \{x \in \Omega \mid \pm(u(t,x) - \mu) \geq 0\}}$$

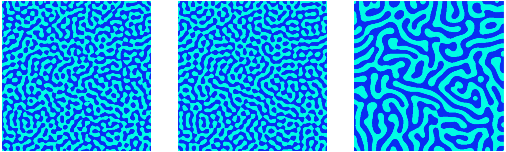




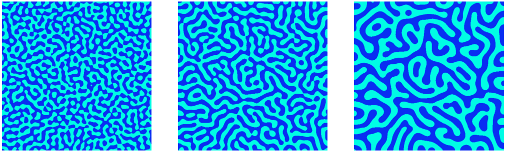
Sample set $X^{+}(t)$ for (CHC) with $\mu = 0$, $\sigma = 0$, and $t = 0.0036$.
The set has $\beta_0 = 26$ components and $\beta_1 = 4$ loops.

The Effects of Thermal Fluctuations

Cahn-Hilliard Model with $\varepsilon = 0.005$ and total mass 0:



Cahn-Hilliard-Cook Model with $\varepsilon = 0.005$, $\sigma = 0.01$ and mass 0:

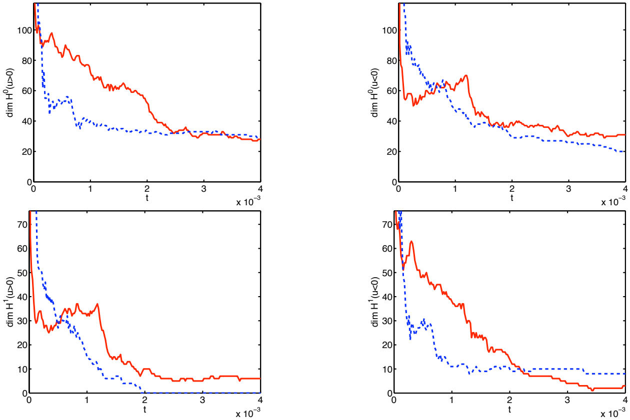


The snapshots are taken at $t = 0.0004$, $t = 0.0012$, $t = 0.0036$.

The dark regions are $X^+(t)$, their complements are $X^-(t)$.

Sample Betti Number Evolution

Betti number evolution for the Cahn-Hilliard model (solid red) and the Cahn-Hilliard-Cook model (dashed blue).



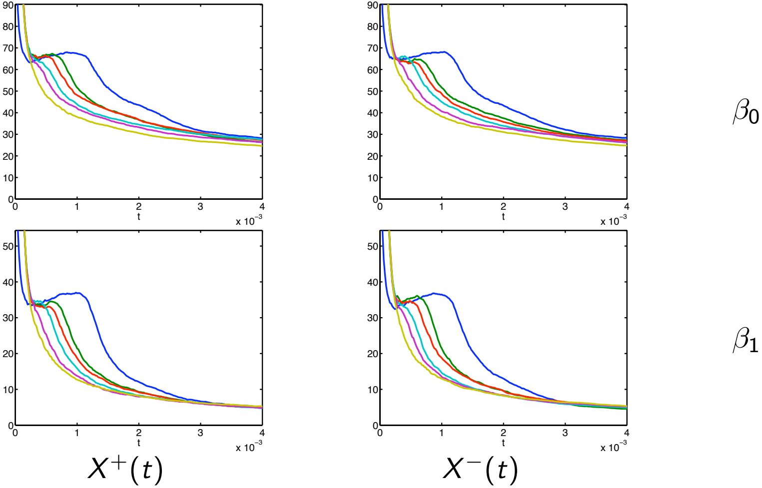
β_0

β_1

$X^+(t)$ $X^-(t)$

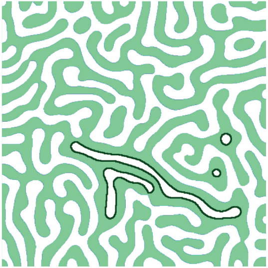
Averaged Betti Number Evolution

From 100 simulations for total mass $\mu = 0$ and a variety of different noise levels σ.



Quantification of Boundary Effects

Combining the Betti number information for $X^{\pm}(t)$ leads to the quantification of boundary effects.

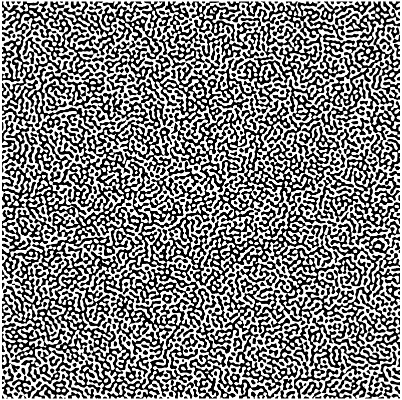


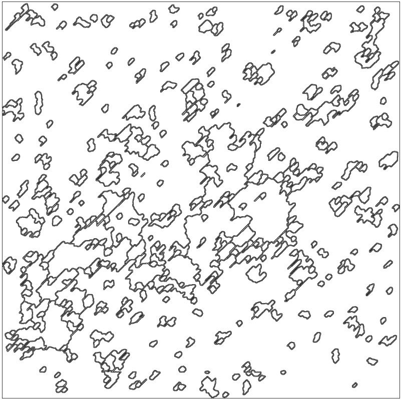
Only white components with black boundary are internal components, all of the remaining white components touch the boundary.

$$\boxed{\begin{aligned} \beta_{\mathrm{int},0}(X^+(t)) &= \beta_1(X^-(t)) \\ \beta_{\mathrm{bdy},0}(X^+(t)) &= \beta_0(X^+(t)) - \beta_1(X^-(t)) \end{aligned}}$$

Visualization of Internal Components

The internal components can be visualized using `homcubes`.

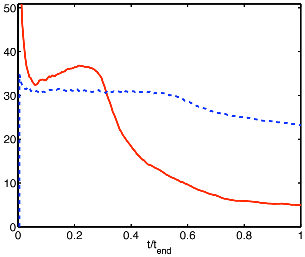




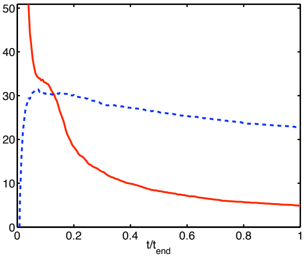
In the figure, $\beta_0 = 526$ and $\beta_1 = 431$, for $\varepsilon = 0.0015$ and $\mu = 0$.

Internal vs. Boundary Components

Averaged evolution curves for the number $\beta_{\mathrm{int},0}$ of internal components and the number $\beta_{\mathrm{bdy},0}$ of components touching the boundary.



$\sigma = 0$



$\sigma = 0.01$

The figures are for $X^{+}(t)$, with $\varepsilon = 0.005$, $\mu = 0$, and 100 samples.

The Averaged Euler Characteristic

- In the two-dimensional setting, the Euler characteristic of the set $X^+(t)$ can be computed as

$$\chi\left(X^+(t)\right) = \beta_0\left(X^+(t)\right) - \beta_1\left(X^+(t)\right)$$

- For mass $\mu = 0$, an inherent symmetry in the Cahn-Hilliard model implies that the averaged Betti numbers satisfy

$$\left\langle \beta_k\left(X^+(t)\right)\right\rangle = \left\langle \beta_k\left(X^-(t)\right)\right\rangle \quad \text{for} \quad k = 0, 1$$

- As a result, the averaged Euler characteristic is given by

$$\boxed{\left\langle \chi\left(X^+(t)\right)\right\rangle = \left\langle \beta_{\mathrm{bdy},0}\left(X^+(t)\right)\right\rangle}$$

The Euler characteristic cannot detect the averaged bulk behavior!

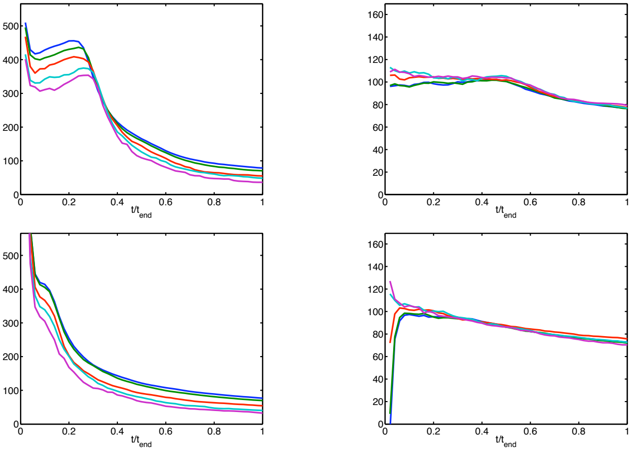
The Effects of Domain Size

- The previous simulations for $\varepsilon = 0.005$ resulted in an average of about 30 internal and 30 boundary components on a unit square during the initial phase separation.
- Rescaling ε can be interpreted as rescaling the size of the base domain for the simulation.
- Additional simulations show that
  - for $\varepsilon = 0.0015$ one obtains an average of about 400 internal and 100 boundary components during the initial phase separation, and
  - for $\varepsilon = 0.01$ one obtains an average of about 6 internal and 15 boundary components during the initial phase separation.

Can the non-monotone bulk behavior still be detected?

The Effects of Domain Size

Variation of ε corresponds to rescaling the underlying domain Ω.



β_0

β_1

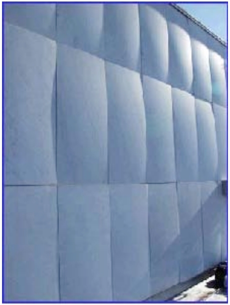
$\beta_{\mathrm{int},0} \cdot (\varepsilon/0.0015)^2$ $\beta_{\mathrm{bdy},0} \cdot \varepsilon/0.0015$

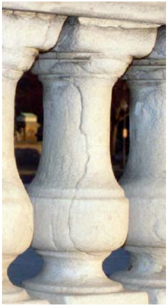
Stress Networks in Polycrystals

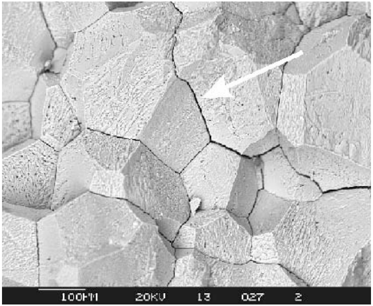
In other situations, the atomic-level microstructure is not the primary object of interest, but certain derived property fields.

Example: Thermal degradation of marble [Weiss et al. (2003)]

Internal stresses in polycrystalline materials can lead to micro-cracking, and ultimately to destruction of components.



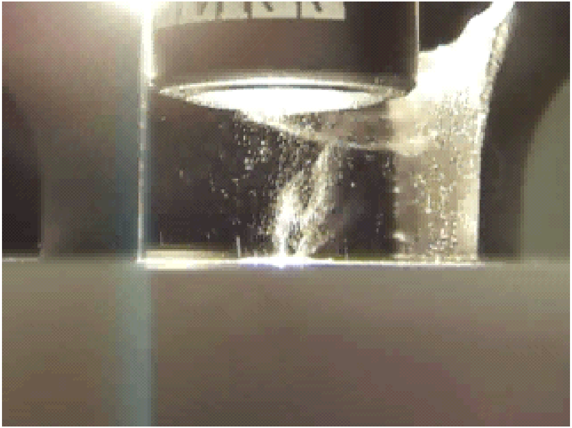




Internal Stresses in β-Eucryptite Composites

Fuller, Reimanis, et al. (2007):

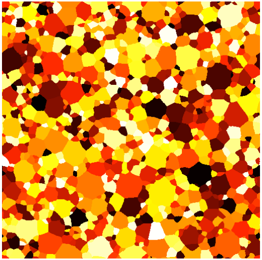
Internal stresses in polycrystals can lead to spontaneous material ejection as a consequence of an indentation.

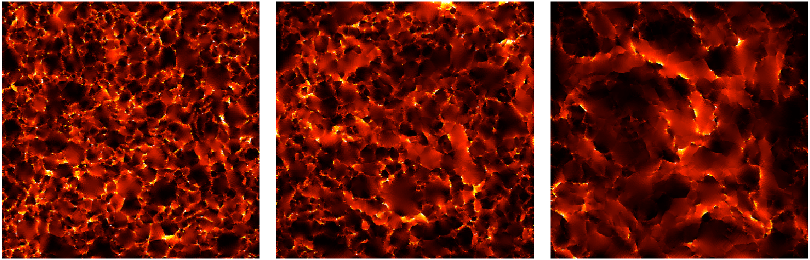


Stress Networks in Polycrystals

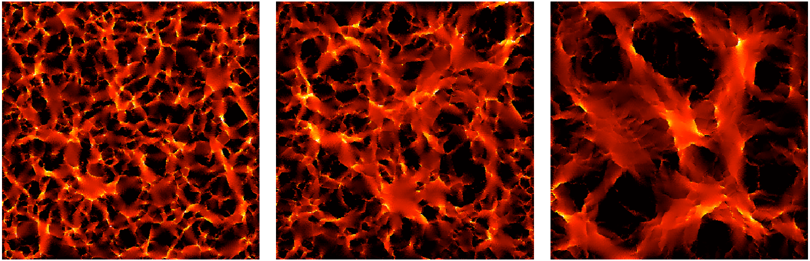
Fuller, Saylor, W. (Acta Materialia, 2009):

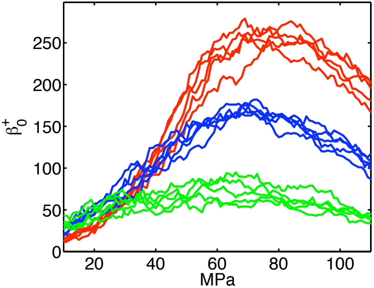
Even identical grain microstructures can lead to considerably different elastic energy density / stress networks, and therefore to different cracking behavior. These differences can be quantified by homology.

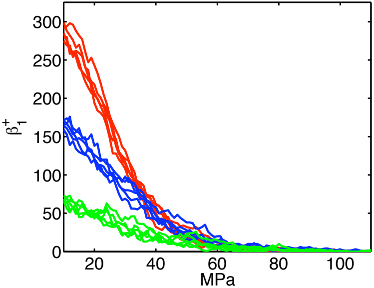




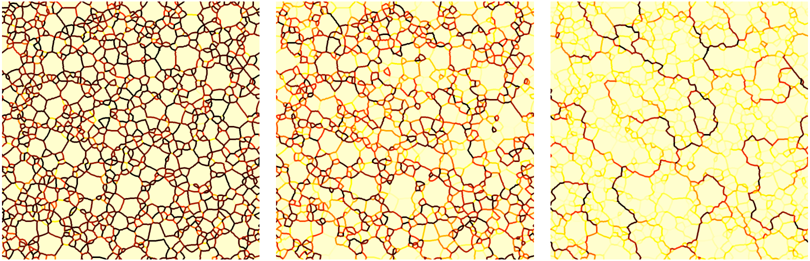
Maximal Principal Stress

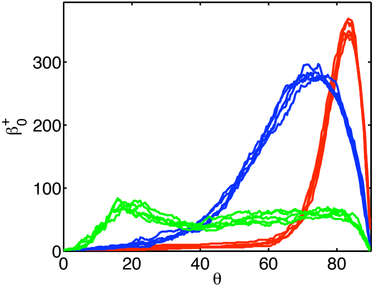


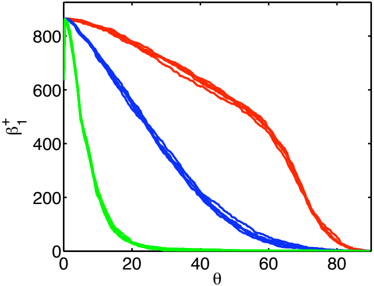




Grain Boundary Misorientations



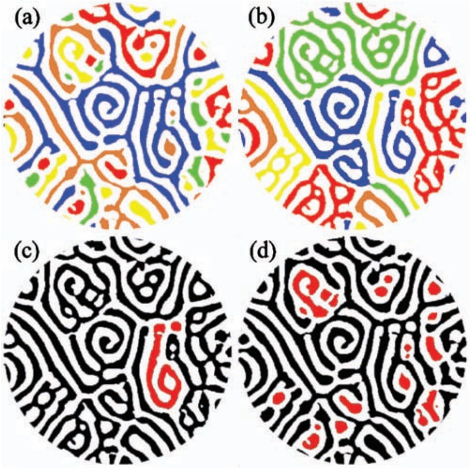




Rayleigh-Bénard Convection Patterns

Krishan, et al. (Physics of Fluids, 2007):

Homology and Symmetry-Breaking in Rayleigh-Bénard convection



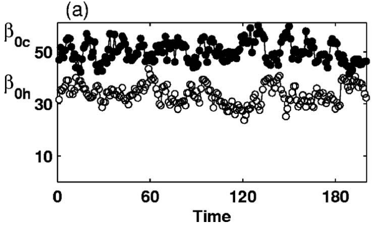
Experimental data:

Visualization of the components and loops for the cold downflow (left column) and the hot upflow (right column).

Experimental Upflow-Downflow Asymmetry

Experimental data:

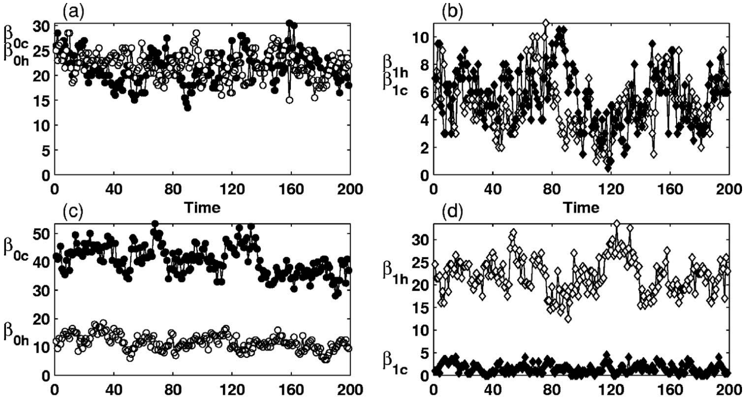
Time series plots of the Betti numbers for the cold downflow and the hot upflow exhibit a surprising asymmetry.



Can this asymmetry be seen in numerical simulations?
Typical simulations employ the Boussinesq approximation...

Breakdown of the Boussinesq Approximation

Betti number time series from both Boussinesq simulations (a, b) and non-Boussinesq simulations (c, d) indicate the breakdown of the Boussinesq approximation.



Thank You!

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