Universality Classes in Coarsening

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October 22, 2009

Universality Classes in Coarsening

Collaborators:

- Andrew Rutenberg, Dalhousie University
- Melinda Gildner, Bucknell → UPenn
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- Sohei Yasuda, Bucknell → Purdue

Bucknell Physics REU

Coarsening . . .

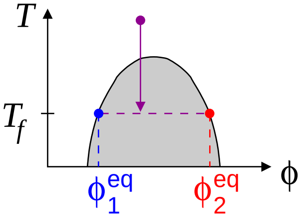
is a nonequilibrium relaxational process in which the characteristic length scale grows with time.

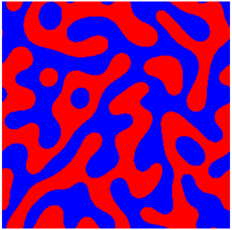
Many examples in nature:

- binary alloys
- polycrystals
- magnetic domains
- binary fluids
- epitaxy
- salad dressing
- polymer blends
- soap froths
- colloids
- liquid crystals
- faceted surfaces
- and more . . .

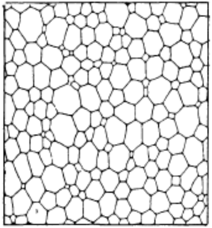
Phase Ordering Dynamics (binary alloys, polymer blends)

- Rapid quench into the forbidden region of a phase diagram
- system responds locally by equilibrating into one of the two phases
- leads to equilibrated domains separated by costly interface
- dissipative dynamics gives coarsening

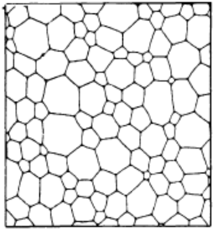




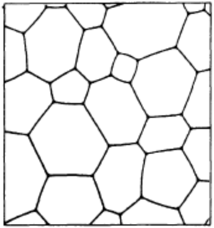
2D Dry Soap Froth



$t = 1.95$ h



$t = 21.5$ h

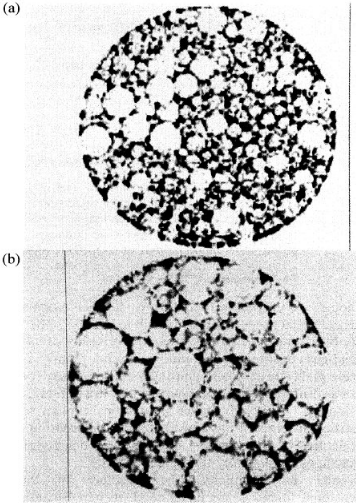


$t = 166$ h

Glazier, Gross, and Stavans, *Phys. Rev. A* **36**, 306 (1987).

Self-similarity!

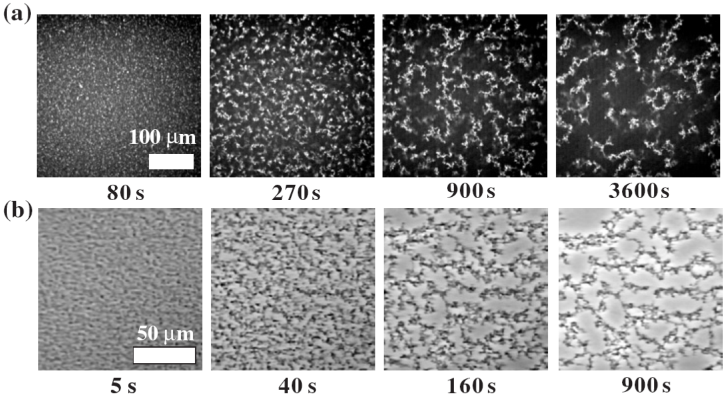
3D Wet Soap Froth



Magnetic Resonance Imaging

Gonata *et al.*, *Phys. Rev. Lett.* **75**, 573 (1995).

(a) Colloidal Suspension and (b) Polymer Solution

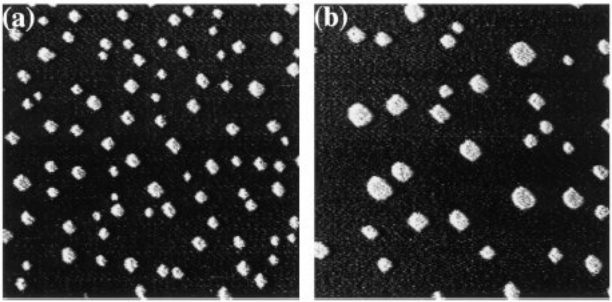


Tanaka, Nishikawa, and Koyama, *J. Phys. Cond. Matt.* **17**, L143 (2005).

Universality!

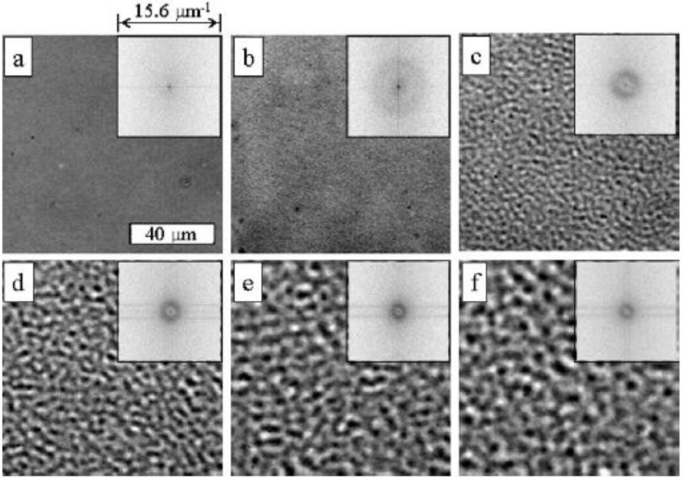
Homoepitaxial Islands

Cu on a Cu(100) surface



Pai *et al.*, *Phys. Rev. Lett.* **79**, 3210 (1997).

Random Copolymers – PEH/PEB

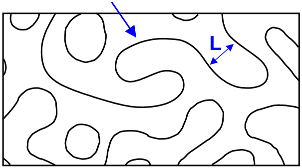


Shimizu *et al.*, *Polymer* **45**, 7061 (2004).

Why is coarsening so common?

Requirements:

- Excess free energy stored in stable, local defects (e.g., domain walls): $F - F_{eq} \propto \rho_{\text{def}}$



- Dissipation: $\frac{dF}{dt} < 0 \quad \Rightarrow \quad \frac{d\rho_{\text{def}}}{dt} < 0$

Result: growing characteristic length $L(t)$

Basic Features of Coarsening

Sharp defects defect size ξ fixed, so for asymptotically late times $L(t) \gg \xi \Leftrightarrow$ sharp-defect limit.

Self-similarity domain structure statistically invariant when rescaled by $L(t)$.

Implies correlation function scaling $C(\mathbf{r}, t) = f\big(\mathbf{r}/L(t)\big)$

Power law growth characteristic scale $L \sim t^{\alpha}$

Universality exponent α determined by only a few general features: conservation laws and nature of order parameter

Coarsening Models I: Kinetic Ising Models

Lattice of spins $s_i = \pm 1$, with hamiltonian $H = -J \sum_{\langle ij \rangle} s_i s_j$

Spins initially random ($T_i = \infty$). Quench at time $t = 0$ to $T < T_c$.

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Glauber Dynamics

- spins flip with probability determined by energy $\Rightarrow$ nonconserved order parameter.

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Glauber Dynamics

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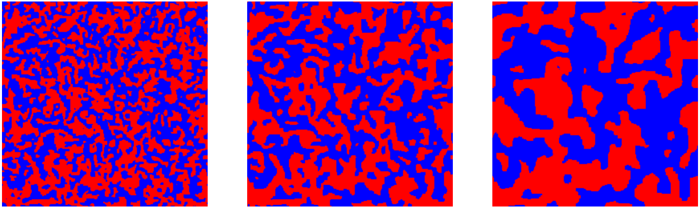
Kawasaki Dynamics

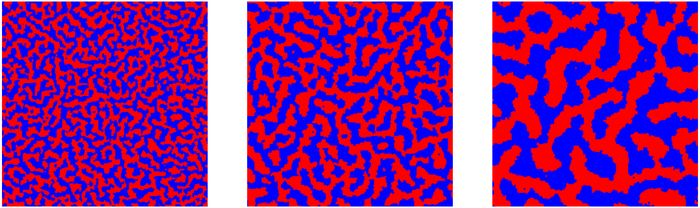
- neighboring spins exchanged $\Rightarrow$ conserved OP.
- additional parameter $\epsilon =$ fraction of spins up
- appropriate for binary mixtures: $\uparrow =$ Fe, $\downarrow =$ Al.

Kinetic Ising Models

Glauber (spin flip): nonconserved OP $\rightarrow L \sim t^{1/2}$



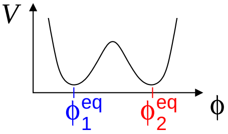
Kawasaki (spin exchange): conserved OP $\rightarrow L \sim t^{1/3}$



Coarsening Models II: Phase Field Models

Field $\phi(\mathbf{x}, t)$ describes local concentration. Free energy functional:

$$F[\phi] = \int d^d x \left\{ \frac{1}{2}(\nabla\phi)^2 + V(\phi) \right\}$$



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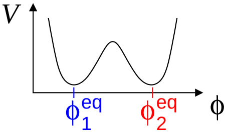

Allen-Cahn equation

Nonconserved OP: $\frac{\partial \phi}{\partial t} = -\frac{\delta F}{\delta \phi} \quad \Rightarrow \quad \frac{\partial \phi}{\partial t} = \nabla^2 \phi - V'(\phi)$

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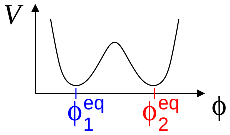

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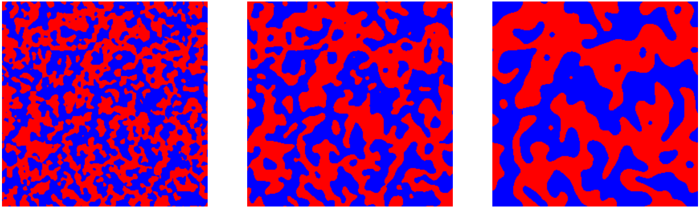
Cahn-Hilliard equation

Conserved OP: $\dfrac{\partial\phi}{\partial t} = -\nabla\cdot\mathbf{J}$ and $\mathbf{J} = -\nabla\dfrac{\delta F}{\delta\phi}$

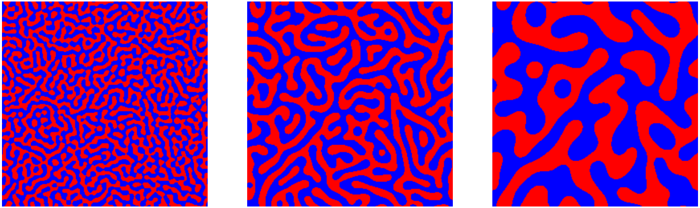
$$\Rightarrow \frac{\partial\phi}{\partial t} = -\nabla^2[\nabla^2\phi - V'(\phi)]$$

Phase Field Models

Allen-Cahn eq: nonconserved OP $\rightarrow L \sim t^{1/2}$



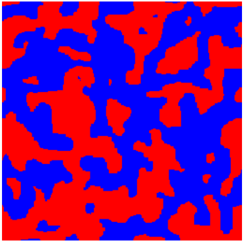
Cahn-Hilliard eq: conserved OP $\rightarrow L \sim t^{1/3}$



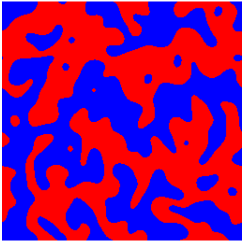
Universality?

$L \sim t^{1/2}$

Glauber

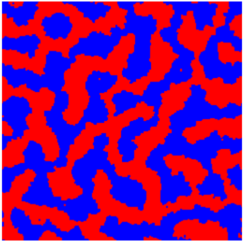


Allen-Cahn

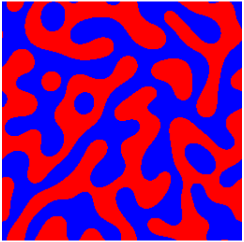


$L \sim t^{1/3}$

Kawasaki



Cahn-Hilliard



Theoretical Challenge

- Self-similar scaling state with universal power law growth generic. Demands explanation!
- Characterizing scaling state a starting point for analysis of real systems. Need universality classes!

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Renormalization Group Scenario

- Critical-like behavior $\Rightarrow$ dynamical RG fixed point controlling the asymptotic dynamics.
- Not (yet) tractable — a strong-coupling fixed point.

How do we proceed?

Two Routes to Progress

Exact Solution — Lifshitz-Slyozov Theory ('58)

- Conserved OP coarsening in dilute $\epsilon \to 0$ limit $\Rightarrow$ isolated droplets
- Derives scaling state, demonstrates its universality.
- Original prediction of $L \sim t^{1/3}$ exponent.

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Assume Scaling, Derive Consequences

- Huse ('86) argued COP $L \sim t^{1/3}$ extends to all ϵ.
- Bray's RG scenario ('89) also gives $L \sim t^{1/3}$.
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So why am I here talking about universality classes?

Bray-Rutenberg $\Rightarrow$ growth exponent $(L \sim t^{\alpha})$ universality classes:

- α depends only on conservation law and nature of order parameter
- does not depend on spatial dimension d, volume fraction ϵ, or microscopic details

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Conventional wisdom: correlation function $C(\mathbf{r}, t)$ or structure factor $S(\mathbf{k}, t)$ has same universality as the growth exponent.

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Not true!

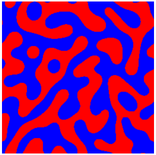
Distinct Universality (for conserved scalar OP)

Quantities that affect the correlation function but not the growth exponent:

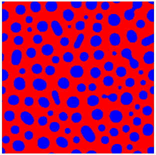
Trivial

- volume fraction ϵ
- spatial dimension d

. . . everyone knew that already.



$\epsilon = 1/2$



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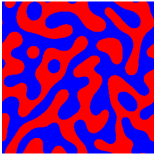

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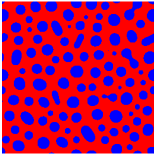
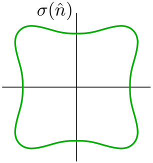


$\epsilon < 1/2$

Less Trivial

- anisotropic surface tension $\sigma(\hat{n})$ (e.g. Ising model)



exact Lifshitz-Slyozov solution for dilute coarsening

[BVL & Rutenberg ‘99; Gildner, Rosenbaum, Fowler, and BVL ’09]

Questions

- Does the scaled correlation function have any universality?
- If so, what are its universality classes?
- And, which quantities belong to exponent universality classes, versus correlation function universality classes?

  [Higher order correlation functions, curvature distribution, autocorrelation exponents, persistence exponents, growth law amplitudes, . . .]

Answer?

Conjecture:

- Growth exponents are a special case. Superuniversal due to constraints

- Correlation function universality reflects domain morphology universality [Ockham, circa 1300], so

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Conjecture:

- Growth exponents are a special case. Superuniversal due to constraints
- Correlation function universality reflects domain morphology universality [Ockham, circa 1300], so

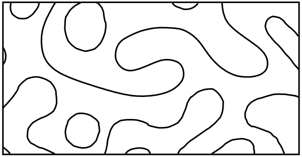
  focus on the domain morphology!
- Domain morphology universality reflects defect (domain wall) dynamics universality, so

  focus on the defect dynamics!

Asymptotic Defect Dynamics

What are the dynamical rules for the interfaces?

For a given domain configuration, e.g.



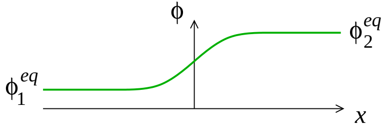
how will it evolve? What is the sequence of future domain configurations?

Use late-time asymptotia to reduce to simpler sharp defect dynamics.

Example: conserved scalar OP with isotropic σ

Step 1. Surface Tension

Consider a flat interface at $x = 0$ with b.c. as shown:



Equilibrium concentration profile given by

$$0 = \mu(\mathbf{x}) = \frac{\delta F}{\delta \phi(\mathbf{x})} = V'(\phi) - c\nabla^2\phi + \ldots$$

Solution $\phi_{\text{int}}(x)$ gives free energy per unit interface:

$$\text{Surface Tension:} \quad \sigma \equiv F[\phi_{\text{int}}(x)]/A$$

For curved interfaces, $\sigma(\kappa) = \sigma + O(\kappa)$

Example: conserved scalar OP with isotropic σ

Step 2. Bulk Mobility

- In bulk $\phi \approx \phi_1^{eq}$, so local chemical potential proportional to the supersaturation:

$$\mu(\mathbf{x}) \sim V''(\phi_1^{eq})\big(\phi(\mathbf{x}) - \phi_1^{eq}\big)$$

- Asymptotic current:

$$\mathbf{J} = -M(\phi)\nabla\mu \sim -M(1)V''(1)\nabla\phi$$

- Gives diffusion equation in bulk:

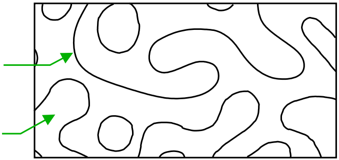
$$\frac{\partial\phi}{\partial t} = -\nabla\cdot\mathbf{J} \sim D\nabla^2\phi$$

- ϕ and μ equilibrate to $\nabla^2\mu$ in time $t_{eq} \sim L^2$

Example: conserved scalar OP with isotropic σ

Step 3. Gibbs-Thomson at interfaces:

$$\mu(\mathbf{x}) = \frac{\sigma}{\Delta\phi_{eq}}\kappa(\mathbf{x}) + O(\kappa^2)$$



Step 4. Quasistatic in bulk: $\nabla^2\mu = 0$ since diffusion field equilibrates faster than interfaces move.

Determines $\mu(\mathbf{x})$ everywhere!

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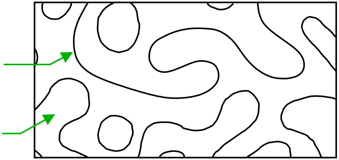

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Step 5. Interface velocity determined by bulk flux to interface:

$$\Delta\phi_{eq}v(\mathbf{x}) = \hat{n}\cdot(\mathbf{J}_+ - \mathbf{J}_-) \Rightarrow \boxed{v(\mathbf{x}) = \frac{M_1\,\hat{n}\cdot\nabla\mu_1 - M_2\,\hat{n}\cdot\nabla\mu_2}{\Delta\phi_{eq}}}$$

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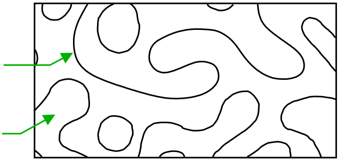

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Huse: $v \sim \dot{L}$, $\nabla\mu \sim 1/L^2$

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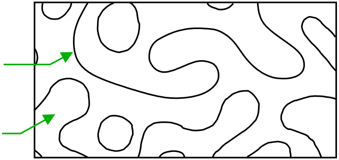

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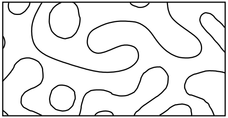
Huse: $v \sim \dot{L}$, $\nabla\mu \sim 1/L^2 \;\Rightarrow\; \dot{L} \sim 1/L^2 \;\Rightarrow\; L \sim t^{1/3}$

Example: conserved scalar OP with isotropic σ

Take case of equal bulk mobilities: $M_1 = M_2 = M$.



- For all such systems $v(\mathbf{x})$ same at each point along the interface, up to an overall factor $M\sigma/(\Delta\phi_{eq})^2$.
- All systems will evolve through the same sequence of configuration: they have the same defect trajectories.
- In rescaled time $\tau = \frac{M\sigma}{(\Delta\phi_{eq})^2} t$, all systems evolve identically!
- If $M_1 \neq M_2$, the above still hold for all systems with the same ratio M_1/M_2.

Domain Morphology Universality

Conjecture: Domain morphology has same universality as the defect trajectories.

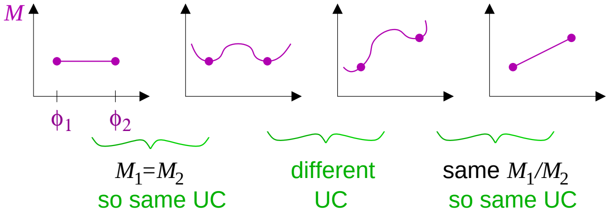
Wrong if

- different trajectories can lead to the same morphology (superuniversal)
- different morphologies possible from same trajectories (history dependent)

Corollary: in rescaled time, growth law $L \sim A\tau^{\alpha}$ is determined by the morphology $\Rightarrow$ the growth law amplitude should have the same universality as the correlation function.

Predicted Universality Classes — conserved scalar OP

- anisotropic $\sigma(\hat{n})$ modifies $\mu(\mathbf{x})$ at interface, so morphology depends on $\sigma(\hat{n}, T)$.
- field-dependent mobility $M(\phi)$, specifically the ratio $M(\phi_1^{eq})/M(\phi_2^{eq})$.



- volume fraction ϵ and spatial dimension d.

Morphology universality determines correlation function, growth law amplitude, persistence exponents, ...

Universality Classes in Coarsening

Asymmetric Cahn-Hilliard Equation

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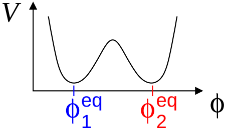
$$F[\phi] = \int d^d x \left\{ \tfrac{1}{2}(\nabla\phi)^2 + V(\phi) \right\}$$

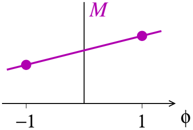
$$\mu(\mathbf{x}) = \frac{\delta F}{\delta\phi(\mathbf{x})} = -\nabla^2\phi + V'(\phi)$$



Conservation: $\dfrac{\partial\phi}{\partial t} = -\nabla\cdot\mathbf{J}$ and $\mathbf{J} = -M(\phi)\nabla\dfrac{\delta F}{\delta\phi}$

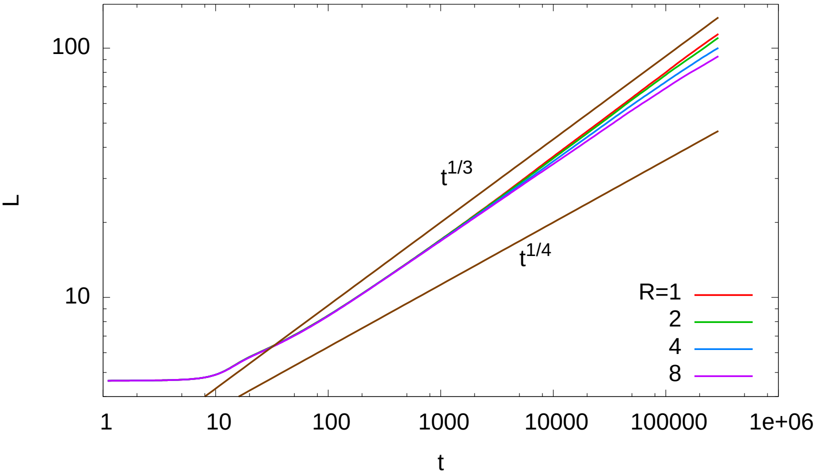
where $M(\phi) = 1 + m\phi$

$\Rightarrow$ asymmetric Cahn-Hilliard Eq.



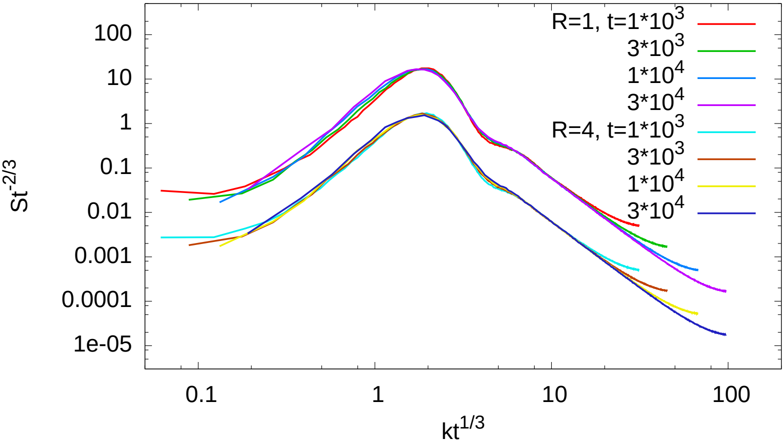
Define $R \equiv \dfrac{M(1)}{M(-1)}$

Power Law Growth of Domain

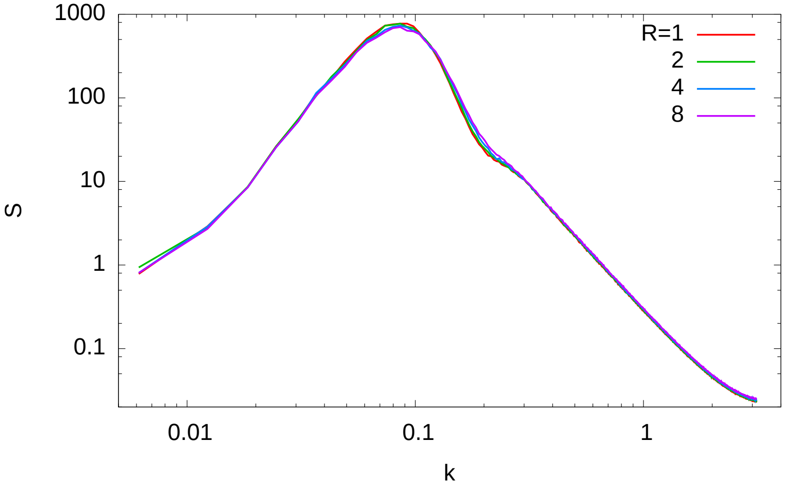


Structure Factor — Scaling Collapse

$$S(\mathbf{k}, t) = t^{2/3}\, g(kt^{1/3})$$

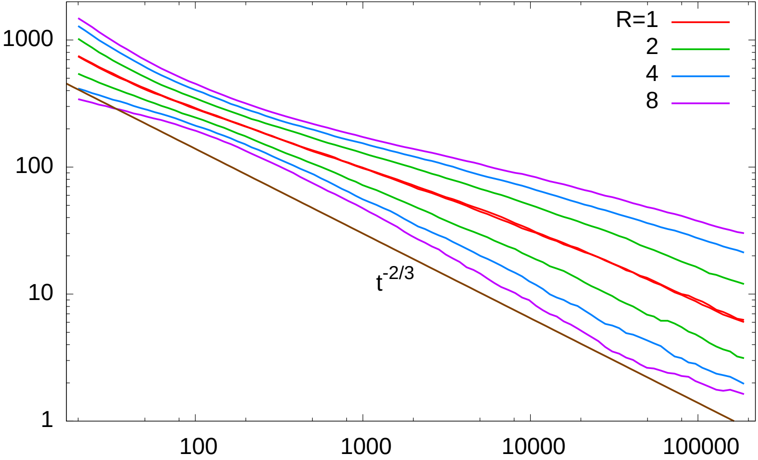


Structure Factor — Different R



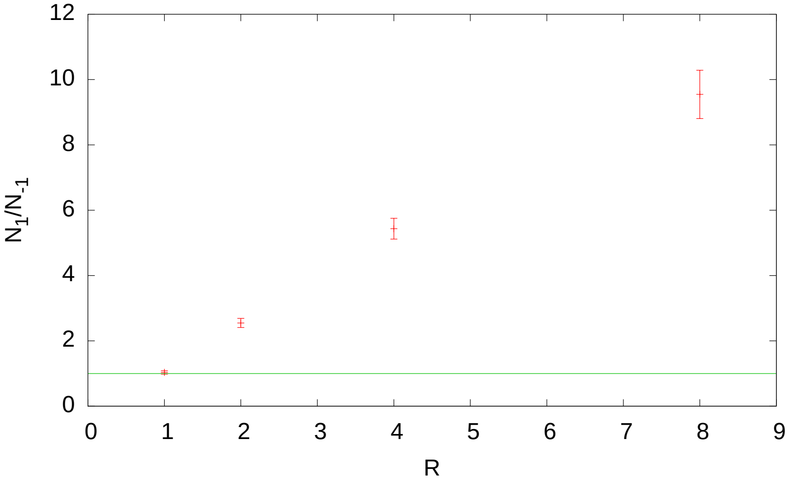
Little R dependence, if there is any!

Number of Domains



Faster phase has more domains

Ratio of Number of Domains at $t = 10^4$



Conclusions

- The growth law exponent and the correlation function do not have the same universality.
- The growth law amplitude and the correlation function do have the same universality, determined by the morphology.
- These universality classes apply to the complete asymptotic scaling state, and might be determined defect dynamics.
- Numerical tests of the asymmetric Cahn-Hilliard equation offer preliminary confirmation.
- Structure factor is not a sensitive measure — need to look at domain number

Future Work

- Generalize defect trajectory analysis (vector order parameter, liquid crystals, hydrodynamics, facets, froths, . . .). With Steven Watson.
- For numerical tests, we need larger system sizes to push runs to later times.
- We'll investigate the Cahn-Hilliard equation with asymmetric potential.