Universality Classes in Coarsening

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Universality Classes in Coarsening

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Bucknell Physics REU
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Coarsening Introduction

Theoretical Picture & Universality Conjecture

Asymptotic Defect Dynamics

Asymmetric Mobility — Numerical Test of Conjecture

Summary and Outlook
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
- facetted 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


Self-similarity!
3D Wet Soap Froth

Magnetic Resonance Imaging

(a) Colloidal Suspension and (b) Polymer Solution


Universality!
Homoepitaxial Islands

Cu on a Cu(100) surface

Why is coarsening so common?

Requirements:

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

Result: growing characteristic length $L(t)$
Basic Features of Coarsening

**Sharp defects** defect size $\xi$ 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

$$C(r, t) = f \left( \frac{r}{L(t)} \right)$$

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

**Universality** exponent $\alpha$ determined by only a few general features: conservation laws and nature of order parameter
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 $T < T_c$. 

Coarsening Models I: Kinetic Ising Models
Lattice of spins $s_i = \pm 1$, with hamiltonian $H = -J \sum_{\langle ij \rangle} s_i s_j$

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**Glauber Dynamics**

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

**Kawasaki Dynamics**
- neighboring spins exchanged $\Rightarrow$ conserved OP.
- additional parameter $\epsilon = \text{fraction of spins up}$
- appropriate for binary mixtures: $\uparrow = \text{Fe}, \downarrow = \text{Al}$. 
Kinetic Ising Models

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

**Kawasaki (spin exchange):** conserved OP $\rightarrow L \sim t^{1/3}$
Field $\phi(x, t)$ describes local concentration. Free energy functional:

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**Allen-Cahn equation**

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

Conserved OP: \[ \frac{\partial \phi}{\partial t} = -\nabla \cdot J \quad \text{and} \quad J = -\nabla \frac{\delta F}{\delta \phi} \]

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

\[ L \sim t^{1/3} \]

Kawasaki

\[ \text{Allen-Cahn} \]

\[ \text{Cahn-Hilliard} \]
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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 $\epsilon$.
- Bray’s RG scenario (’89) also gives $L \sim t^{1/3}$.
- Bray-Rutenberg energy scaling approach (’94) $\Rightarrow$ growth exponents.
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- Bray-Rutenberg energy scaling approach (’94) $\Rightarrow$ growth exponents. **Explains universality classes!**
Bray-Rutenberg ⇒ growth exponent \( (L \sim t^\alpha) \) universality classes:

- \( \alpha \) depends only on conservation law and nature of order parameter
- does not depend on spatial dimension \( d \), volume fraction \( \epsilon \), or microscopic details
Bray-Rutenberg $\Rightarrow$ growth exponent $(L \sim t^\alpha)$ universality classes:

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But which quantities are universal?

Conventional wisdom: correlation function $C(r, t)$ or structure factor $S(k, t)$ has same universality as the growth exponent.
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But which quantities are universal?

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

Not true!
Distinct Universality (for conserved scalar OP)

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

**Trivial**

- volume fraction $\epsilon$
- spatial dimension $d$

...everyone knew that already.

$\epsilon = 1/2$  
$\epsilon < 1/2$
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... everyone knew that already.

$$\epsilon = 1/2 \quad \epsilon < 1/2$$

**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, ...]
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!
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What are the dynamical rules for the interfaces?

For a given domain configuration, e.g.

![Diagram](image)

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 $\sigma$

**Step 1. Surface Tension**

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

Equilibrium concentration profile given by

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

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

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

For curved interfaces, $\sigma(\kappa) = \sigma + O(\kappa)$. 
Step 2. Bulk Mobility

- In bulk $\phi \approx \phi_{1}^{eq}$, so local chemical potential proportional to the supersaturation:

$$\mu(x) \sim V''(\phi_{1}^{eq})(\phi(x) - \phi_{1}^{eq})$$

- Asymptotic current:

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

- Gives diffusion equation in bulk:

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

- $\phi$ and $\mu$ equilibrate to $\nabla^{2}\mu$ in time $t_{eq} \sim L^{2}$
Example: conserved scalar OP with isotropic $\sigma$

**Step 3. Gibbs-Thomson** at interfaces:

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

**Step 4. Quasistatic** in bulk: $\nabla^2 \mu = 0$

since diffusion field equilibrates faster than interfaces move.

Determines $\mu(x)$ everywhere!
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**Step 5. Interface velocity** determined by bulk flux to interface:

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

$Huse$:

$v \sim \dot{L}$,

$\nabla \mu \sim 1/L^2$ \Rightarrow $\dot{L} \sim 1/L^2$ \Rightarrow $L \sim t^{1/3}$
Step 3. **Gibbs-Thomson** at interfaces:

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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 $\sigma$

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

- For all such systems $v(x)$ 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 $M_1/M_2$. 
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.
- anisotropic $\sigma(\hat{n})$ modifies $\mu(x)$ at interface, so morphology depends on $\sigma(\hat{n}, T)$.

- field-dependent mobility $M(\phi)$, specifically the ratio $M(\phi_{eq}^1)/M(\phi_{eq}^2)$.

- volume fraction $\epsilon$ and spatial dimension $d$.

Morphology universality determines correlation function, growth law amplitude, persistence exponents, . . . .
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Asymmetric Cahn-Hilliard Equation

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

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

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

Conservation:

$$ \frac{\partial \phi}{\partial t} = -\nabla \cdot J \quad \text{and} \quad J = -M(\phi)\nabla \frac{\delta F}{\delta \phi} $$

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

$\Rightarrow$ asymmetric Cahn-Hilliard Eq.

Define $R \equiv \frac{M(1)}{M(-1)}$
Power Law Growth of Domain
\[ S(k, t) = t^{2/3} g(kt^{1/3}) \]
Structure Factor — Different $R$

Little $R$ dependence, if there is any!
Number of Domains

Faster phase has more domains

$t^{-2/3}$
Ratio of Number of Domains at $t = 10^4$
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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.