Coarsening

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In collaboration with

Theory : J. J. Arenzon (Porto Alegre), A. J. Bray (Manchester),
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Experiments : I. Dierking (Manchester), M. B. Ros (Zaragoza)
PRL 07, PRE 07, EPL 08 and in preparation

Virginia Tech, May 2008.

Plan

1. Very quick review of Coarsening phenomena

   Non-conserved order parameter ; ex. para-ferro transition.

   Conserved order parameter ; ex. phase separation.

2. **Old** : the scaling hypothesis & the typical domain radius.

   Analytical and numerical results.

3. **New** : **details on the domain conformations**.

   Analytical and numerical results.

4. Why should one look at this problem ?

   Non-equilibrium dynamics, glassy systems.

5. Work in progress.

The standard Ising model

$$H = -J \sum_{\langle ij \rangle} s_i s_j \ ,$$

Ising, 1925

- The ‘classical’ spins s_i take bimodal values, $s_i = \pm 1$.
- The sum $\sum_{\langle ij \rangle}$ runs over nearest neighbours on a d dimensional, typically hypercubic, lattice.
- $J > 0$ is the coupling strength.

In equilibrium at $T < T_c(d)$ the system magnetizes : $|m_{eq}(T)| > 0$.

2nd order phase-transition at $T_c(d)$.

Evolution

The system is in contact with a thermal bath

Thermal agitation

Non-conserved order parameter $m(t,T) \neq$ ct

e.g. single spin flips with Glauber or Monte Carlo stochastic rules.

Development of magnetization in a ferromagnet.

Conserved order parameter $m(t,T) = m(0,T) =$ ct

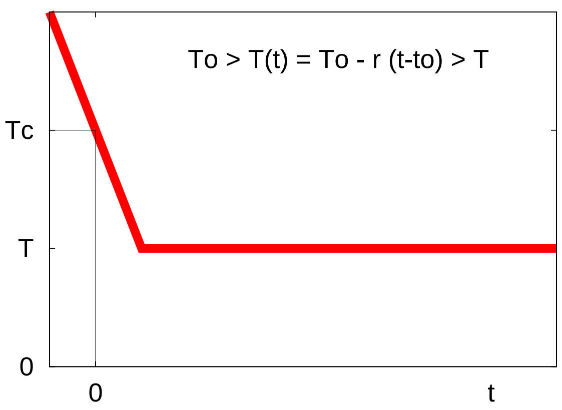
e.g. pair of antiparallel spin flips with stochastic rules.

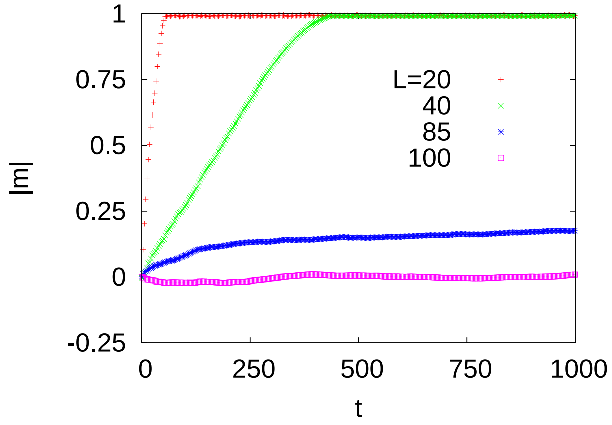
Phase separation in binary fluids.

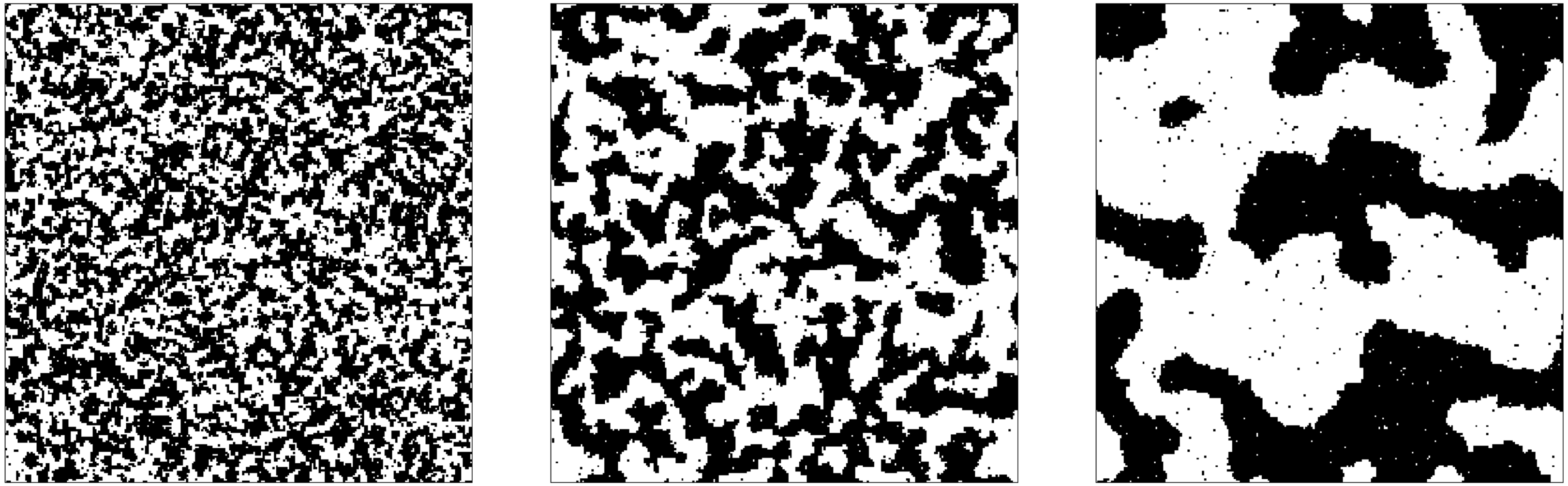
Domain growth

A rapid quench below T_c

Non-conserved order parameter







Phase separation

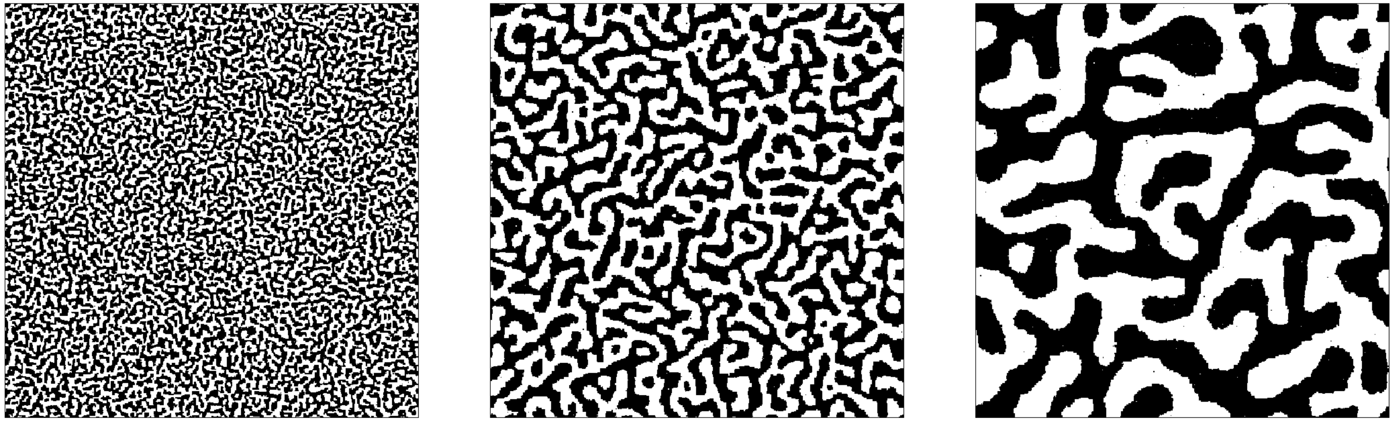
Spinodal decomposition in binary mixtures

A spieces $\equiv$ spin up ; B species $\equiv$ spin down

$2d$ Ising model with Kawasaki dynamics at T

after a rapid quench from $T_0 \to \infty$

locally conserved order parameter



50 : 50 composition ; Rounder boundaries

Scaling theory

At late times there is a single length-scale, the typical radius of the domains $\mathcal{R}(T,t)$*, such that the domain structure is (in statistical sense) independent of time when lengths are scaled by* $\mathcal{R}(T,t)$*, e.g.*

$$C(r,t) \equiv \langle\, s_i(t) s_j(t)\,\rangle\big|_{|\vec{x}_i-\vec{x}_j|=r} \sim m_{eq}^2(T)\; f\left(\frac{r}{\mathcal{R}(T,t)}\right),$$

$$C(t,t_w) \equiv \langle\, s_i(t) s_i(t_w)\,\rangle \sim m_{eq}^2(T)\; f_c\left(\frac{\mathcal{R}(T,t)}{\mathcal{R}(T,t_w)}\right),$$

etc. when $r \gg \xi(T)$, $t, t_w \gg t_0$ and $C < m_{eq}^2(T)$.

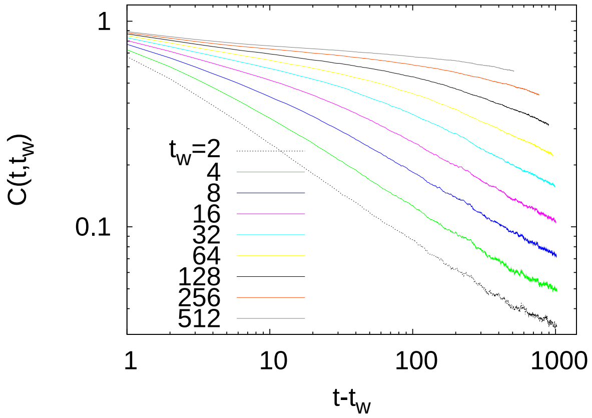
Suggested by experiments and numerical simulations. Proved for

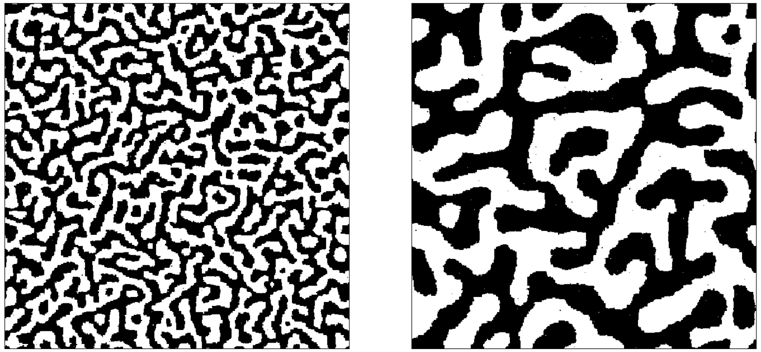
- Ising chain with Glauber dynamics.
- Langevin dynamics of the $O(N)$ model with $N \to \infty$, and the spherical ferromagnet.

Review Bray, 1994.

Self correlation

$$C(t,t_w) = N^{-1}\sum_{i=1}^{N} s_i(t)s_i(t_w)$$





$$C(t,t_w) = \underbrace{C_{st}(t-t_w)}_{\text{Equil. fluct. in domains}} + \underbrace{C_{ag}\left(\frac{\mathcal{R}(T,t)}{\mathcal{R}(T,t_w)}\right)}_{\text{Domain wall motion}}$$

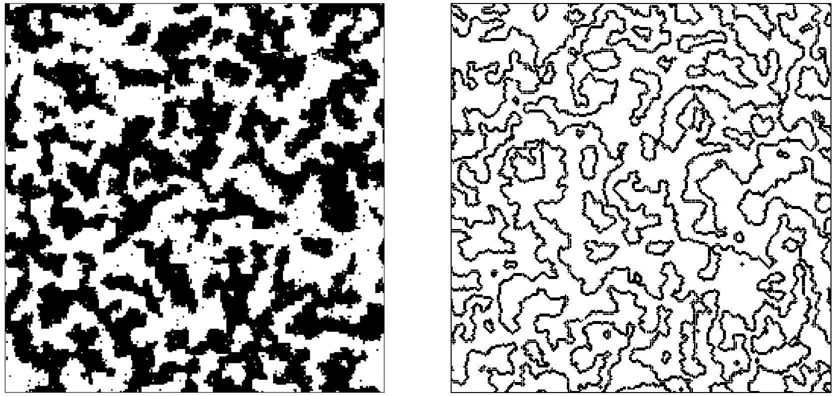
Geometry

What happens locally ?

Basic question : what does $\mathcal{R}(T,t)$ really mean ?

Can we compute, *e.g.* the number of domains with size A at time t per unit area of the system (L^2) ? Focus on $d=2$.

An instantaneous configuration $t=32$ MCs, $T=1.5$



Domains Walls

So typical means...

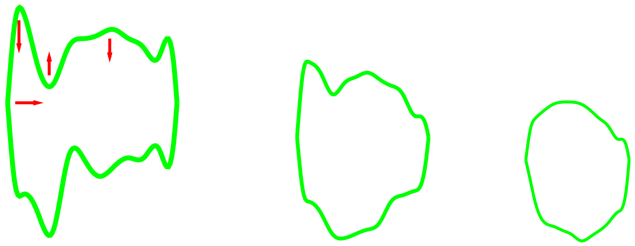
Arenzon, Bray, LFC, Sicilia, PRL 07

Non-conserved order parameter

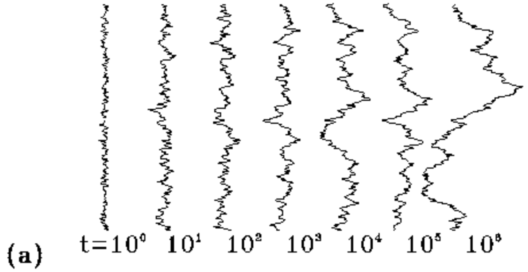
(1) the non-conserved problem is purely curvature driven at $T = 0$:

$$\vec{v} \propto -\kappa \hat{n} \, ;$$

(2) Walls move *independently* of each other **Allen & Cahn, 79**

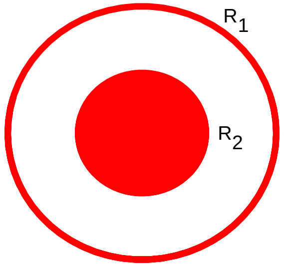


(3) Domain wall roughening ($T > 0$)



$\mathcal{R}(T,t) \propto \sqrt{\lambda_d(T)t}$, and $\lambda_d(T)$ decreases for increasing T .

Domain & hull-enclosed areas



Two hull-enclosed areas

$$A_1 = \pi R_1^2$$
$$A_2 = \pi R_2^2$$

Two domains

$$A_1 = \pi(R_1^2 - R_2^2)$$
$$A_2 = \pi R_2^2$$

Hull-enclosed areas : the interior of a domain boundary.

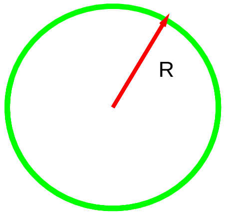
- Typically hull-enclosed areas tend to be larger than domain areas ($A_1^h > A_2^h$).
- There are as many hull-enclosed as domain areas (two).
  - Each spin belongs to one and only one domain (*e.g.* spin at the center).
  - A spin can be within more than one hull (*e.g.* spin at the center).

Non-conserved order parameter

The hull-enclosed area t-dependence

Take a sphere with radius R,

area $A = \pi R^2$



The time-variation of the *hull area*, $\frac{dA}{dt} = 2\pi R \, \frac{dR}{dt}$, in the case $v = -\frac{\lambda}{2\pi}\kappa$, with the curvature $\kappa = \frac{1}{R}$, is just constant

$$\frac{dA}{dt} = -\lambda$$

In general, $\frac{dA}{dt} = \oint \vec{v} \wedge d\vec{\ell} = \oint v d\ell$. The local wall-velocity, v, is proportional to the local geodesic curvature, κ, and the Gauss-Bonnet theorem implies $\oint \kappa d\ell = 2\pi$ for a planar $2d$ manifold with no holes. Therefore, the hull-enclosed area decreases with constant velocity for *any* geometry.

Non-conserved order parameter

The hull-enclosed area pdf evolution

Since all hull-enclosed areas decrease independently of one another, the number of hulls-enclosed areas A at time t is given by

$$n_h(A,t) = \int dA_0 \; \delta(A - A(t,A_0)) \, n_h(A_0,t_0)$$

where $n_h(A_0,t_0)$ is the initial distribution and $A(t,A_0)$ is the area at time t given that the area at the initial time t_0 was A_0.

For convenience we normalize by the area of the full system, L^2.

Thus, we need $A(t,A_0)$ – that we just computed for hulls-enclosed areas – and the initial pdf $n_h(A_0,t_0)$.

Non-conserved order parameter

The hull-enclosed area distribution in $d = 2$

Each hull area : $\frac{dA}{dt} = -\lambda$. Thus $A(t, A_0) = A_0 - \lambda(t - t_0)$.

- Quench from an infinite temperature ⇔ random initial condition,

  $s_i = \pm 1$ with $p = \frac{1}{2}$; close to critical percolation, p_c, in $d = 2$.

- Quench from equilibrium at T_c : Ising cluster hulls at criticality.

The equilibrium hull area distribution at p_c and T_c are

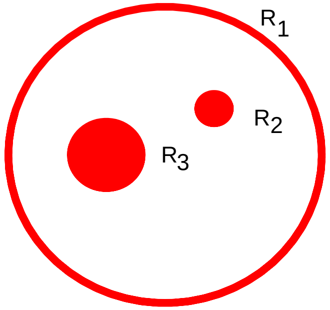
$$n_h(A_0, t_0) \sim \frac{(2)c_h}{A_0^2} \; , \qquad c_h = \frac{1}{8\pi\sqrt{3}} \qquad\qquad (a^2 \ll A_0 \ll L^2)$$

Conformal field theory, scaling & numerical checks **Cardy & Ziff, 03.**

Non-conserved order parameter

Domain area t-dependence

An example



$$A_i(t) = A_i(t_0) - \lambda(t - t_0)$$

while $A_i > 0$

$i = 1, 2, 3$ (Hulls) .

- Hulls with initial area smaller than λt will have disappeared at t.
- Hulls with initial area larger than λt will have decreased by λt.

$$\frac{dA_d}{dt} = \frac{dA_1}{dt} - \frac{dA_2}{dt} - \frac{dA_3}{dt} = -\lambda[1 - \nu(t)]$$

The outer (white) domain area grows while its hull area shrinks.

$\nu(t)$ instantaneous number of internal domain walls (2 in the ex.)

Non-conserved order paramater

The domain area distribution in $d = 2$

- For the domain area $\frac{dA_d}{dt} = -\lambda\,[1-\nu(t)]$ where $\nu(t)$ is the number of internal walls of the chosen domain. One can approximate it in a 'mean-field' manner [$O(c_h)$ approximation] as

$$\nu(t) \sim \langle\, \nu(t)\, \rangle = A_h(t) \int_0^{A_h(t)} dA'\; n_h(A', t)$$

- The initial domain distribution is

$$n_d(A_0, t_0) \sim \frac{c_d\; a^{2(\tau-2)}}{A_0^{\tau}} \qquad\qquad (a^2 \ll A_0 \ll L^2)$$

with $\tau = 379/187 \sim 2.027$ at T_c ; $\tau' = 187/91 \sim 2.055$ at p_c ;

c_d is not known analytically.

Stella & Vanderzande, 89 ; Duplantier & Saleur, 89 ; Janke & Schakel, 05.

Non-conserved order parameter

The predictions

$$n_h(A,t) \equiv \frac{(2)c_h}{(A+\lambda t)^2} \qquad\qquad n_d(A,t) \approx \frac{(2)c_d\,(\lambda_d t)^{\tau-2}}{(A+\lambda_d t)^{\tau}}$$

in the long time limit and for large areas such that $a^2 \ll A \ll L^2$.

Note that we derived (!) the expected scaling forms :

$$n_h(A,t) = (\lambda t)^{-2}\, f_h\left(\frac{A}{\lambda t}\right) \qquad\qquad n_d(A,t) \approx (\lambda_d t)^{-2}\, f_d\left(\frac{A}{\lambda_d t}\right) .$$

The new parameters are $c_d = c_h + O(c_h^2)$ and $\lambda_d = \lambda + O(c_h)$.

Moreover, the sum rules,

$$N_h(t) = N_d(t) \qquad\qquad \int dA\, A\, n_d(A,t) = 1$$

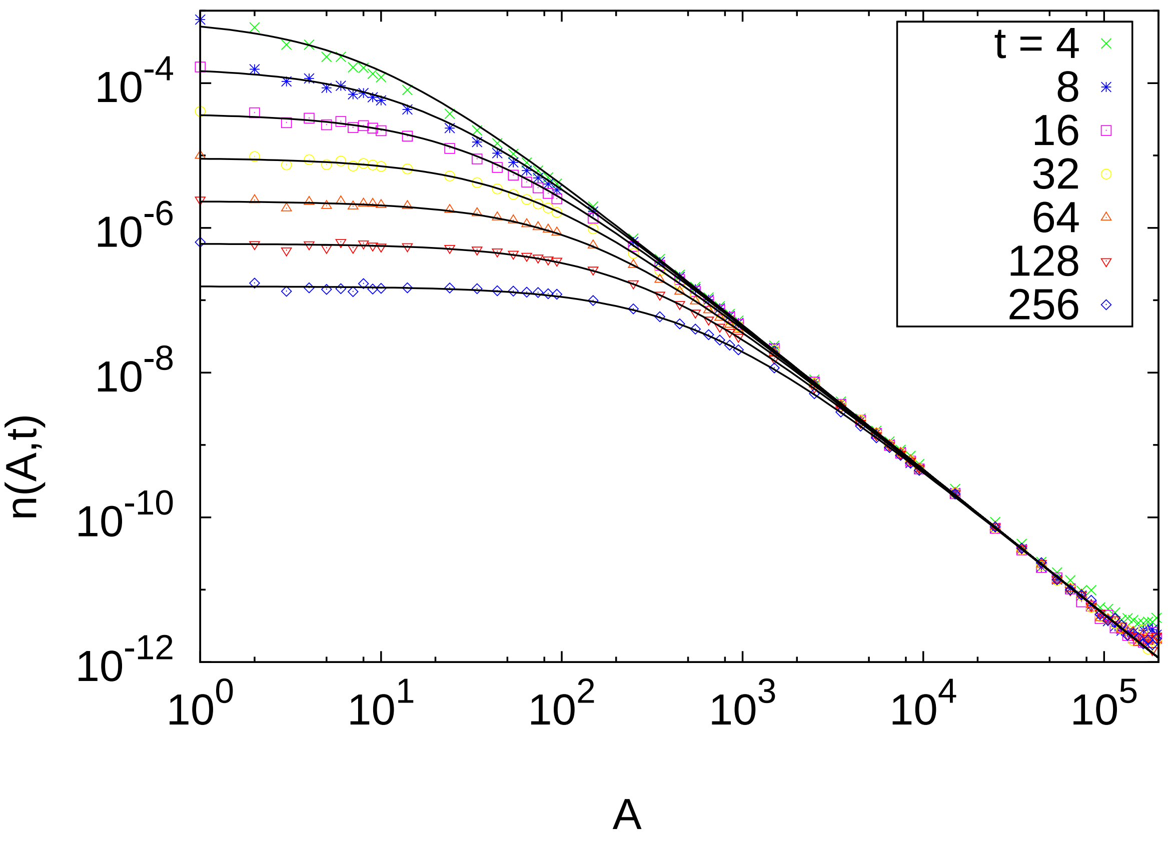
relate c_h to τ (or τ') ! **Arenzon, Bray, LFC, Sicilia, PRL 07, PRE 07.**

Non-conserved order parameter

Number density of (finite) *hull-enclosed areas* per unit area

$T = 0$ dynamics after a quench from $T_0 \to \infty$

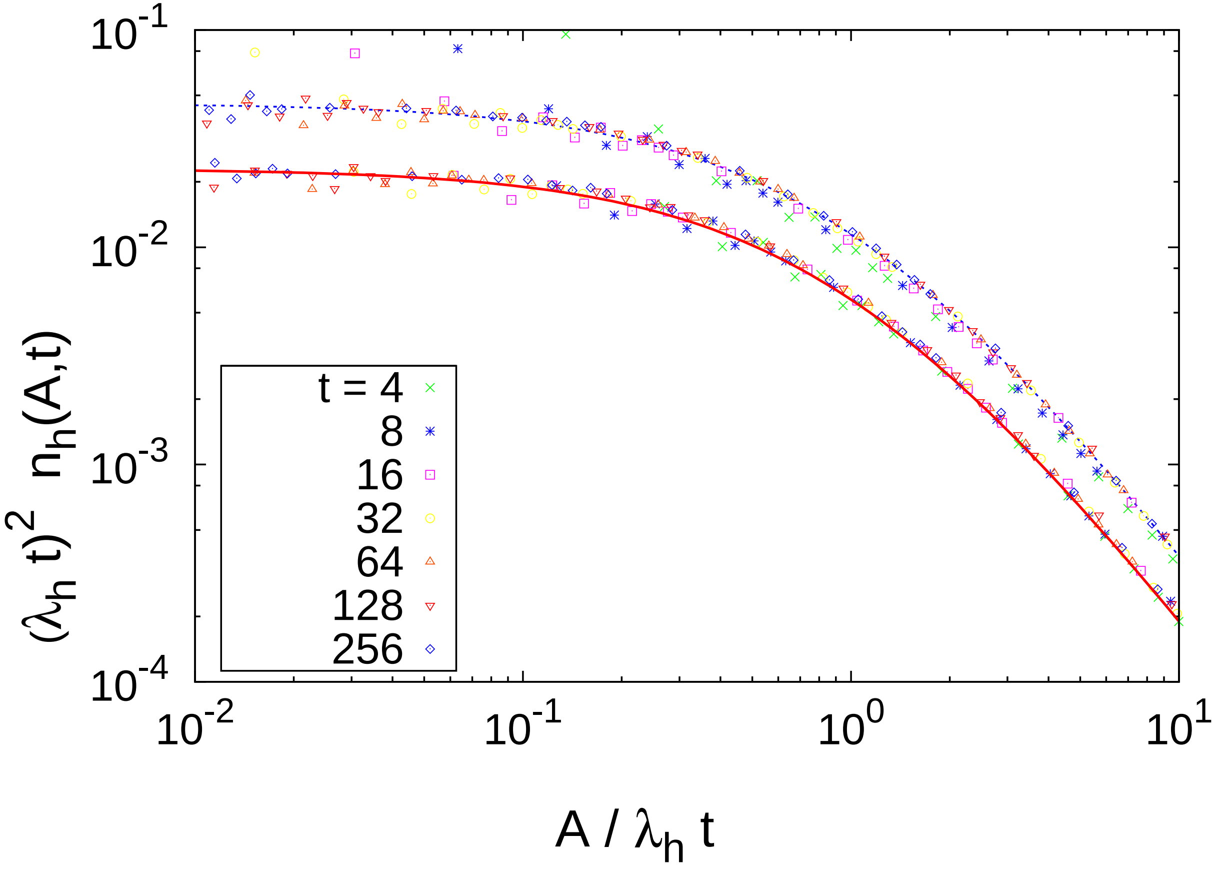
$L = 10^3$; 2×10^3 samples



Non-conserved order parameter

Number density of (finite) *hulls* per unit area

$T = 0$; quenches from $T_0 \to \infty$ and T_c

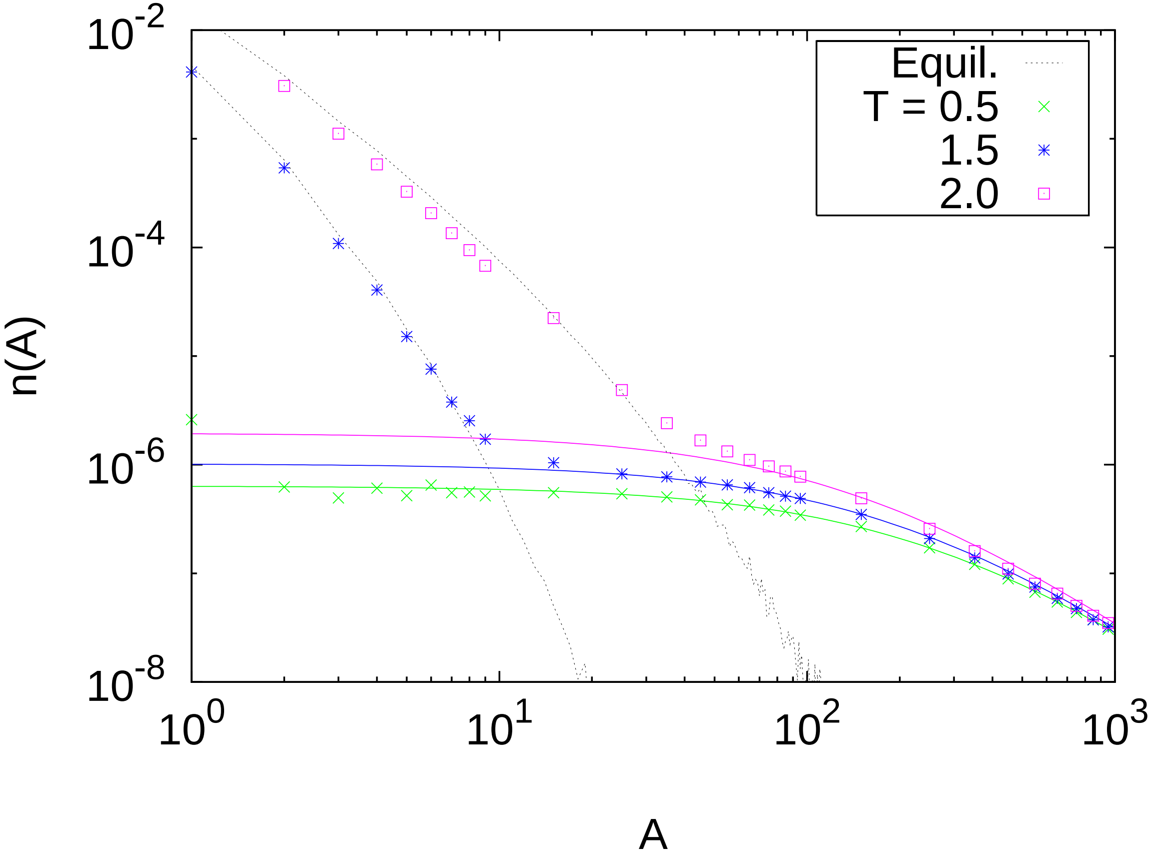


Difference between c_h at $T_0 = T_c$ and $2c_h$ at $T_0 \to \infty$.

Non-conserved order parameter

Number density of (finite) *domains* per unit area

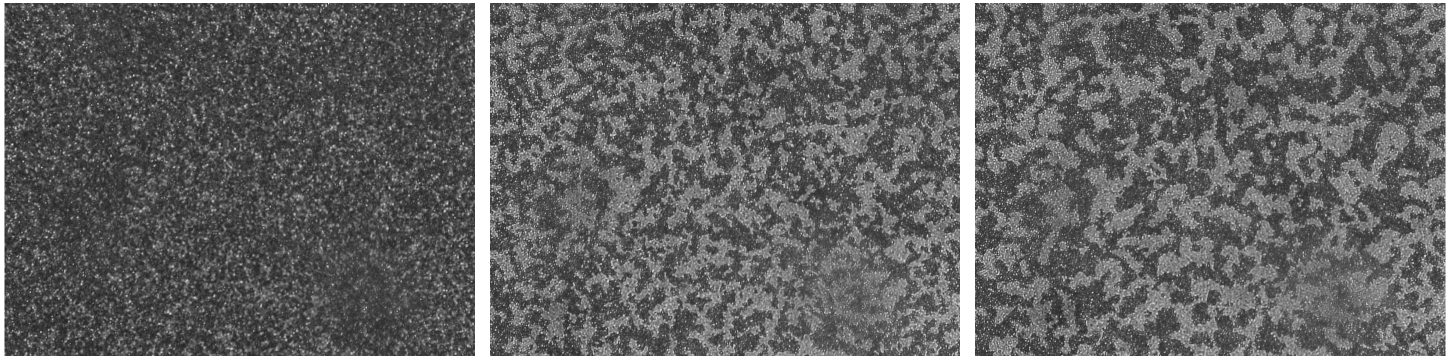
$T > 0$ dynamics after a quench from equilibrium at T_c



Experiments

$2d$ liquid crystal

After a rapid quench



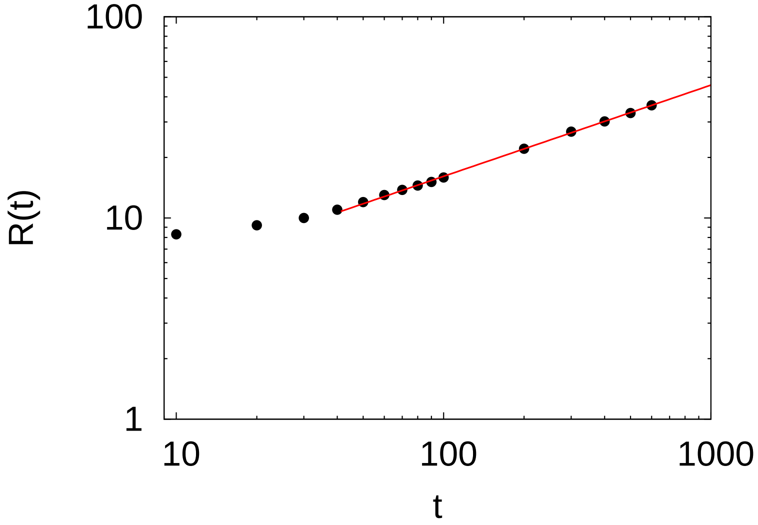
Domains of two chiralities

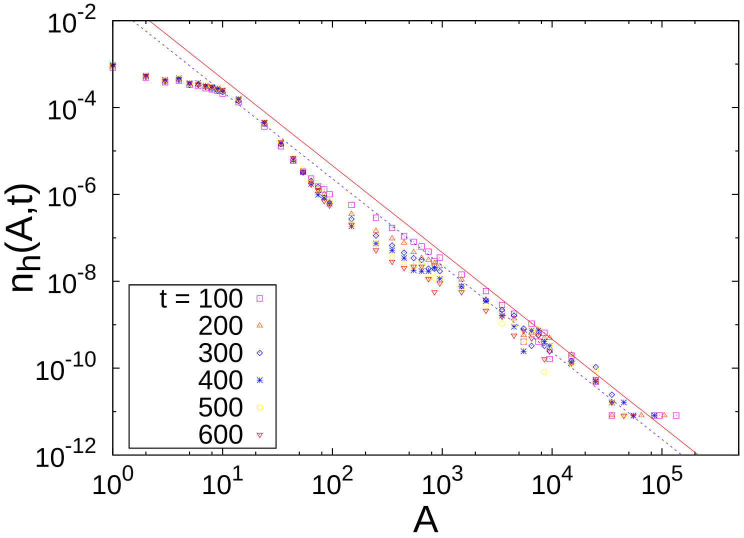
- Global constraint : total chirality is conserved.
- Microscopic mechanism for domain growth is not known.
- Sample provided by **M. B. Ros (Zaragoza)**
- Experimental set-up due to **I. Dierking (Manchester)**.

Experiments

Growth of chiral domains in a slice of a liquid crystal

$T \ll T_c$; quench from high $T_0 \gg T_c$





$R(t,T) \sim t^{0.45}$

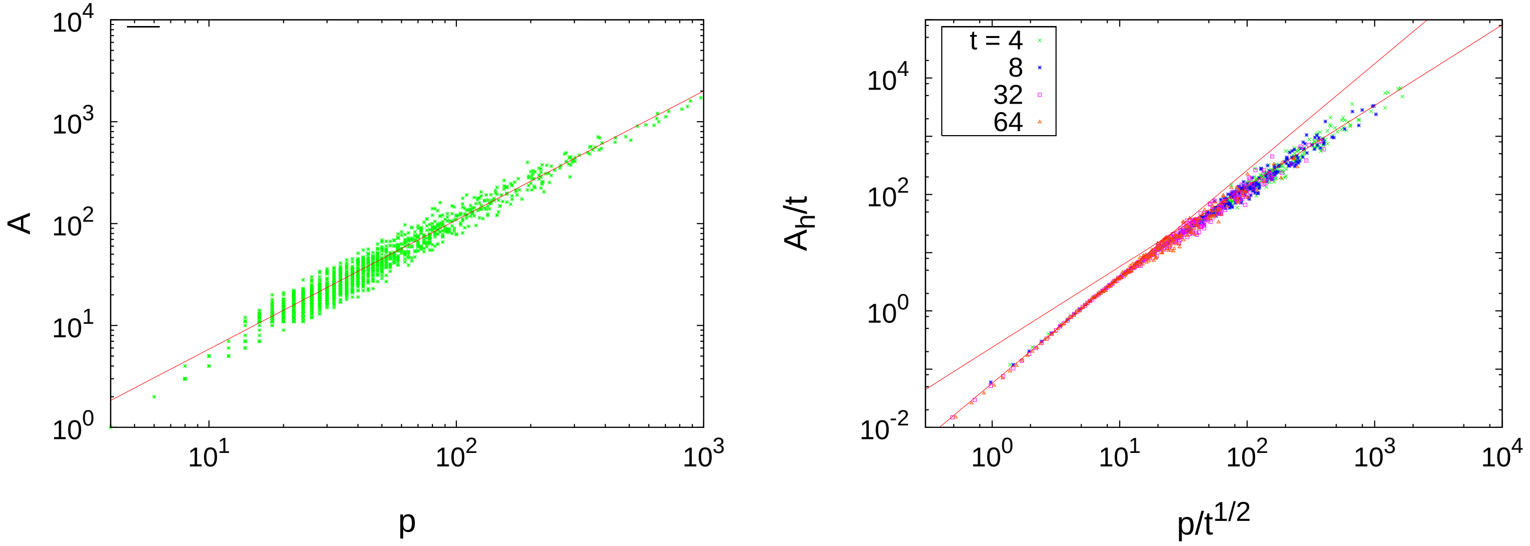
Finite size effects & data collection.

Arenzon, Dierking, Sicilia, Bray, LFC, Ros, 08

Non-conserved order parameter

Areas and perimeters

$T = 0$ dynamics after a quench from equilibrium at $T_0 = T_c$



$$\frac{A}{\lambda t} \propto \left(\frac{p}{\sqrt{\lambda t}}\right)^{\alpha}$$

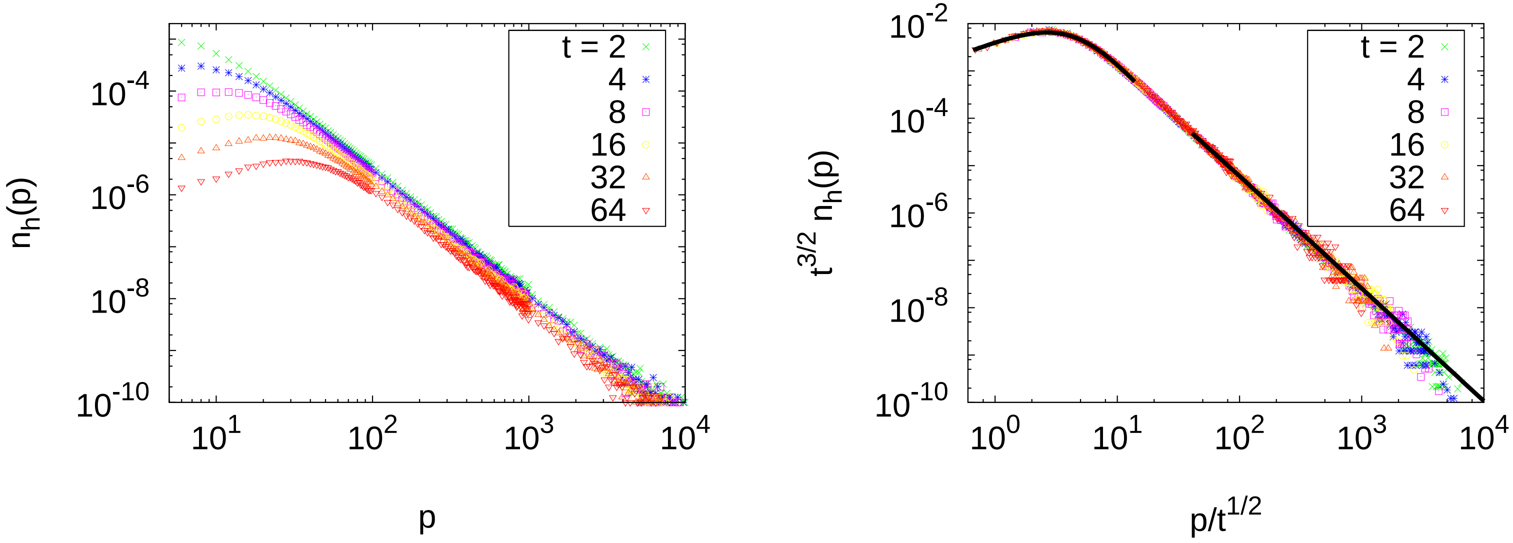
Large structures keep the initial condition geometry, $\alpha \sim 1.5$.

Small structures get regular $\alpha \sim 1.8$.

Non-conserved order parameter

Perimeter distributions

$T = 0$ dynamics after a quench from equilibrium at $T_0 = T_c$



The lines are the analytic predictions for short and long perimeters.

Scaling, $(\lambda t)^{3/2} n_h(p,t) = f(p/\sqrt{\lambda t})$, found.

Conserved order parameter

Mechanisms and growing length

- Surface diffusion : walk on interface from higher to lower curvature regions.

- Bulk diffusion : activated detachment, diffusion through matrix of opposite phase, attachment to the surface of the same or another domain.

- Small areas ($A \ll \mathcal{R}^2(t,T) \sim t^{2/3}$) diluted in opposite phase evaporate as $A^{3/2}(t) = A_0^{3/2} - C(t-t_0)$.

- Large areas ($A \gg \mathcal{R}^2(t,T) \sim t^{2/3}$) capture matter and grow also as $A^{3/2}(t) = A_0^{3/2} + C(t-t_0)$.

Lifshitz-Slyozov, 61 ; Wagner, 61 ; Huse, 86

Conserved order parameter

The predictions

- The large structures keep the statistics of the initial condition.
- The small structures can be considered independently from one another.

  Then, $A^{3/2}(t) = A_0^{3/2} - C(t-t_0)$ applies.

  From $n(A,t) \approx \int dA_0 \, \delta(A - A(t,A_0)) \, n(A_0,t_0)$ one finds

$$(\lambda t)^{2\tau/3} \, n_{d,h}(A,t) \approx \frac{(2) c_{d,h} \, a^{2(\tau-2)} \left[\frac{A}{(\lambda t)^{2/3}}\right]^{1/2}}{\left\{1 + \left[\frac{A}{(\lambda t)^{2/3}}\right]^{3/2}\right\}^{(2\tau+1)/3}}$$

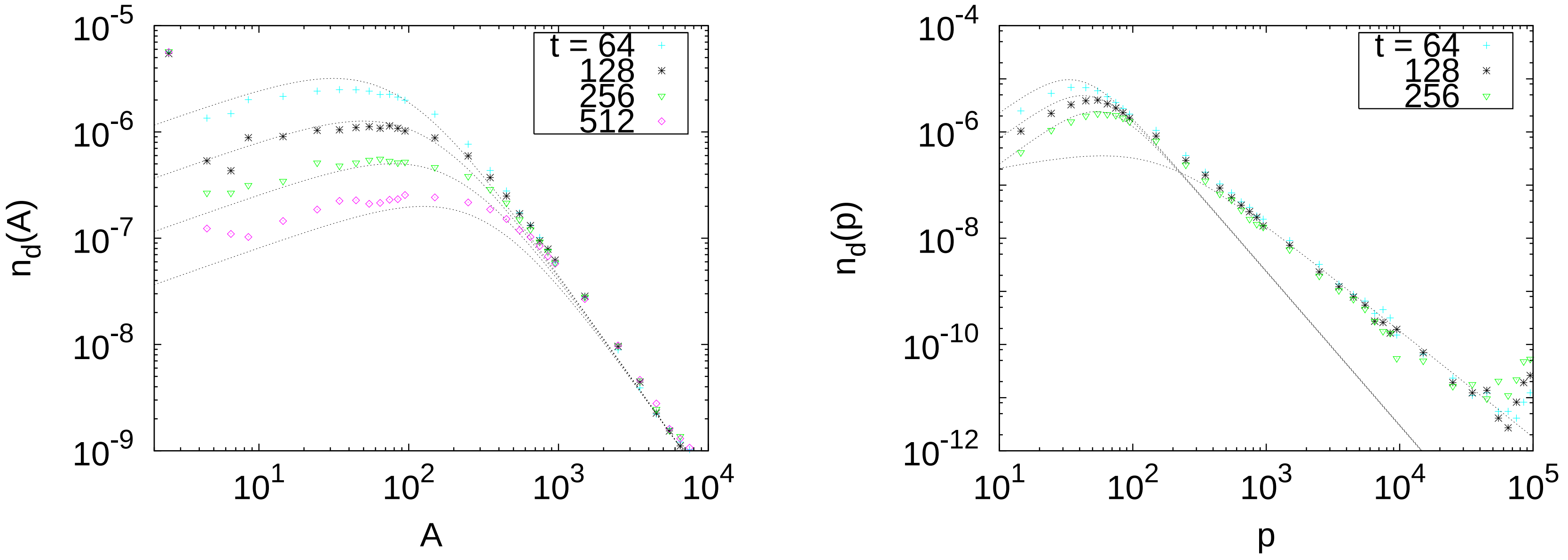
with $\tau = 2$ for hull-enclosed areas and $\tau \approx 2$ for domains

Sarrazin, Sicilia, Arenzon, Bray, LFC, 08

Conserved order parameter

Numerical tests

Domain area and perimeter density



Sarrazin, Sicilia, Arenzon, Bray, LFC, 08

Summary

Non-conserved order parameter

- **Exact** results for hull-enclosed area pdfs. **We proved scaling !**
- Approximate results for domain area pdfs. Consistent with scaling.
- Approximate results for hull and domain perimeter pdfs. Also consistent with scaling.
- The typical length-scale is not so typical after all :

  no maximum and power-law tails in $n_{h,d}(A, t)$;

  there is a maximum in $n_{h,d}(p, t)$ but still power-law tails.
- Large structures keep the statistics of the initial condition.
- Small structures become round and ‘feel’ the microscopic dynamics.

Summary

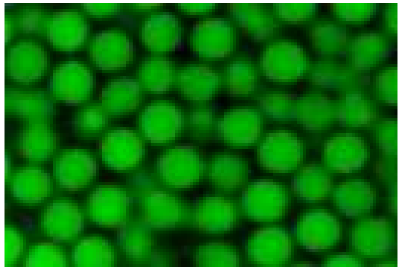
Conserved order parameter

- The pdf of domain areas satifies scaling ;

  small areas : it matches the Lifshitz-Slyozov-Wagner dilute-limit result.

  large areas : it is given by the initial condition distribution.

- **Relate these results to dynamic fluctuations in glasses**.



e.g. Chamon, LFC, Fabricius, Iguain, Weeks, 08

- Other coarsening problems ? Hydrodynamic interactions in fluids, coupled chaotic maps, *etc.*

Simulations

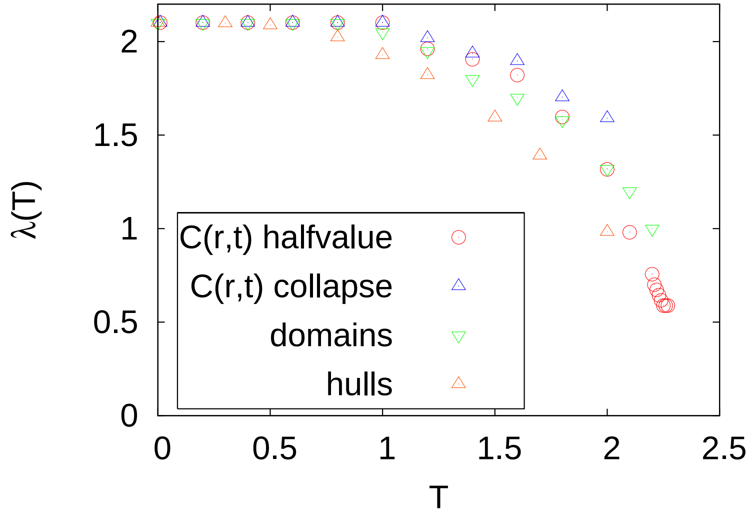
- $2d$ Ising model on a square lattice with periodic boundary conditions.
- Monte Carlo (MC) dynamics with heat-bath updates.
- $L = 10^3$, 2×10^3 samples, one time step corresponds to a MC sweep.
- Critical initial conditions generated with the Swendsen-Wang cluster algorithm to avoid critical slowing down.
- Hoshen-Kopelman algorithm to identify the domains.
- Our algorithm to identify the hulls inspired by the one used in

R. M. Ziff, cond-mat/0510633, StatPhys22.

Non-conserved order parameter

The typical length-scale ⇔ a typical area

$$\mathcal{R}(T,t) \sim \sqrt{\lambda(T)\, t} \qquad \Leftrightarrow \qquad A(T,t) \sim \lambda(T)\, t$$

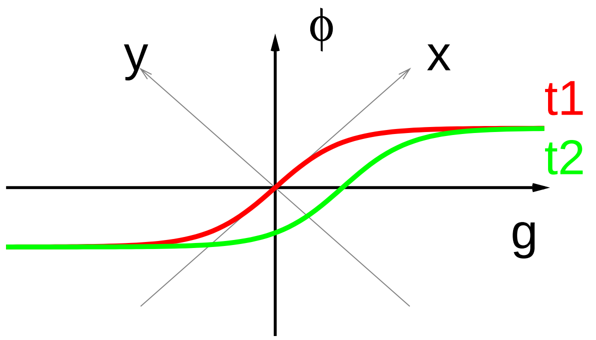


NB the exponent $\frac{1}{2}$ is independent of T and the details of the dynamics, lattice, *etc.* as long as the order parameter is non-conserved & there is no disorder.

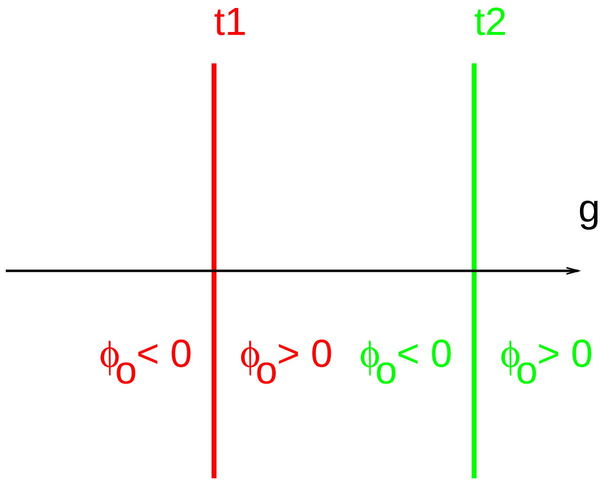
The T-dependence in $\lambda(T)$ is due to the roughening of the domain walls.

Non-conserved order parameter

The Allen-Cahn $T = 0$ equation



Domain wall profile



View from the top

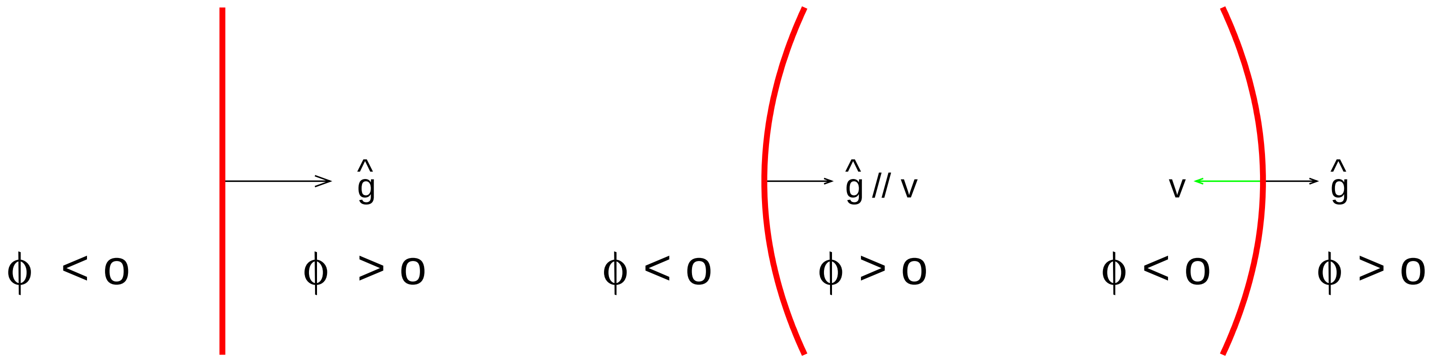
$$\frac{\partial\phi(\vec{x},t)}{\partial t} = -\left.\frac{\partial\phi(\vec{x},t)}{\partial g}\right|_t \left.\frac{\partial g}{\partial t}\right|_\phi , \qquad \vec{\nabla}\phi(\vec{x},t) = \left.\frac{\partial\phi(\vec{x},t)}{\partial g}\right|_t \hat{g} ,$$

$$\nabla^2\phi(\vec{x},t) = \left.\frac{\partial^2\phi(\vec{x},t)}{\partial g^2}\right|_t + \left.\frac{\partial\phi(\vec{x},t)}{\partial g}\right|_t \vec{\nabla}\cdot\hat{g}.$$

Using $\frac{\partial^2\phi(\vec{x},t)}{\partial g^2}|_t = V'(\phi)$ in the GL equation : $v \equiv \partial_t g|_\phi = -\vec{\nabla}\cdot\hat{g}$.

Velocity of a quasi-planar wall

Time-dependent Ginzburg-Landau



$$v = -\vec{\nabla} \cdot \hat{g} = -K$$

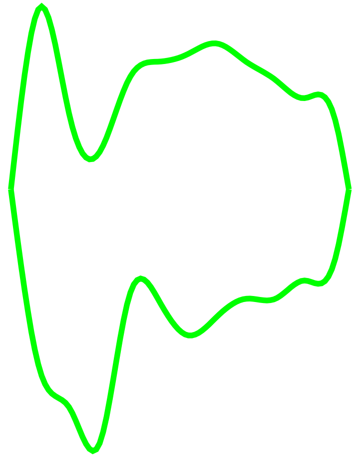
where $\hat{g}$ points in the direction $\phi > 0$ and

K is the mean curvature measured from the phase $\phi < 0$.

Allen & Cahn, 79.

Non-conserved order parameter

A generic hull in $d = 2$



with radius R, area A and perimeter L.

The time-variation of the *hull area*, $\frac{dA}{dt} = \oint \vec{v} \wedge d\vec{\ell} = \oint v d\ell$, in the case $v = -\frac{\lambda}{2\pi}\kappa$, with κ the *geodesic curvature*, is *also* constant

$$\frac{dA}{dt} = -\lambda$$

due to the Gauss-Bonnet theorem $\int_A K dA + \int_{\partial A} \kappa d\ell = 2\pi\chi(A)$ that simply becomes $\oint \kappa d\ell = 2\pi$ for a planar $2d$ manifold with no holes.

Non-conserved order parameter

A spherical hull in $d = 3$

Take a sphere with radius R, volume $V = \frac{4}{3}\pi R^3$ and surface $A = 4\pi R^2$.

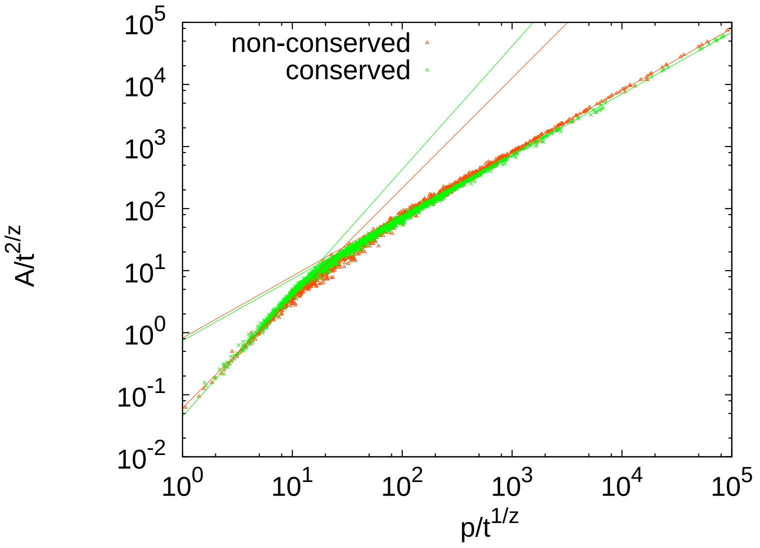
The time variation of the *hull*-enclosed volume, $\frac{dV}{dt} = 4\pi R^2 \, \frac{dR}{dt}$, in the case $v = -\frac{\lambda}{2\pi}\kappa$, with κ the *mean* curvature, *is not* constant :

$$\frac{dV}{dt} = -2R \propto -V^{1/3} \; .$$

Guess : $\frac{dV}{dt} \sim -V^{1/3}$ for generic geometries.

Conserved vs non-conserved

Areas vs. perimeters



The exponent for the small structures is slightly different

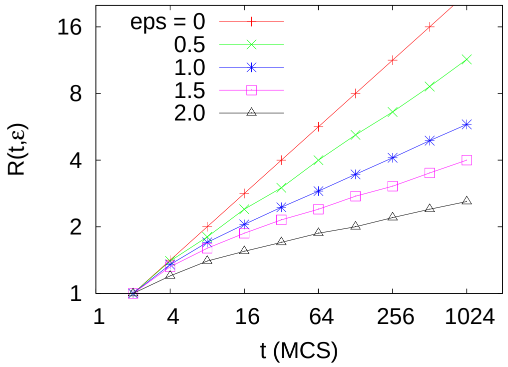
(The fit runs over the same interval)

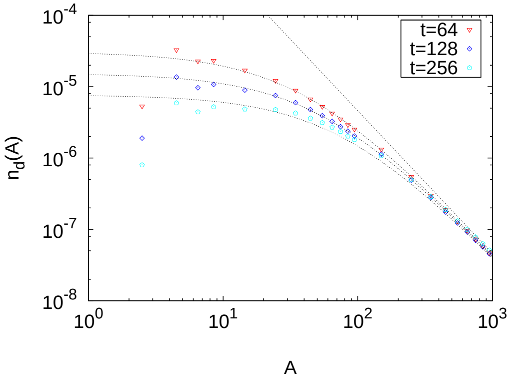
$\alpha_{non-cons} \approx 1.8$ $\alpha_{cons} \approx 2.$

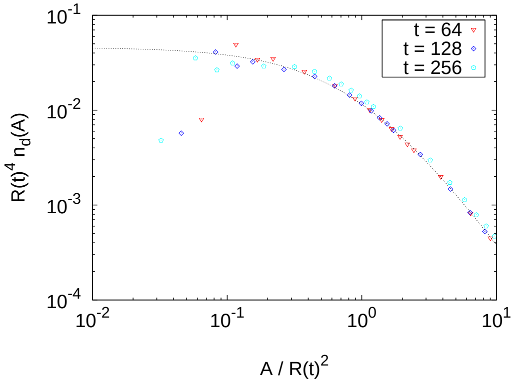
Random ferromagnet

$H = -\sum_{\langle ij \rangle} J_{ij} s_i s_j$, J_{ij} uniform distributed in $[2-\epsilon, 2+\epsilon]$

with $|\epsilon| \leq 2$ at $T = 0.4$.





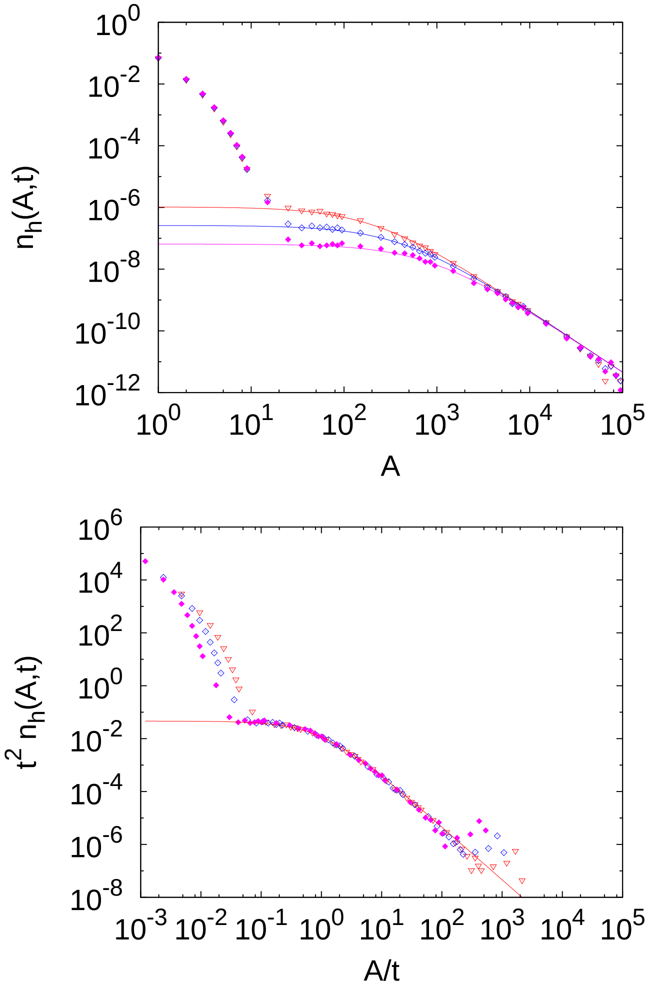


Super-universality applies, scaling with $\langle A \rangle \propto \mathcal{R}^2(t, T, \epsilon)$.

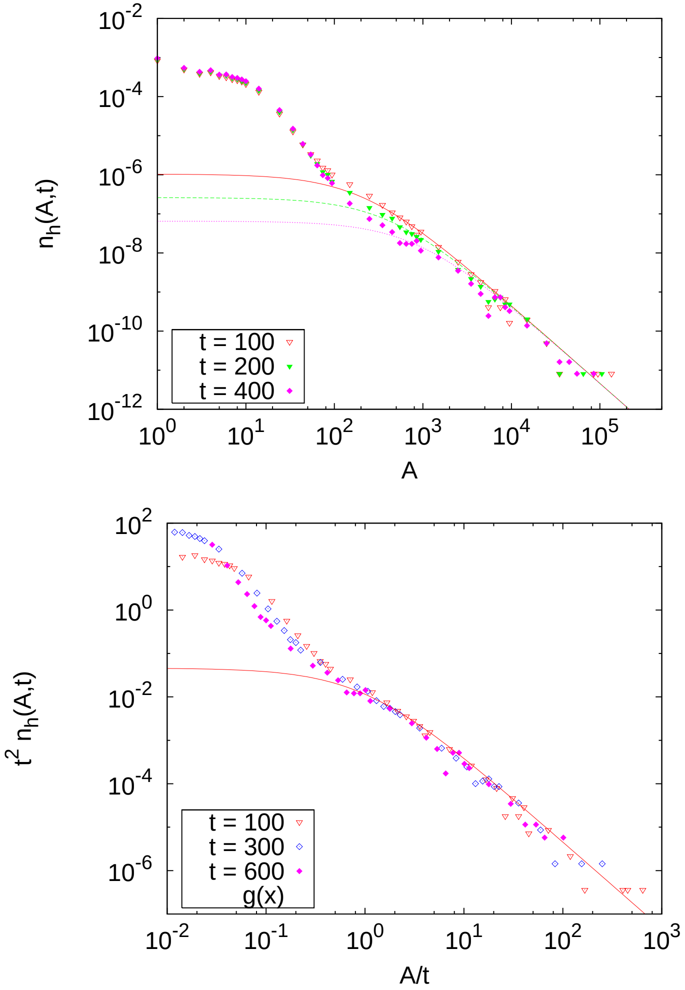
A. Sicilia, J. J. Arenzon, A. J. Bray, LFC, 07

Experiments

Growth of chiral domains in a slice of a liquid crystal



Simulations



Experiments