Spinodal Decomposition

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Contents

Spinodal decomposition

- Quench by instantaneous cooling
  - System enters unstable State
- Relaxation to equilibrium - Spinodal Decomposition

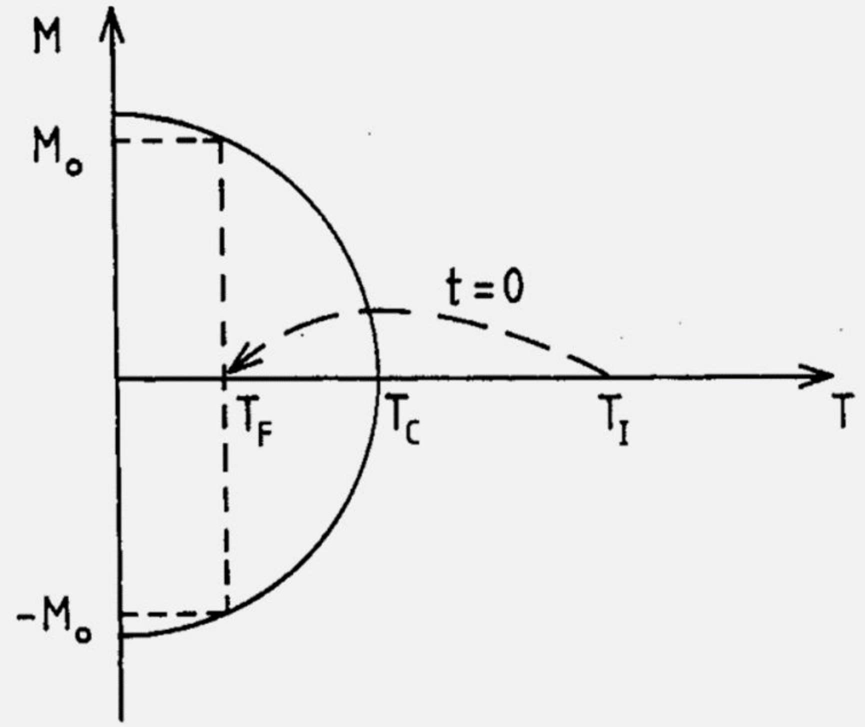


Figure 1: Graph of Magnetisation vs Temperature we, cool the system below the critical temperature,into an unstable state and wait for it to relax to equilibrium magnetisation

"Theory of Phase Ordering Kinetics", A. J. Bray, Advances in Physics, 51, 481 (2002).

Spinodal decomposition in Physics

- Ising model
- Granular media
- Conserved order - separation of polymer species in mixture
- Spinodal Architected Materials

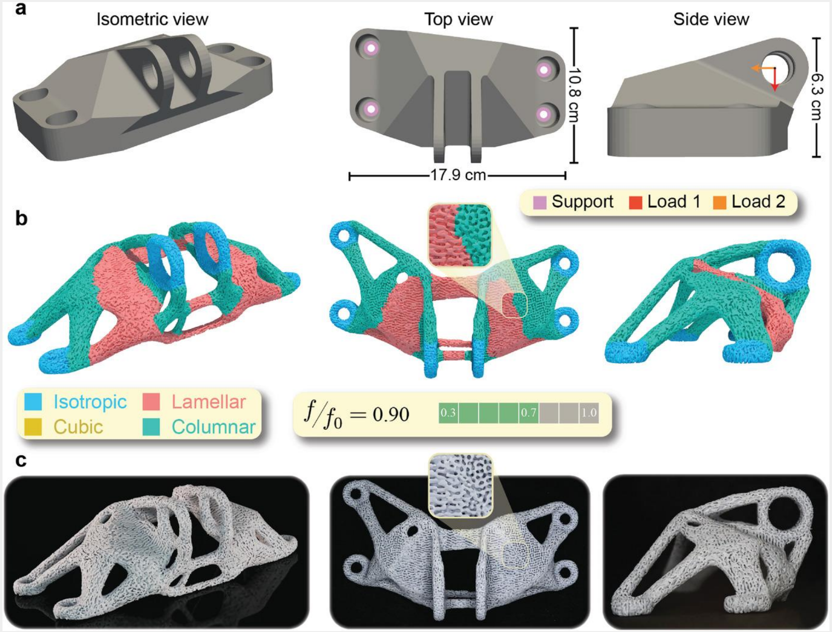


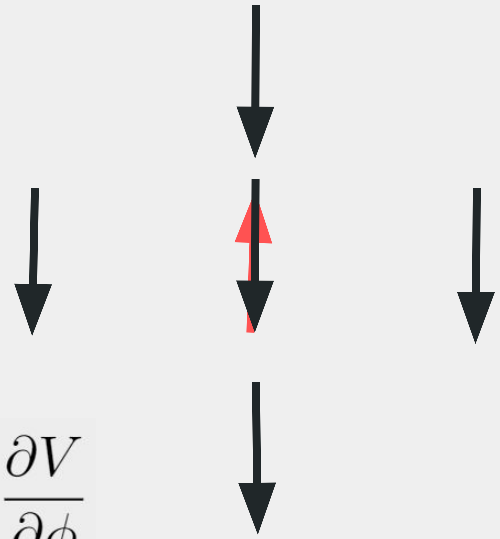
Figure 2:A jet engine bracket produced using spinodal designed materials

Senhora, F. V., Sanders, E. D., Paulino, G. H., Optimally-Tailored Spinodal Architected Materials for Multiscale Design and Manufacturing. *Adv. Mater.* 2022

2D Ising Model with Non-Conserved Order

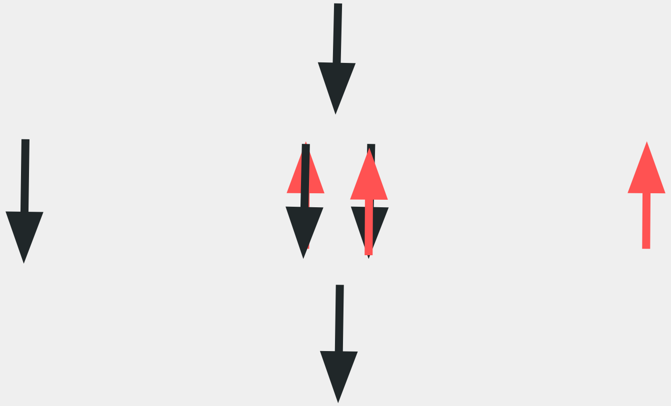
$$H = -\sum_{\langle i,j \rangle} J \sigma_i \sigma_j$$

Model A



$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi - \frac{\partial V}{\partial \phi}$$

Model B



$$\frac{\partial \phi}{\partial t} = -\nabla^2 \left(\nabla^2 \phi - \frac{\partial V}{\partial \phi} \right)$$

Monte Carlo

- Generate random (high T) $N \times N$ lattice of spins and set up parameters (non-zero T quenching)
- 1 Monte Carlo Step (MCS):
  - Choose random spin
  - Calculate Energy change from flipping it by neighbour interactions
  - Compare r = $e^{-\frac{\Delta E}{T}}$ to random number R from 0 to 1:
    - If r > R - flip spin
    - Else - pass
  - Works by decrease in energy giving r>1 so always r>R, otherwise probabilistic
  - Repeat for N^2 attempts.
- Satisfies Metropolis:

$$p = \begin{cases} 1, & \Delta E < 0 \\ e^{-\frac{\Delta E}{T}}, & \Delta E > 0 \end{cases}$$

J. M. Yeomans, Statistical mechanics of phase transitions., Oxford science publications (Clarendon Press, Oxford, England, 1992)

Ginzburg-Landau Theory

- Non-conserved order parameter φ describes net magnetisation of a region
  - Coarse-graining of a system
  - Continuous variable
- Free energy form:

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

- Time evolution of φ minimises F

$$\frac{\partial \phi}{\partial t} = -\frac{\delta F}{\delta \phi}$$

- With T=0 quenching potential, Ginzburg-Landau equation (numerically solved)

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi + \phi(1 - \phi^2)$$

“Theory of Phase Ordering Kinetics”, A. J. Bray, Advances in Physics, 51, 481 (2002).

Dynamic Scaling Exponent z

- Allen-Cahn equation gives $$v \propto \frac{1}{L}$$
- Single length scale implies $$v = \frac{dL}{dt} \propto \frac{1}{L}$$
- Scaling regime $\xi \equiv L$ so we find $L \propto t^{\frac{1}{2}}$
- Fractal self-similarity

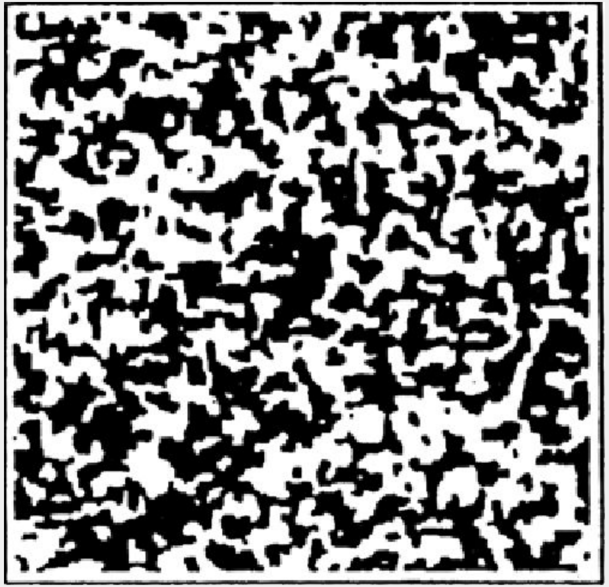
"Theory of Phase Ordering Kinetics", A. J. Bray, Advances in Physics, 51, 481 (2002).
"Universality and scaling for the structure factor in dynamic order-disorder transitions", G. Brown, P.A. Rikvold, M. Grant. Phys. Rev. E 58, 5501 (1998)..

Structure Factor

- The structure factor S(k,t) characterises the size of ordered domains

$$S_{\mathrm{TDGL}}(\boldsymbol{k},t) = |\mathscr{F}(\phi(\boldsymbol{x},t))|^2$$
$$S_{\mathrm{MC}}(\boldsymbol{k},t) = |\mathscr{F}(s(\boldsymbol{x},t))|^2$$

Early times



Late times

Images: “Theory of Phase Ordering Kinetics”, A. J. Bray, Advances in Physics, 51, 481 (2002).

Structure Factor and Scaling form giving Dynamical Scaling

The scaling hypothesis suggests

$$S(k,t) = a(t)f(kt^{\alpha})$$

As S(k,t) is normalised for all values of t

$$\int_0^\infty S(k,t)kdk = \int_0^\infty a(t)f(kt^{\alpha})kdk = 1$$

We make the substitutions

$$y = kt^{\alpha},\, dk = t^{-\alpha}dy$$

Limits independent of t, so

$$t^{-2\alpha}a(t)\int_0^\infty yf(y)dy = 1$$

For the scaling form to be normalizable for all t a(t) must be an power law

$$S(k,t) = t^{2\alpha}f(kt^{\alpha})$$

K. Hassan, M. Hassan, and N. Pavel, Dynamic scaling, data-collapse and self-similarity in barab ́ asi-albert net-works,(2011)

Consequences of dynamic scaling

From our expression for
S-weighted average of k

$$\langle|\boldsymbol{k}(t)|\rangle = \frac{\sum S(|\boldsymbol{k}|,t)|\boldsymbol{k}|^2 \mathrm{d}k}{\sum S(|\boldsymbol{k}|,t)|\boldsymbol{k}|\mathrm{d}k}$$

$$\langle|\boldsymbol{k}(t)|\rangle = \frac{2\pi}{L(t)}$$

Substituting

$$S(k,t) = t^{2\alpha} f(kt^{\alpha})$$

The function of y can be ignored as
that will just end up as some constant

$$\frac{2\pi}{L(t)} = t^{-\alpha} \frac{\int_0^\infty f(y) y^2 dy}{\int_0^\infty f(y) y dy}$$

And using the same substitutions for y we
end up with our scaling relationship between
the domain length and time

$$L(t) \sim t^{\alpha},\ \alpha \equiv \frac{1}{z}$$

K. Hassan, M. Hassan, and N. Pavel, Dynamic scaling, data-collapse and self-similarity in barab ́ asi-albert net-works, CoRR abs/1101.4730 (2011)

Excess Energy in Domain Walls

$$\Delta E = 2J - \frac{J}{N^2} \sum_{\langle i,j \rangle} s_i(t) s_j(t)$$

- Extra energy in domain walls
- Ground state energy when all aligned - within one domain
- Decreases to 0 over time, but can get stuck and never equilibrate
- Scales as $\Delta E \propto L^{-1} \propto t^{-\frac{1}{2}}$ for Model A systems

K. Humayun and A. J. Bray, - “Non-equilibrium dynamics of the ising model for t \leq tc, Journal of Physics A: Mathematical and General 24, 1915 (1991).

Method

- MC with J=1 and $T = 0.1T_c$
- Optimisation and periodicity
- TDGL T = 0 quench
- Annuli averaging
- Initial conditions
- Finite size effect

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi + \phi(1 - \phi^2)$$

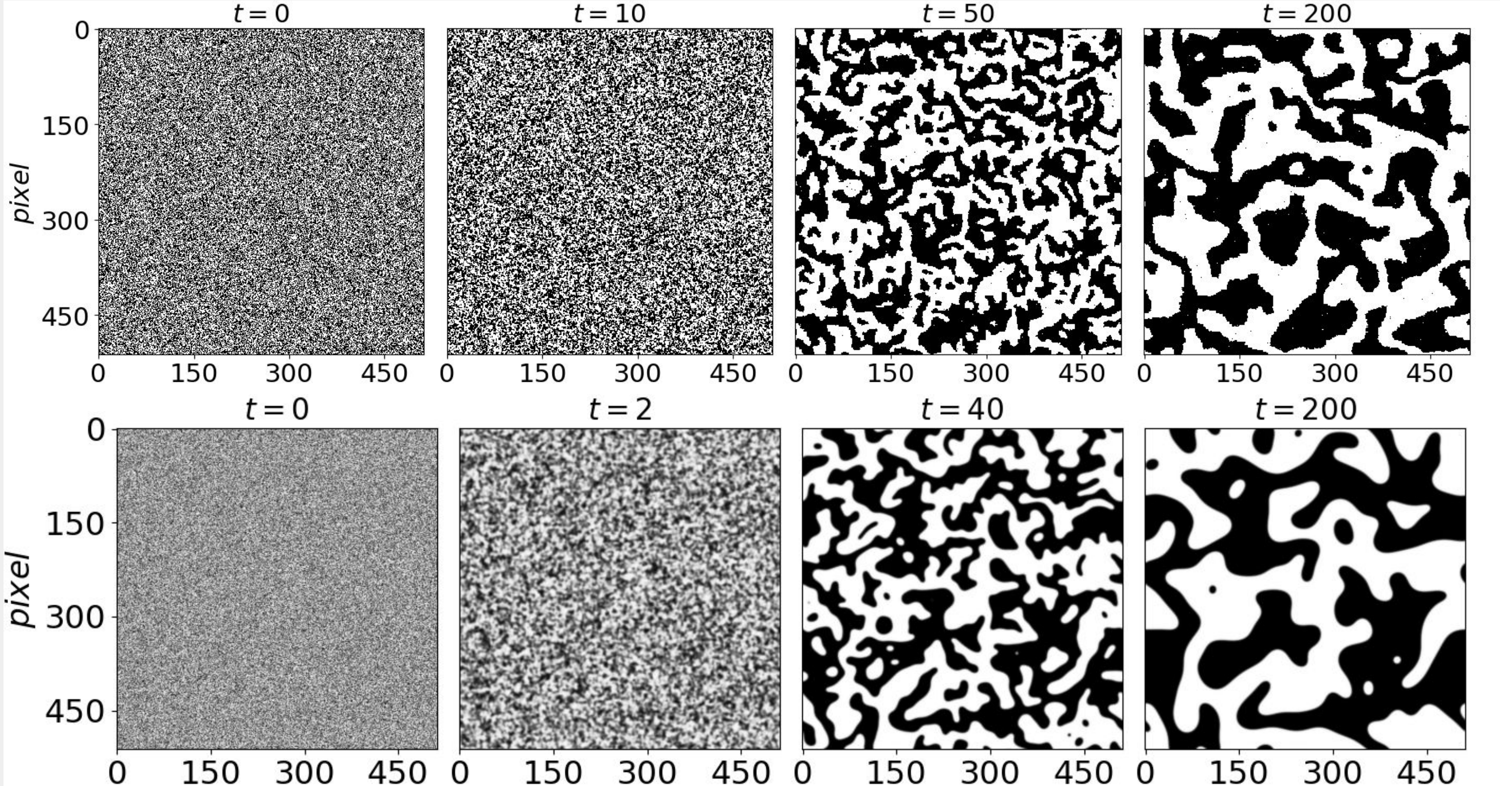
$$\langle |\boldsymbol{k}(t)| \rangle = \frac{\sum S(|\boldsymbol{k}|, t) |\boldsymbol{k}|^2 \mathrm{d}k}{\sum S(|\boldsymbol{k}|, t) |\boldsymbol{k}| \mathrm{d}k}$$

$$\langle |\boldsymbol{k}(t)| \rangle = \frac{2\pi}{L(t)}$$

Results - Simulations

MC

TDGL



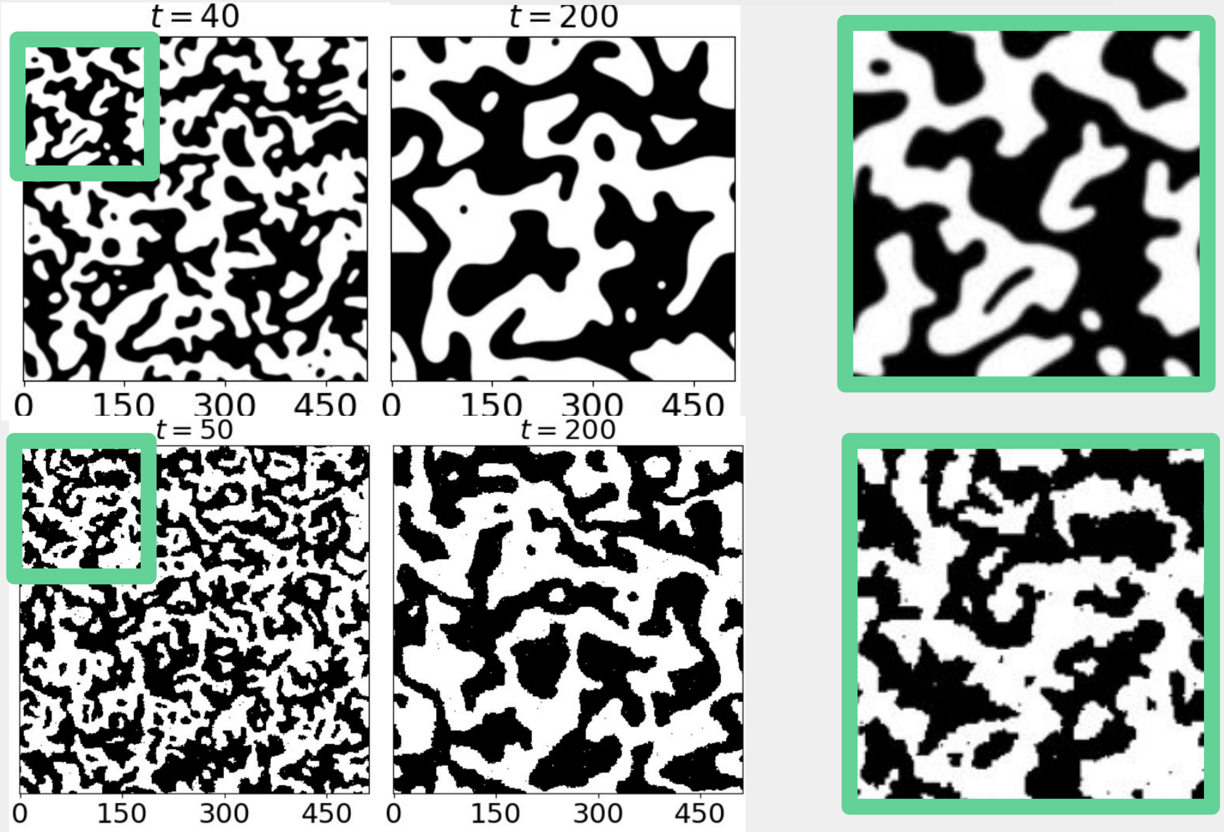
512x512

Self Similarity

$$S(k,t) = a(t)f(kt^{\alpha})$$

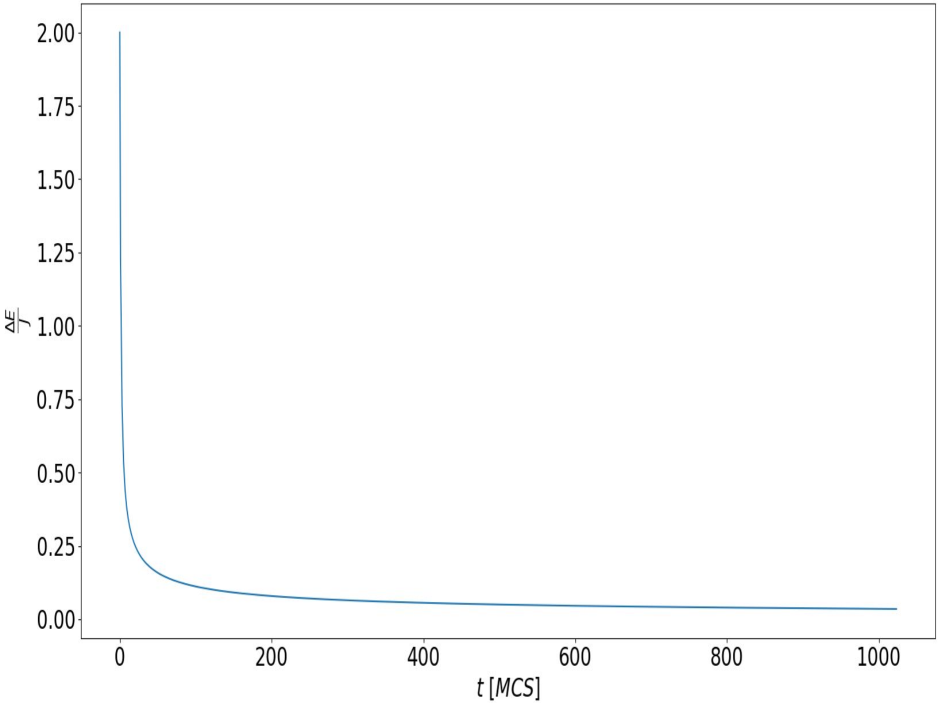
MC

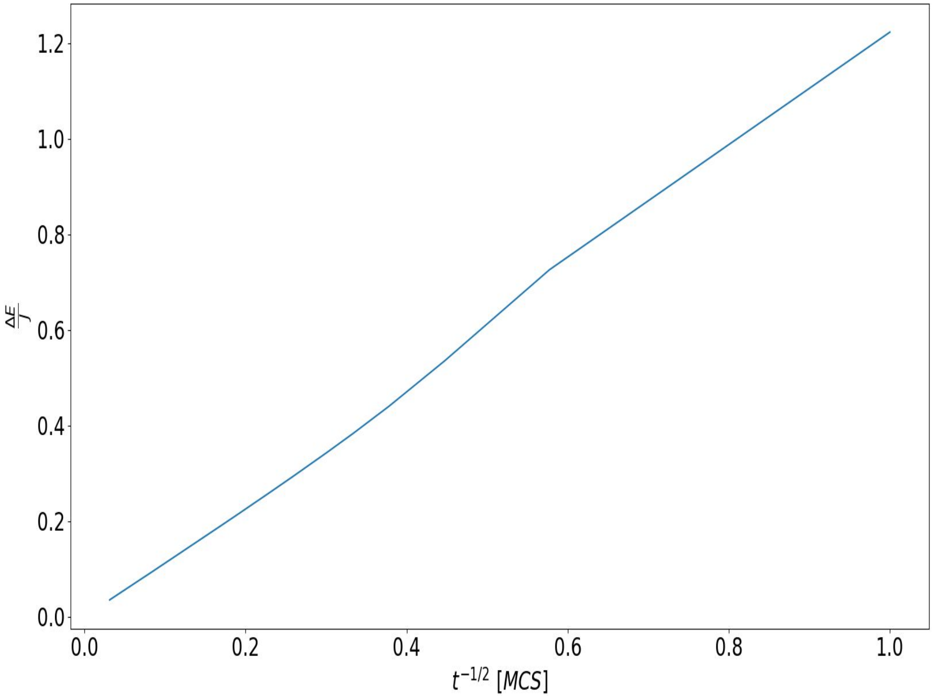
TDGL



Results - Excess Energy

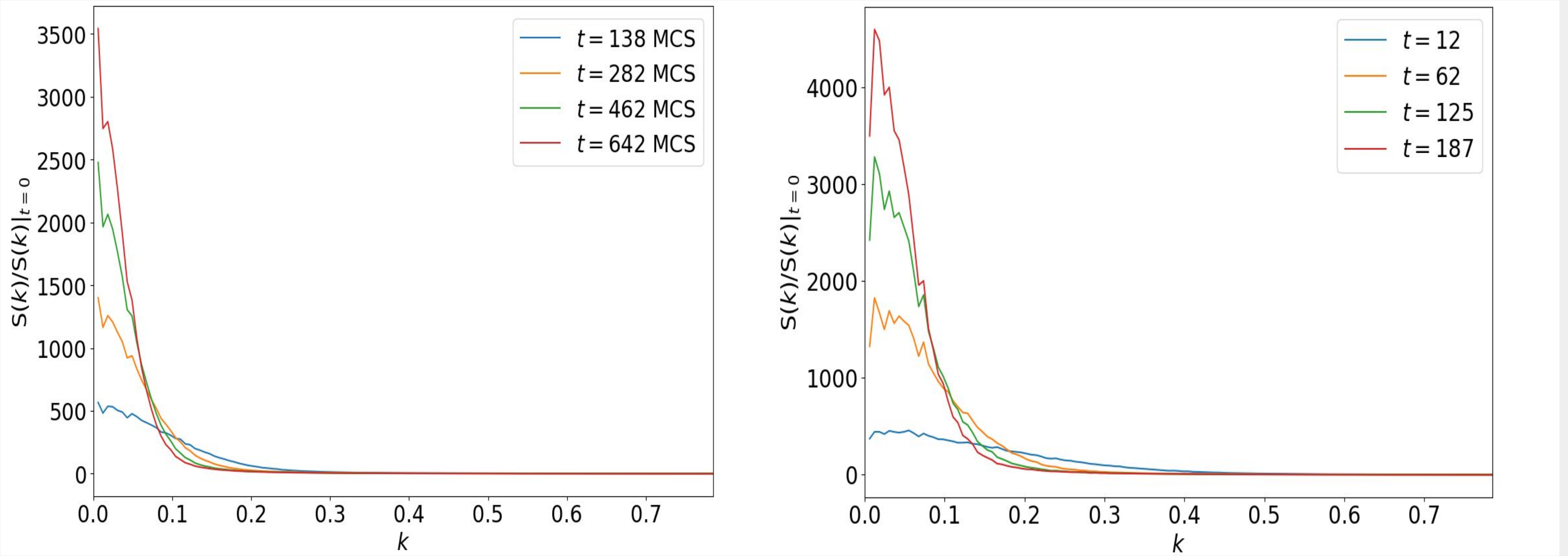
$$\Delta E = 2J - \frac{J}{N^2} \sum_{\langle i,j \rangle} s_i(t) s_j(t)$$





Results - Unscaled Structure Factors

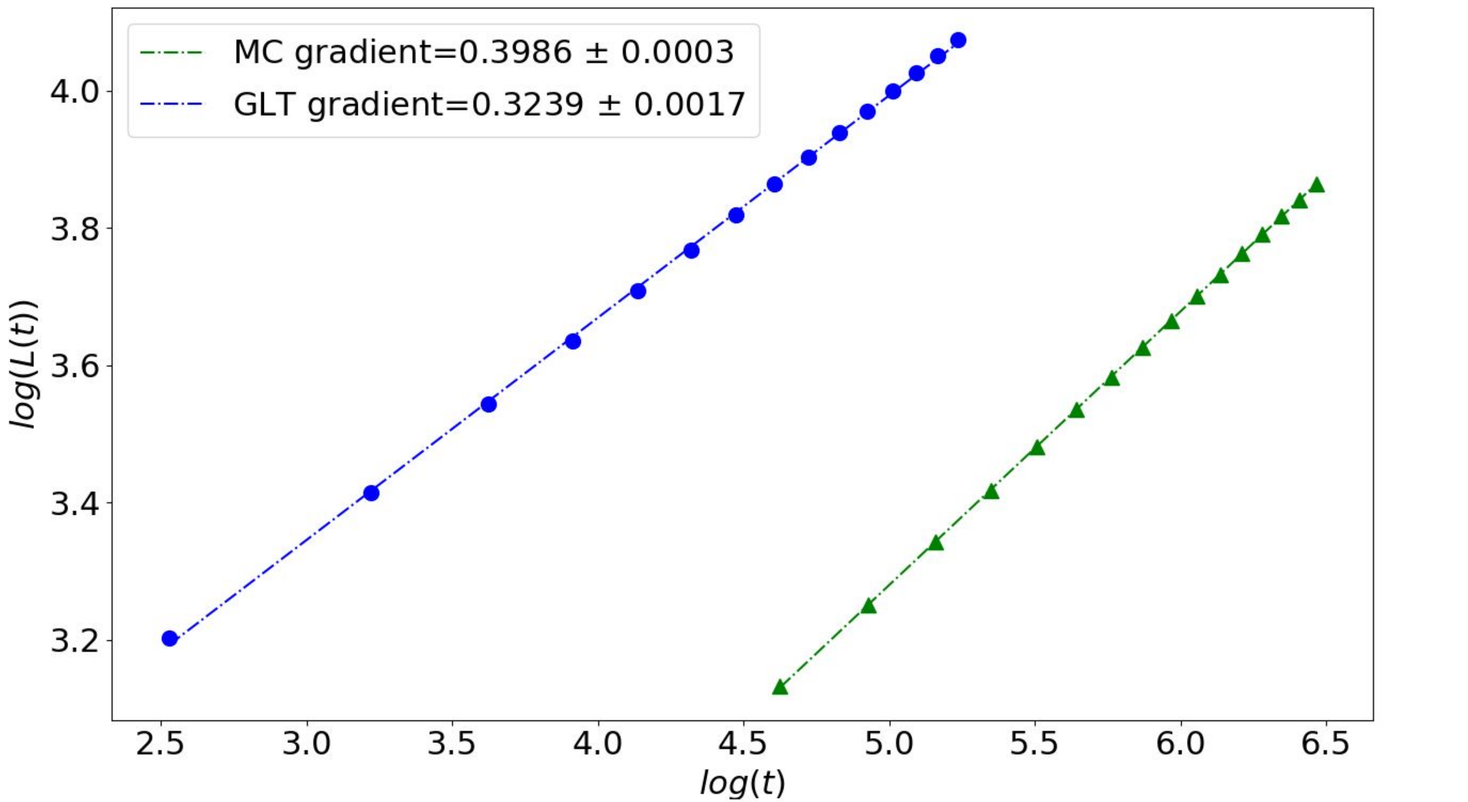
- Over time, fewer small-scale regions



Results - Domain Size Scaling

TDGL - 10 repeats, 512x512

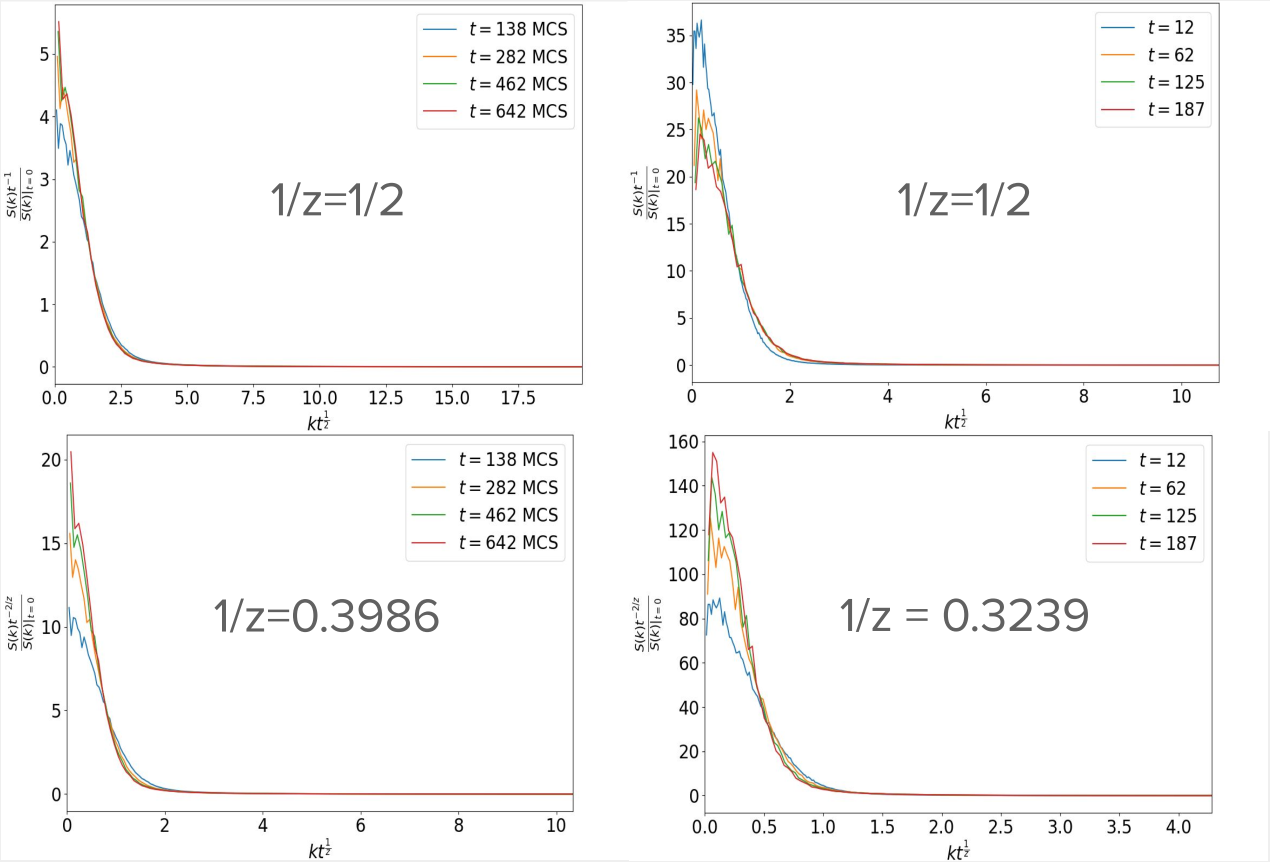
MC - 60 repeats, 1024x1024



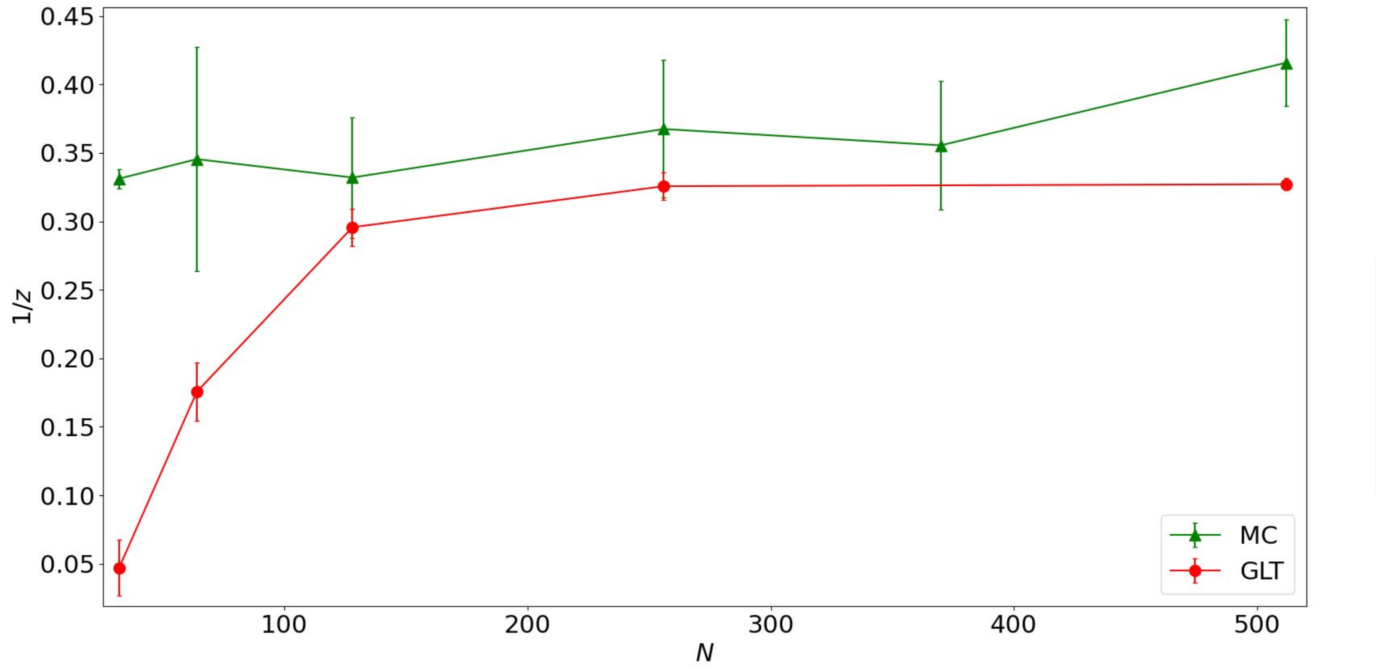
Results - Scaled Structure factors

MC

TDGL



Convergence and representative errors



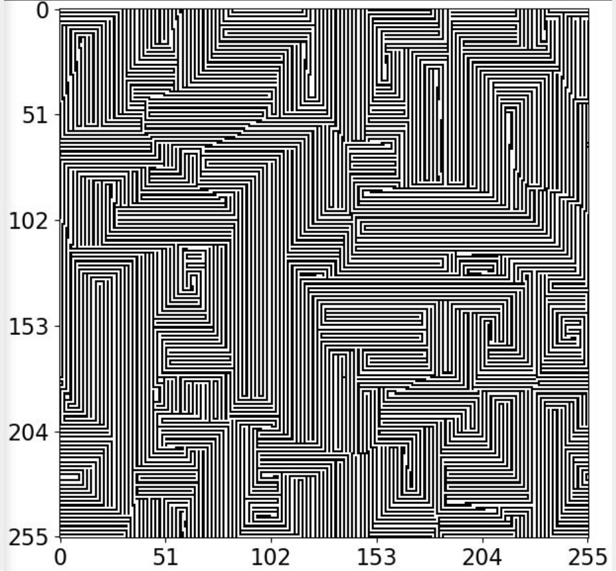
final results

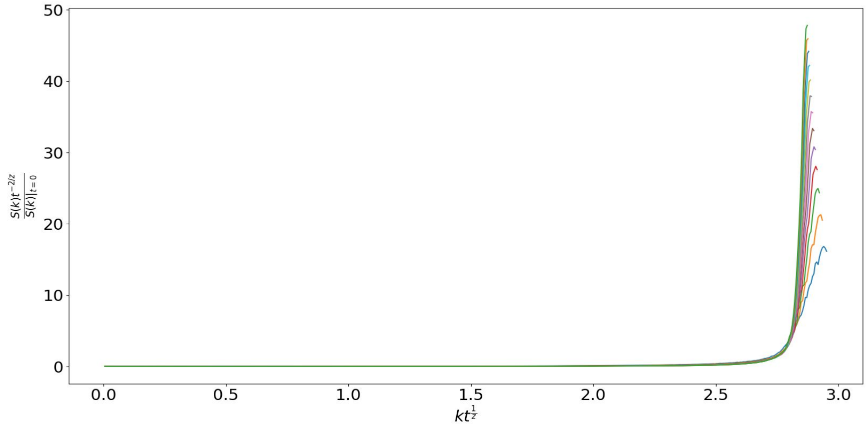
$$\frac{1}{z_{\mathrm{MC}}} = 0.416 \pm 0.032$$

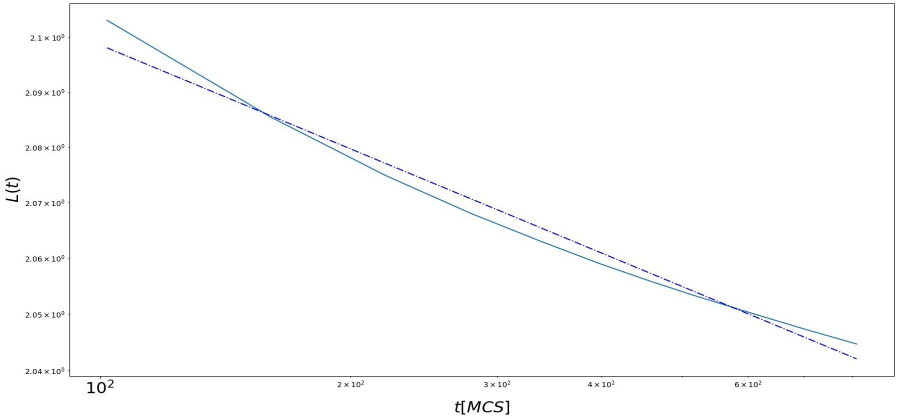
$$\frac{1}{z_{\mathrm{TDGL}}} = 0.327 \pm 0.004$$

Extensions - Frustrated Models

$$m = -0.013 \pm 0.001$$

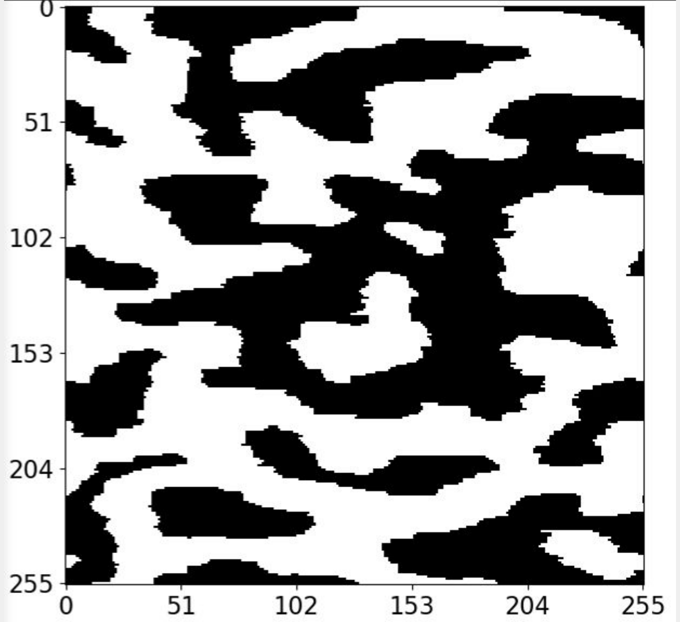


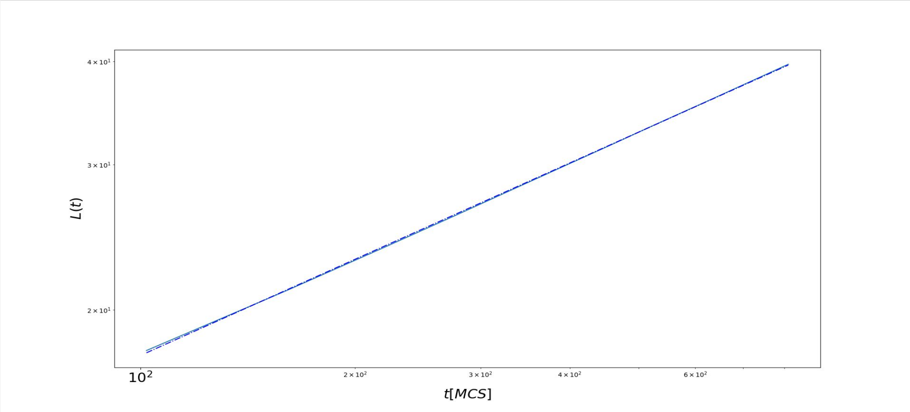


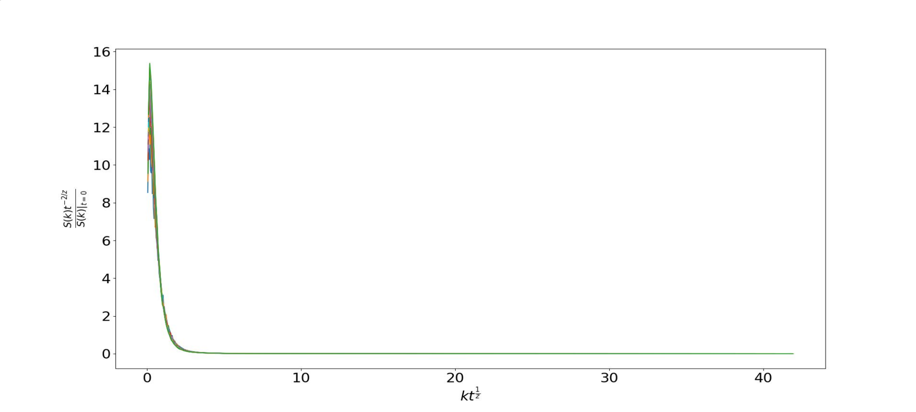


Extension - Anisotropic models

$$m = 0.387 \pm 0.001$$







Outlook

- More repeats over initial conditions
- Excess Energy in TDGL
- Include noise in TDGL quenching to match Monte Carlo
- Continue with mentioned extensions

K. Humayun and A. J. Bray, - “Non-equilibrium dynamics of the ising model for t \leq tc, Journal of Physics A: Mathematical and General 24, 1915 (1991).

Thanks for listening! - Take Home:

1. Spinodal Decomposition - Phase Separation
2. Domain wall motion minimises excess energy
    a. Gets stuck and never reaches equilibrium
3. Growth of domains scales as $L \propto t^{\frac{1}{2}}$
    a. Arises from Scaling Form of Structure Factor
    b. Or by Allen-Cahn equation of propagation from curvature
4. Anisotropic Models
5. Frustrated Models
6. Topics still relevant to current research

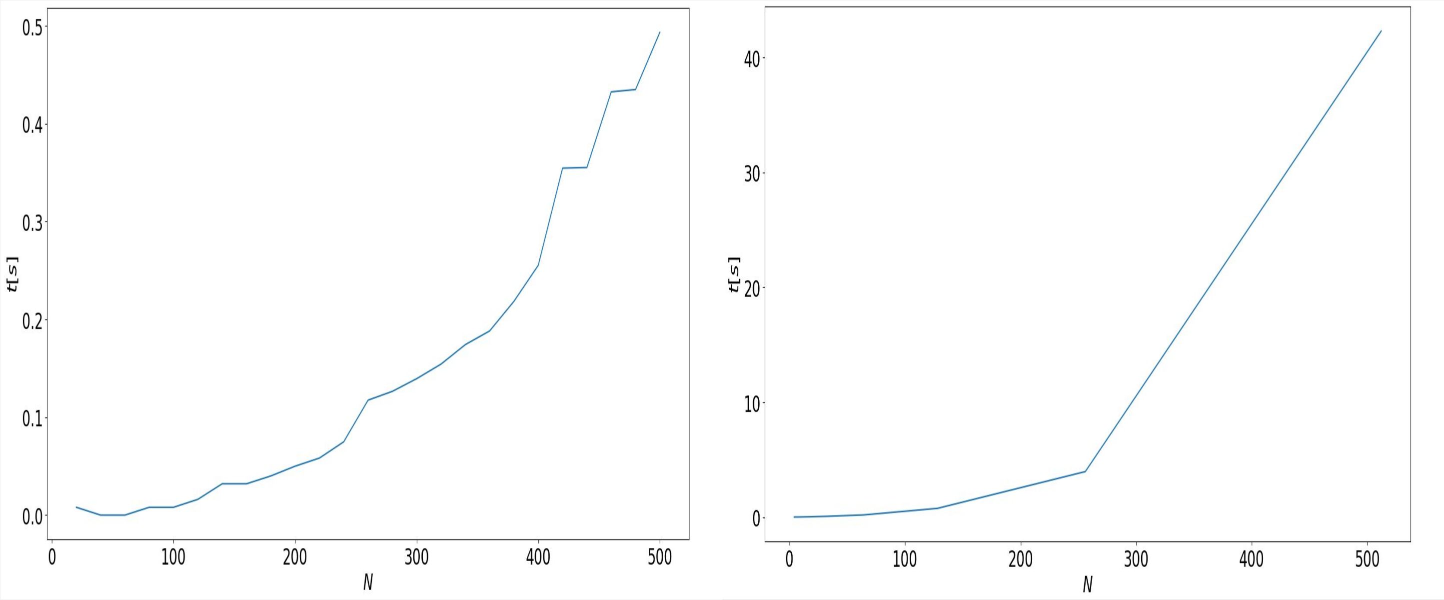
Any Questions?

POSSIBLE QUESTION SLIDES FOLLOW

Excess energy in TDGL

$$\Delta E = 1 - \frac{1}{N^2} \int |\nabla^2 \phi| d\boldsymbol{x}$$

Code time scaling - MC



Code Time Scaling - TDGL