UCSD

2D Spinodal Decomposition in Forced Turbulence:

Structure Formation in a Challenging Analogue of 2D MHD Turbulence

1

Xiang Fan[1], P H Diamond[1], Luis Chacon[2], Hui Li[2]

[1] University of California, San Diego

[2] Los Alamos National Laboratory

This material is based upon work supported by the U.S. Department of Energy Office of Science under Award Number DE-FG02-04ER54738.

Overview

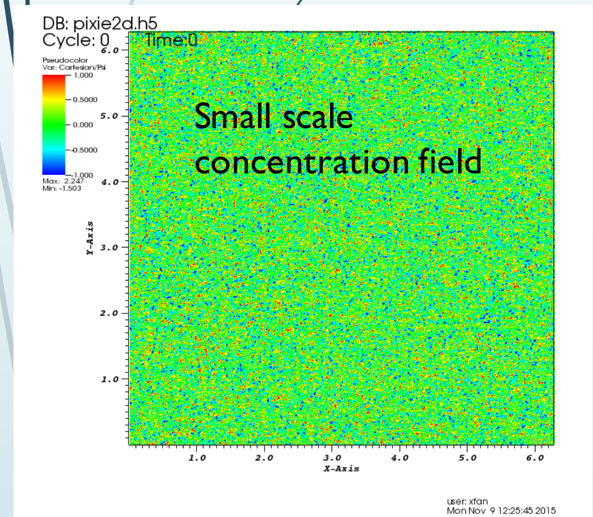
- Spinodal decomposition (SD) is an analogue to 2D MHD in terms of dynamics and turbulence, with many similarities and some differences.
- We study and compare the *turbulence spectra*, *turbulent transport* and *memory* of the two systems.
- Both are multi-scale problems, with bi-directional cascades. Memory is critical to nonlinear transfer and transport in both.
- The mean square concentration in 2D SD has an inverse cascade, which is an analogue to the mean square magnetic potential inverse cascade in 2D MHD. The fluid blob coalescence process in spinodal decomposition is similar to magnetic flux blob coagulation in 2D MHD.
- The characteristic length scale of blobs grows if unforced. If external forcing at large scale is present, the turbulence can break up large blobs into small ones. This can arrest the growth of the blob length scale, and meso-scale structure can be formed.

Outline

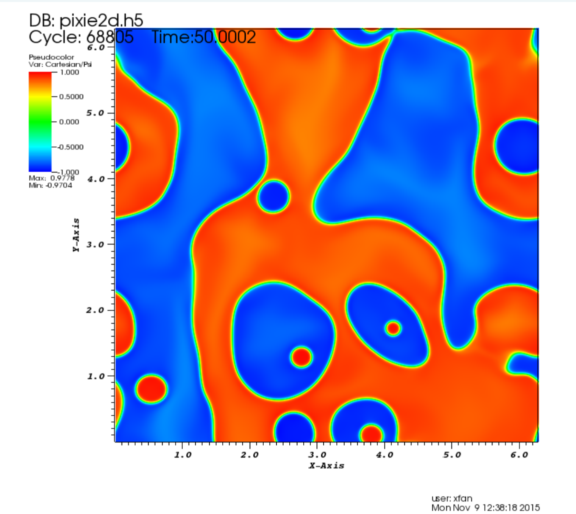
- Introduction
  - What is Spinodal Decomposition (SD)?
  - Why should a plasma physicist care? 2D SD is a challenging analogue to 2D MHD
- Basic Theory and comparison to 2D MHD
  - Basic Equations for Spinodal Decomposition
  - Ideal Conserved Quantities
  - Waves in SD and MHD
  - Length Scales of Spinodal Decomposition Turbulence
  - Turbulent Transport
- Simulation Results and comparison to 2D MHD
  - Simulation Setup
  - H_ψ/H_A spectrum
  - Length Scale Growth
  - PDF of ψ/A
- Conclusion
- Future work

Introduction

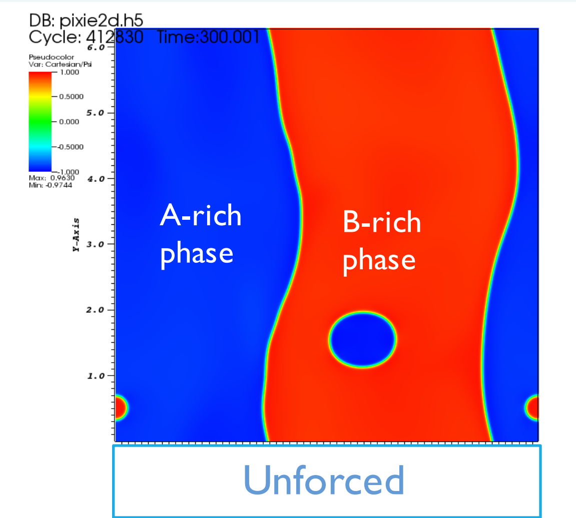
- **Spinodal decomposition (SD)** is a second order phase transition for a binary fluid mixture, to pass from one thermodynamic phase to two coexisting phases. For example, at high enough temperature, water and oil can form a single thermodynamic phase, and when it's cooled down, the separation of oil-rich and water-rich phases occurs.
- Below is a simulation demonstration for an unforced case (Run 1). The plots are time evolution of pseudo-color plots of concentration field.



In the beginning, the system is cooled down to just below the critical temperature, and keeps isothermal later on. Initially the concentration field is a random distribution of 1 or -1.

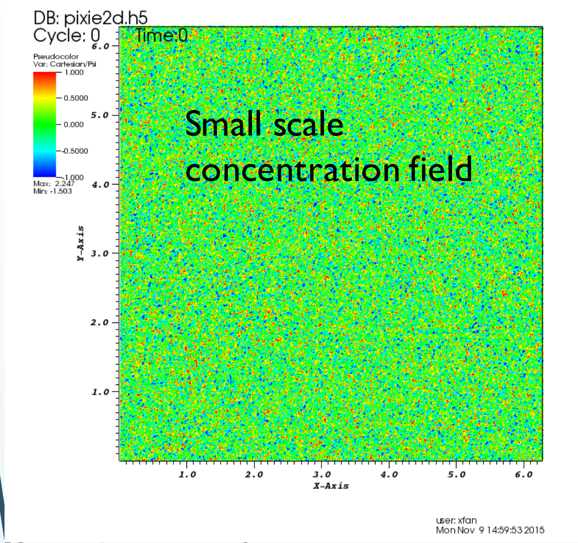


The blob coalescence process occurs.

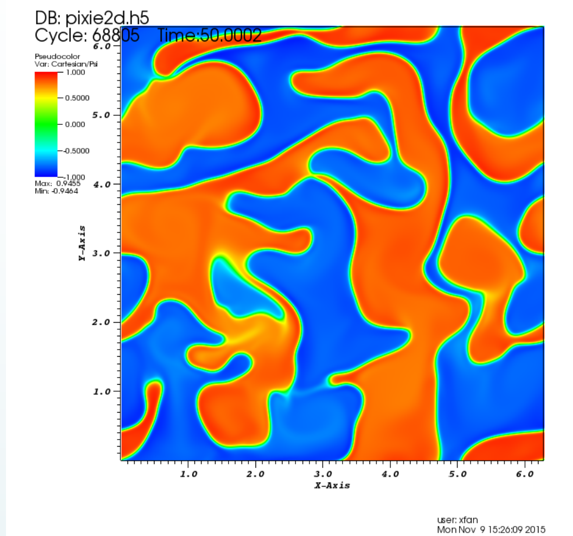


Finally the blob length scale reaches the system size. A-rich phase and B-rich phase are saperated completely.

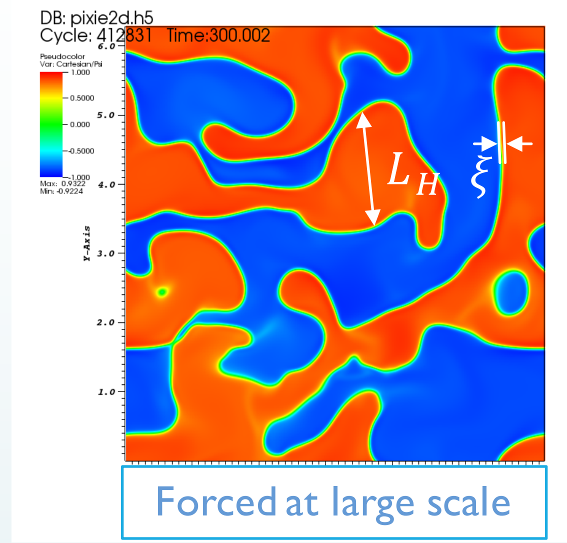
Introduction



The same small scale concentration field initial condition as the unforced case.



The blob coalescence process occurs.



Meso-scale structure is formed, and the saturated blob length scale is the Hinze Scale L_H.

- Above is a simulation demonstration for a case forced at large scale (Run 2).
- The most interesting point for plasma physicists is that the governing equations for 2D SD have many similarities to 2D MHD equations, though are more challenging.
- The study of 2D SD is a different way to understand 2D MHD turbulence, and offers additional challenges.

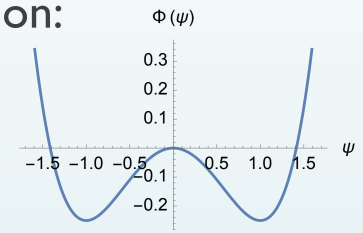
Introduction

- Physicists are interested in Spinodal Decomposition for more than 50 years.
- [Ruiz 1981] first pointed out the similarities between Spinodal Decomposition and 2D MHD.
- [Furukawa 2000] found that for unforced low viscous 2D Spinodal Decomposition, the blob length scale grows as a power law: $L(t) \sim t^{2/3}$.
- [Berti 2005] discovered that the blob coalescence process in 2D Spinodal Decomposition can be arrested by sufficiently strong external forcing at large scale.
- [Perkelar 2014] did a Lattice-Boltzmann simulation on 3D Spinodal Decomposition. They verified that the saturated length scale is the Hinze scale. They studied the Energy spectrum in that case, and observed in the inertial range the energy content is suppressed compared to pure fluid turbulence spectrum.
- The usual application for spinodal decomposition is in alloy manufacture.

Basic Equations for SD

- Define the concentration field $\psi(\vec{r},t) \stackrel{\text{def}}{=} [\rho_A(\vec{r},t) - \rho_B(\vec{r},t)]/\rho$. $\psi = -1$ means A-rich phase, $\psi = 1$ means B-rich phase.
- The governing equation for SD is derived from the Ginzburg-Landau theory, the general theory for second order phase transition, with ψ being the order parameter. Below is the free energy for SD, where ξ is a parameter that describes the strength of the interaction:

$$\Phi(\psi) = \int d\vec{r}\left(-\frac{1}{2}\psi^2 + \frac{1}{4}\psi^4 + \frac{\xi^2}{2}|\nabla\psi|^2\right)$$



Chemical potential $\mu = \frac{\delta\Phi(\psi)}{\delta\psi} = -\psi + \psi^3 - \xi^2\nabla^2\psi$ Fick's Law: $\vec{J} = -D\nabla\mu$

$$\therefore \frac{d\psi}{dt} + \nabla\cdot\vec{J} = 0 \Rightarrow \frac{d\psi}{dt} = D\nabla^2\mu = D\nabla^2(-\psi + \psi^3 - \xi^2\nabla^2\psi)$$

Cahn-Hilliard Equation

- The fluid velocity comes in the Cahn-Hilliard Eqn via the convection term. The surface tension enters the fluid equation of motion as a force:

$$\partial_t\vec{v} + \vec{v}\cdot\nabla\vec{v} = -\frac{\nabla P}{\rho} - \psi\nabla\mu + \nu\nabla^2\vec{v}$$

Basic Equations for SD

- The governing equations for incompressible 2D Spinodal Decomposition are:

$$\partial_t \psi + \vec{v} \cdot \nabla \psi = D \nabla^2 (-\psi + \psi^3 - \xi^2 \nabla^2 \psi)$$
$$\partial_t \omega + \vec{v} \cdot \nabla \omega = \frac{\xi^2}{\rho} \vec{B}_\psi \cdot \nabla \nabla^2 \psi + \nu \nabla^2 \omega$$

$-\psi$: Negative diffusion term
ψ^3: Self nonlinear term
$-\xi^2 \nabla^2 \psi$: Hyper-diffusion term

With $\vec{v} = \hat{z} \times \nabla \phi, \omega = \nabla^2 \phi, \vec{B}_\psi = \hat{z} \times \nabla \psi, j_\psi = \xi^2 \nabla^2 \psi$

- The governing equations for incompressible 2D MHD are:

$$\partial_t A + \vec{v} \cdot \nabla A = \eta \nabla^2 A$$
$$\partial_t \omega + \vec{v} \cdot \nabla \omega = \frac{1}{\mu_0 \rho} \vec{B} \cdot \nabla \nabla^2 A + \nu \nabla^2 \omega$$

A: Simple diffusion term

With $\vec{v} = \hat{z} \times \nabla \phi, \omega = \nabla^2 \phi, \vec{B} = \hat{z} \times \nabla A, j = \frac{1}{\mu_0} \nabla^2 A$

- Note that the magnetic potential A is a scalar in 2D
- MHD with a constant hyper-resistivity is more similar to SD.
- *Differences:*
  - 2D SD contains negative diffusion, nonlinear diffusion and hyper-diffusion, these additional terms offer more challenges compared to 2D MHD.
  - By definition $\psi \in [-1,1]$, while A doesn't have such restriction

2D SD	2D MHD
ψ	A
ξ^2	$1/\mu_0$
D	η

Ideal Conserved Quantities $(D, \eta = 0; \nu = 0)$

- 2D MHD

1. Energy:

$$E = \int (\frac{v^2}{2} + \frac{B^2}{2\mu_0}) d^2x$$

2. Mean Square Magnetic Potential

$$H_A = \int A^2 \, d^2x$$

3. Cross Helicity

$$H_C = \int \vec{v} \cdot \vec{B} d^2x$$

- 2D SD

1. Energy:

$$E = \int (\frac{v^2}{2} + \frac{\xi^2 B_\psi^2}{2}) d^2x$$

2. Mean Square Concentration

$$H_\psi = \int \psi^2 \, d^2x$$

3. Cross Helicity

$$H_C = \int \vec{v} \cdot \vec{B}_\psi \, d^2x$$

Dissipation of Conserved Quantities

- 2D MHD

1. Energy:

$$\frac{dE_{MHD}}{dt} = -\eta \int \mu_0 j^2 \, \mathrm{d}^2x - \nu \int \omega^2 \, \mathrm{d}^2x$$

2. Mean Square Magnetic Potent

$$\frac{dH_A}{dt} = -2\eta \int B^2 \, \mathrm{d}^2x$$

3. Cro

$$\frac{dH_{C,MHD}}{dt} = -(\nu + \eta) \int \mu_0 j \omega \, \mathrm{d}^2x$$

Note that the energy E_{MHD} and mean square magnetic potential H_A can only decrease in unforced case.

- Spinodal Decomposition

1. Energy: $\boxed{-\psi + \psi^3 - \xi^2 \nabla^2 \psi}$

$$\frac{dE}{dt} = -D \int (-\xi^{-2} j_\psi^2 + 6\psi B_\psi^2 j_\psi + 3\xi^{-2}\psi^2 j_\psi^2 + (\nabla j_\psi)^2) \, \mathrm{d}^2x - \nu \int \omega^2 \, \mathrm{d}^2x$$

2. Mean Square Concentration:

$$\frac{dH_\psi}{dt} = -2D \int [-B_\psi^2 + 3\psi^2 B_\psi^2 + \xi^{-2} j_\psi^2] \, \mathrm{d}^2x$$

3. Cross Helicity: $\boxed{-\psi + \psi^3 - \xi^2 \nabla^2 \psi}$

$$\frac{dH_C}{dt} = -\nu \int -\xi^{-2} j_\psi \omega \, \mathrm{d}^2x - D \int (\xi^{-2} j_\psi - 3\psi^2 \xi^{-2} j_\psi - 6\psi B_\psi^2 + \nabla^2 j_\psi)\omega \, \mathrm{d}^2x$$

Note that the energy E and mean square concentration H_ψ will NOT always decrease in unforced case.

Actually in all unforced runs, H_ψ increases monotonically, with an upper bound of 1.

Waves in SD and MHD

- The linear dispersion relation in 2D MHD is:

$$\omega(k) = \pm\sqrt{\frac{1}{\mu_0\rho}}\,|\vec{k}\times\vec{B}_0| - \frac{1}{2}i(\eta+\nu)k^2$$

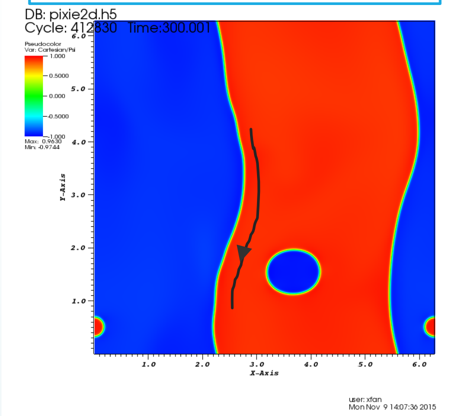
Alfven Wave

- The linear dispersion relation in 2D SD is:

$$\omega(k) = \pm\sqrt{\frac{\xi^2}{\rho}}\,|\vec{k}\times\vec{B}_{\psi 0}| - \frac{1}{2}i(CD+\nu)k^2$$

SD Wave

The SD wave propagates along the $\vec{B}_{\psi 0}$ field line:



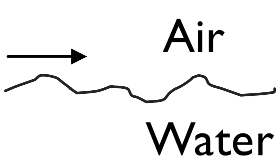
Where C is a dimensionless coefficient which could be either positive or negative depending on k :

$$C \equiv [-1 - 6\psi_0\nabla^2\psi_0/k^2 - 6(\nabla\psi_0)^2/k^2 - 6\psi_0\nabla\psi_0\cdot i\mathbf{k}/k^2 + 3\psi_0^2 + \xi^2k^2]$$

When $CD+\nu > 0$, the wave is a damping wave; when $CD+\nu < 0$, it is an instability.

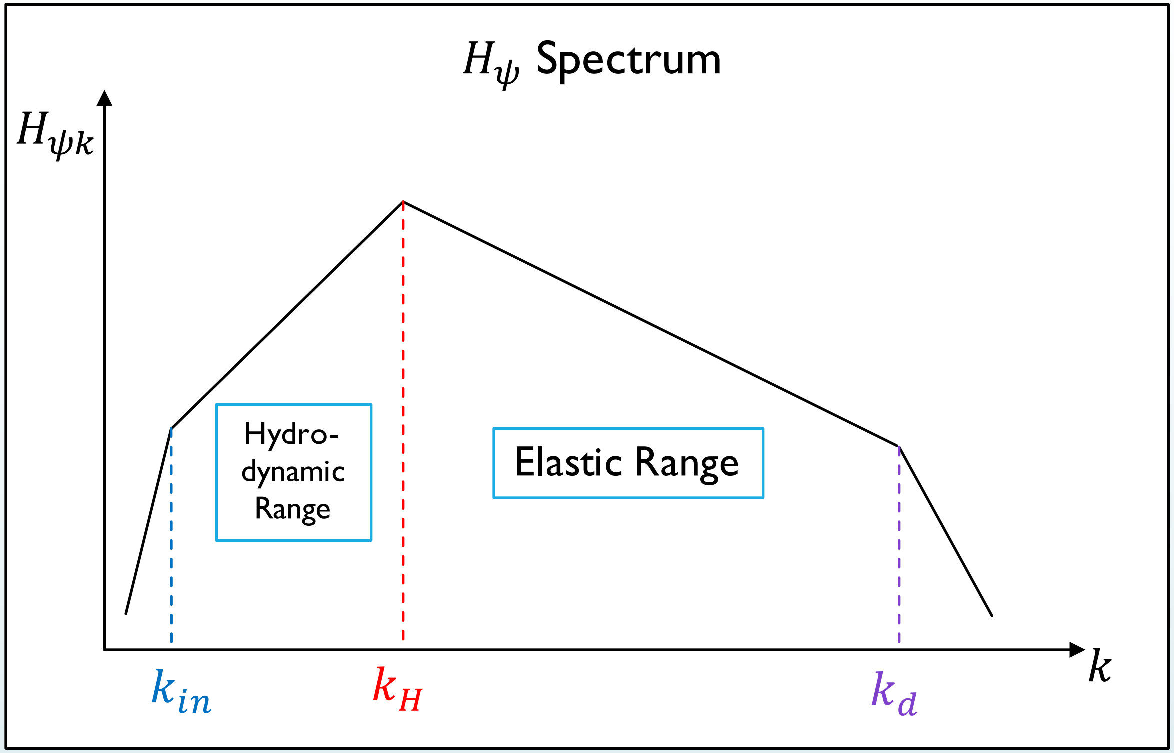
The SD wave is like a capillary wave: it only propagates along the boundary of the two fluids, where the gradient of concentration $\vec{B}_{\psi 0} \neq 0$. Surface tension offers restoring force.

Capillary Wave:



The SD wave is similar to Alfven wave: they have similar dispersion relation; they both propagates along $\vec{B}_0$ field lines; both magnetic field and surface tension act like an elastic restoring force.

Length Scales of SD Turbulence



Hinze Scale: $L_H \sim (\frac{\rho}{\sigma})^{-3/5} \epsilon^{-2/5} \sim (\frac{\rho}{\xi})^{-3/5} \epsilon^{-2/5}$. It's the length scale with the balance between the turbulent kinetic energy (break up large blobs) and surface tension energy (stick small blobs together). For scales smaller than Hinze scale (i.e. in the elastic range), the blobs tend to coalesce by surface tension, while for scales larger than Hinze scale, the blobs tend to break up by turbulence.

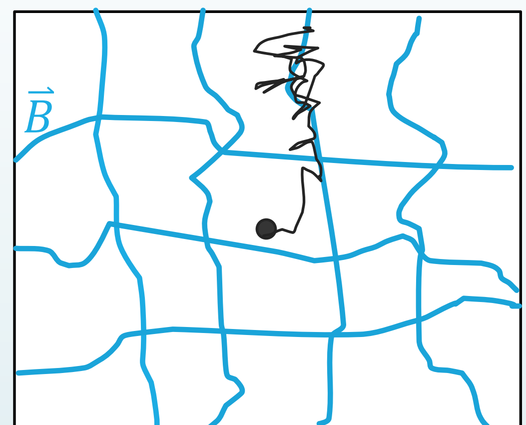
Dissipation Scale: $L_d = L_{IK} = (\nu^2 v_A/\epsilon)^{1/3}$, where v_A is the analogue to Alfven speed. This expression is an analogue to the MHD dissipation scale by Iroshnikov–Kraichnan (IK) theory: $T_l \sim \frac{(\tau_l)^2}{\tau_A} \sim \frac{(L_{IK})^2}{\nu}$.

Turbulent Transport

MHD

- Zeldovich Theorem $\langle B^2 \rangle = \frac{\eta_T}{\eta} \langle B \rangle^2$ in MHD implies even a weak mean magnetic field can result in a large mean square fluctuation. [Diamond 2010]
- Elastization in MHD: small scale magnetic field will result in enhanced memory.

Pure hydrodynamics



MHD, with strong small scale magnetic field lines

- Turbulent transport (η_T, ν_T) in MHD with even a weak large scale magnetic field is suppressed by the enhanced memory. [Cattaneo 1994, Tobias 2007]
- In the elastic range in the spectra, the enhanced memory effect dominates and stops the forward energy cascade.

Turbulent Transport

SD

- Initial ideas on Spinodal Decomposition: based on the following similarities between MHD and SD, we expect the suppression of turbulent transport by enhanced memory also occurs in SD:

MHD	SD
Magnetic field lines offer elasticity	Surface tension offers elasticity
Magnetic flux blob coagulation	Blob coalescence process
Inverse cascade of mean square magnetic potential	Inverse cascade of mean square concentration
There is an elastic range where magnetic energy dominates	There is an elastic range where surface tension energy dominates

- The study of effective diffusivity D_T and effect viscosity ν_T in 2D SD turbulence and the effect of memory is ongoing.
- Also similar to the drag reduction in flexible polymers in dilute solution.

Simulation Setup

- Pixie2d code [Chacon 2002] is used to simulate the system. Pixie2d originally solves the 2D MHD equation, and now is modified to be able to solve the spinodal decomposition equation, too. It is a Direct Numerical Simulation that solves the following equations in real space:

$$\partial_t \psi + \vec{v} \cdot \nabla \psi = D\nabla^2(-\psi + \psi^3 - \xi^2 \nabla^2 \psi) + F_\psi$$

$$\partial_t \omega + \vec{v} \cdot \nabla \omega = \frac{\xi^2}{\rho} \vec{B}_\psi \cdot \nabla \nabla^2 \psi + \nu \nabla^2 \omega + F_\omega$$

With $\vec{v}=\hat{z}\times\nabla\phi$, $\omega = \nabla^2\phi$, $\vec{B}_\psi = \hat{z}\times\nabla\psi$, $j_\psi = \xi^2\nabla^2\psi$

- Initial condition: by default ψ in each cell is assigned to 1 or -1. randomly; $\phi = 0$ everywhere. Other initial conditions are also considered.
- Boundary condition: doubly periodic.
- External force for either ψ or ϕ: an isotropic homogeneous force that has a wave number k_{in}:

$$F = F_0 \sin(k_{in} \cos\theta\, x + k_{in} \sin\theta\, y + \varphi)$$

where θ and φ are both random number in $[0, 2\pi)$, they are random angle and random phase respectively.

H_A Spectrum

MHD

- Assuming a constant energy transfer/dissipation rate ϵ, the IK theory gives the energy spectrum for forward energy cascade: $E_k = C_{IK}(\epsilon v_A)^{1/2} k^{-3/2}$, thus by dimensional analysis the H_A spectrum is:

$$H_{Ak} = C_{IK}(\epsilon v_A)^{1/2} k^{-7/2}$$

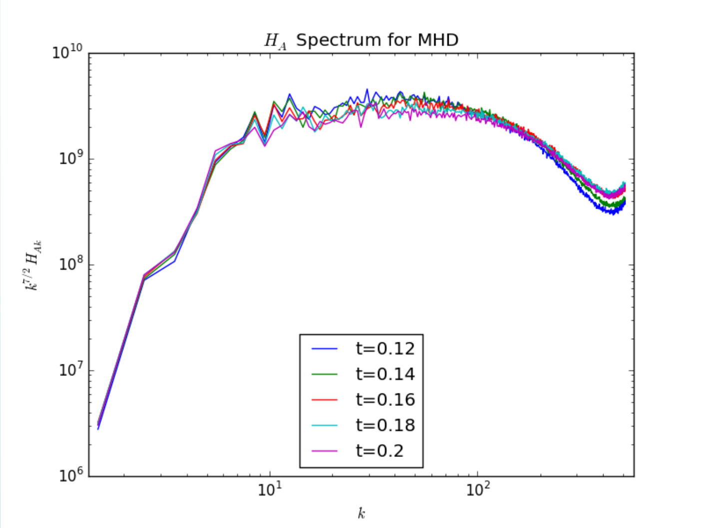
Forward Energy Cascade

- Assuming a constant H_A transfer/dissipation rate ϵ_{HA}, by dimensional analysis we obtain the mean square potential energy spectrum for inverse H_A cascade:

$$H_{Ak} \sim {\epsilon_{HA}}^{2/3} k^{-7/3}$$

Inverse H_A Cascade

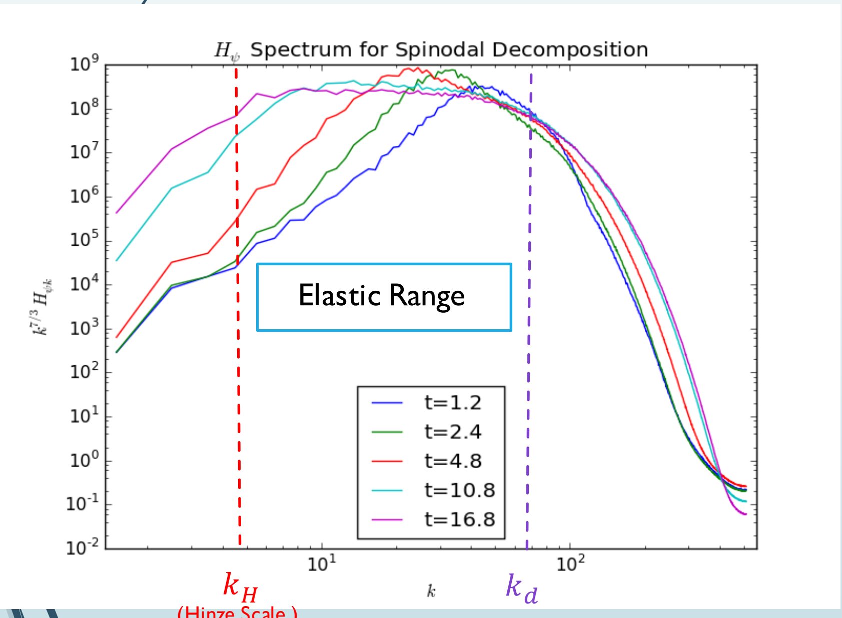
- We obtain the correct 2D MHD forward energy cascade exponent $-7/2$ with this code. Initial condition: large scale A field and ϕ field. See the right figure (Run 5).

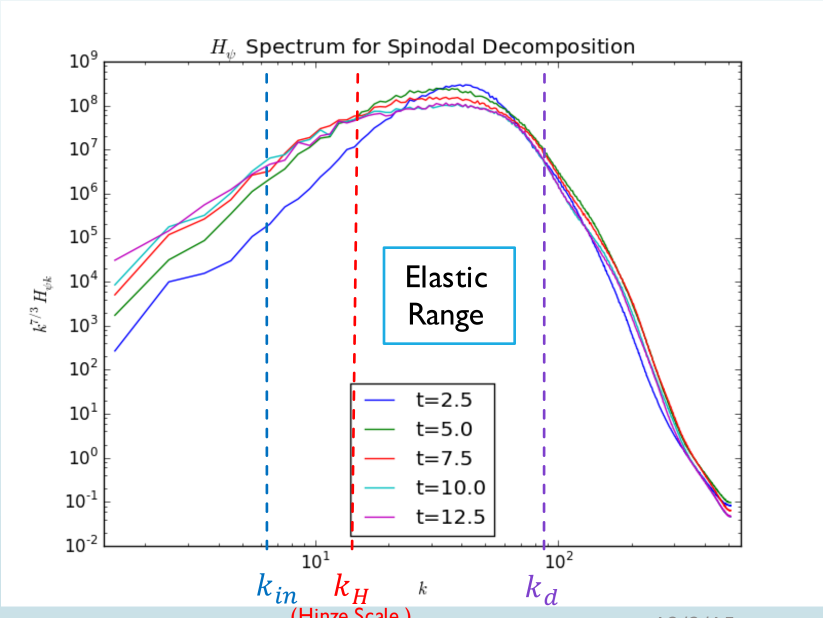


H_ψ Spectrum

SD

- The unforced mean square concentration H_ψ spectrum has an exponent $-7/3$ ($H_{\psi k} \sim {\epsilon_{H\psi}}^{2/3} k^{-7/3}$). See the left figure (Run 7). This result suggests an inverse H_ψ cascade in SD, and is consistent with the blob coalescence process.
- When ϕ is forced at large scale (k_{in}=4), at scales smaller than Hinze scale, the mean square concentration H_ψ spectrum still has the exponent $-7/3$, See the right figure (Run 8). The elastic range is shortened because the Hinze Scale becomes smaller.

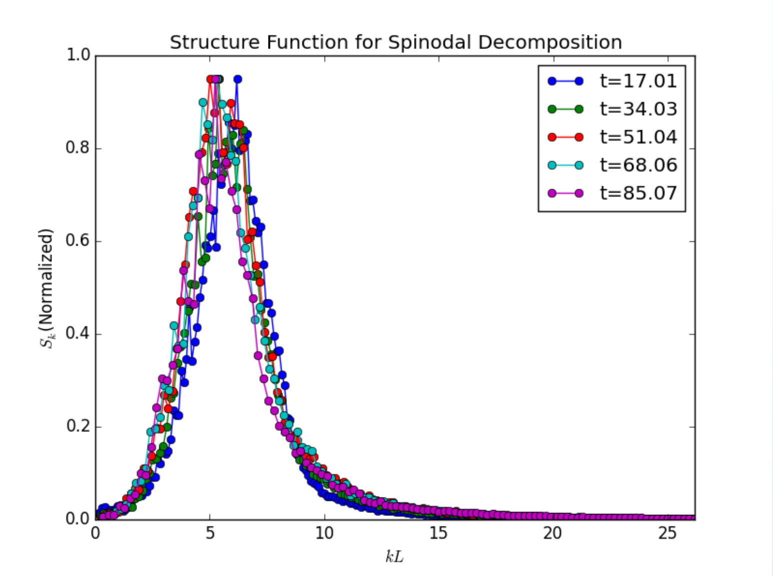




Length Scale Growth

SD

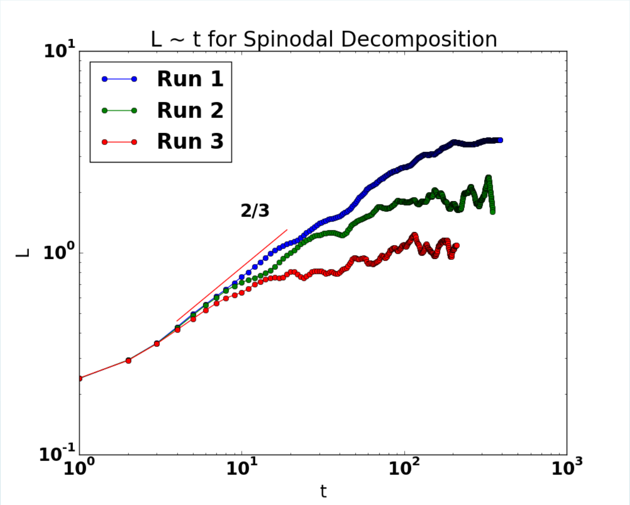
- For spinodal decomposition, define Structure function as
$$S_k(k,t) \stackrel{\text{def}}{=} < |\psi_{\vec{k}}(\vec{k},t)|^2 >$$
- Then define the blob length scale by
$$L(t) = 2\pi \frac{\int S_k(k,t)dk}{\int kS_k(k,t)dk}$$
- We see there is a clear peak in the structure function. This verifies there is a single definite blob structure length scale in the SD turbulence [Furukawa 2000]. See the right figure (Run 4).

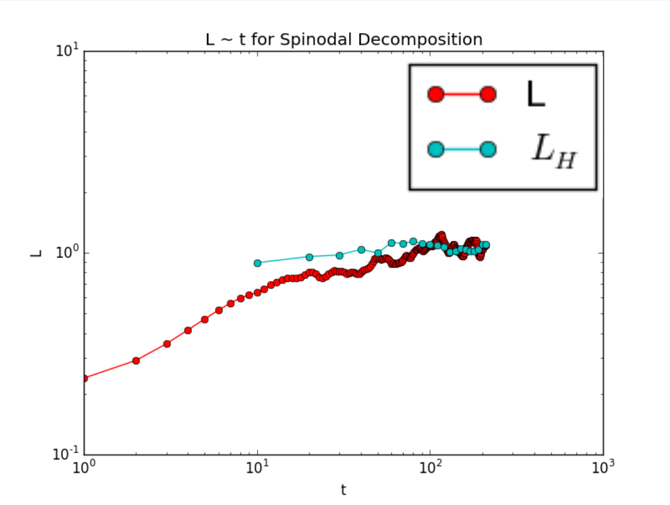


Length Scale Growth

SD

- The blob length scale grows with time as a power law if unforced: $L(t) \sim t^{2/3}$. Derivation: $\vec{v} \cdot \nabla \vec{v} \sim \frac{\xi^2}{\rho} \nabla^2 \psi \nabla \psi \Rightarrow \frac{\dot{L}^2}{L} \sim \frac{\sigma}{\rho} \frac{1}{L^2}$. [Kendon 2001]
- When external force is present, the growth of length scale can be arrested. The larger the external force is, the smaller the saturated length scale becomes. [Berti 2005]
- The saturated length scale is related to the Hinze Scale (the balance between the turbulent kinetic energy and surface tension energy). See the right figure (Run 3).



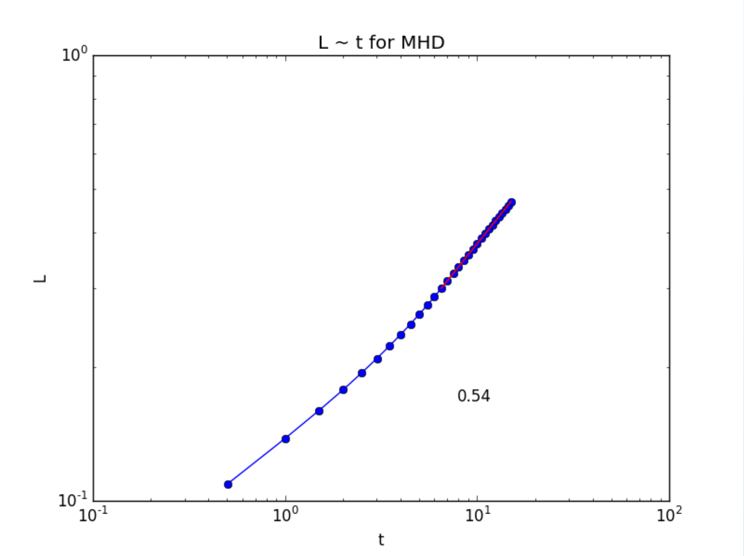


Length Scale Growth

MHD

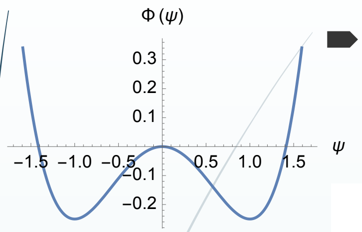
- Given similar small scale A field initial conditions, the previous structure function evolution and the blob length scale growth arguments for 2D SD also apply to 2D MHD.
- By similar argument, we obtain the length scale growth for 2D MHD: $L(t) \sim t^{1/2}$. Derivation: $\vec{v} \cdot \nabla \vec{v} \sim \frac{1}{\rho} \vec{j} \times \vec{B} \Rightarrow \frac{\dot{L}^2}{L} \sim \frac{1}{\mu_0 \rho} \frac{A^2}{L^3}$.
- The simulation result verifies the exponent $1/2$, see the figure below (Run 6).
- This is a new result for 2D MHD illuminated by the study of Spinodal Decomposition.

2D SD	2D MHD
$S_k(k,t) \stackrel{\text{def}}{=} < \lvert\psi_{\vec{k}}(\vec{k},t)\rvert^2 >$	$S_k(k,t) \stackrel{\text{def}}{=} < \lvert A_{\vec{k}}(\vec{k},t)\rvert^2 >$
$L(t) = 2\pi \frac{\int S_k(k,t)dk}{\int k S_k(k,t)dk}$	$L(t) = 2\pi \frac{\int S_k(k,t)dk}{\int k S_k(k,t)dk}$



PDF of ψ/A

SD vs MHD



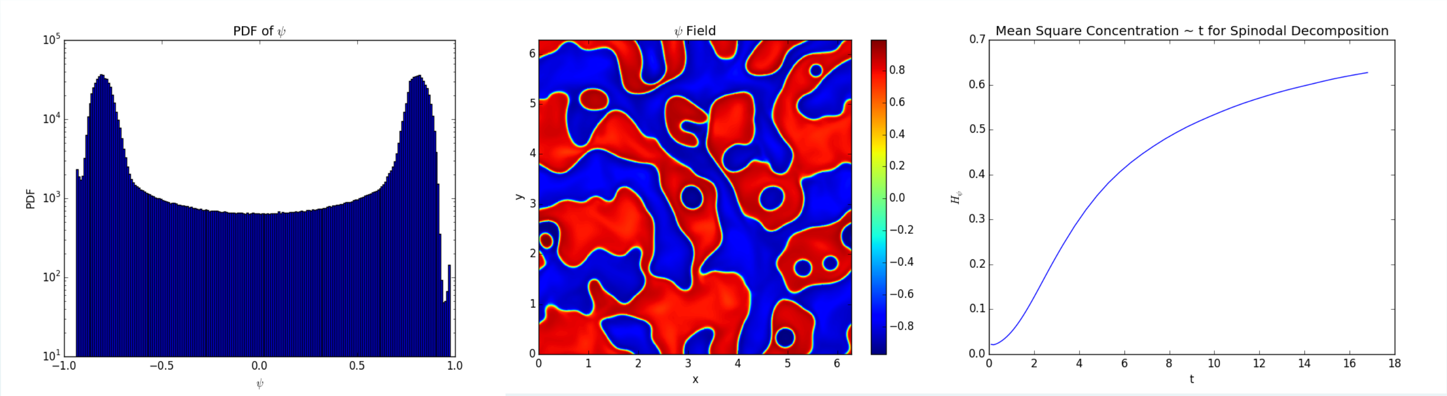
SD:

Unforced

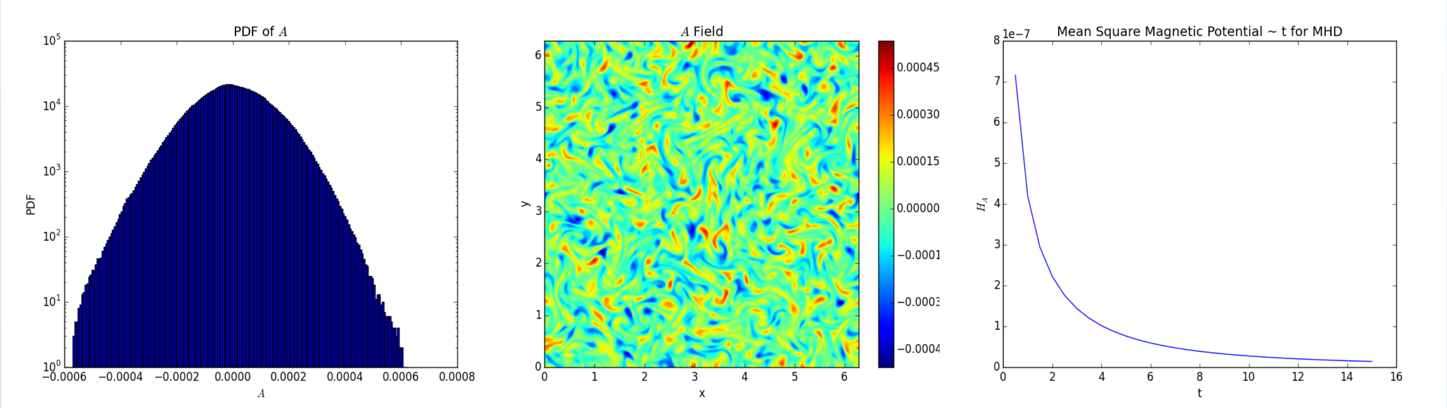
MHD:

Unforced

- The Probability Density Function (PDF) of concentration ψ for unforced spinodal decomposition has sharp peaks at ± 1. This shape is mainly due to the well shape of the free energy $\Phi(\psi)$. See the upper figure below (Run 7).



- The PDF for magnetic potential A for 2D MHD has one peak at 0. See the lower figure below (Run 6). This is an interesting difference between spinodal decomposition and 2D MHD.



UCSD

22

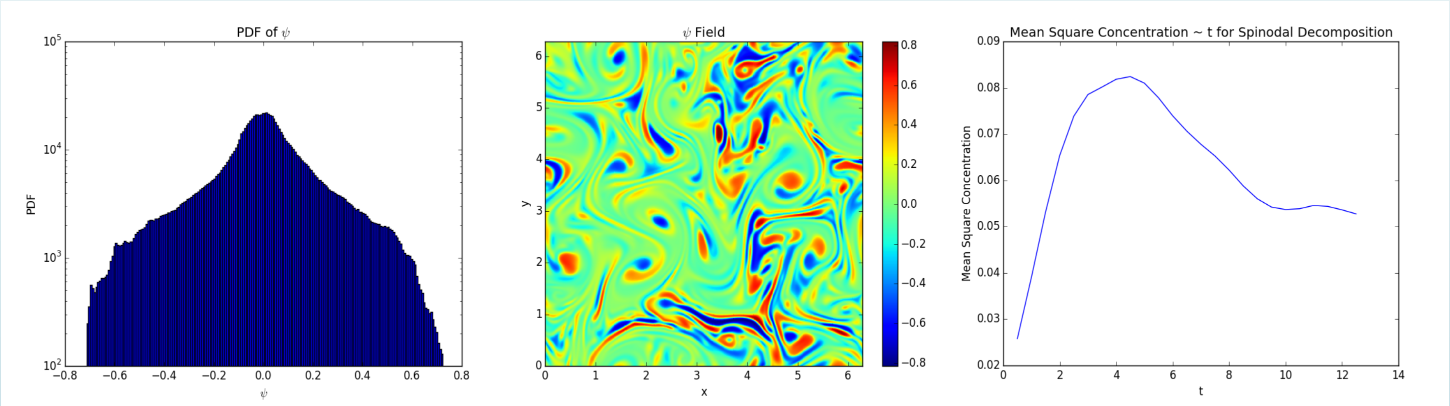
PDF of ψ

SD

- The PDF of concentration ψ for spinodal decomposition may change its shape dramatically when external forcing is large enough. See the lower figure below (Run 8), the only change from the previous PDF of ψ is the presence of external forcing.
- [Náraigh 2007] observed similar phenomena in a passive Cahn-Hilliard flow simulation. An issue raised: why do I see the same phenomena in an active flow simulation? What's the role of the advection term in Cahn-Hilliard Eqn?
- It seems that the phase transition is reversed by large enough external forcing. This may be the noise-induced phase transition.

SD:

Strongly forced



Conclusion

- The mean square concentration H_ψ spectrum in unforced spinodal decomposition has an exponent $-7/3$ in the elastic range.
- The mean square concentration H_ψ spectrum in large scale forced spinodal decomposition still has an exponent $-7/3$ in the elastic range. The elastic range is shortened because the Hinze Scale becomes smaller.
- The blob length scale in spinodal decomposition grows as $L(t) \sim t^{2/3}$ for unforced case. When external forcing is present, the length scale growth saturates at the Hinze scale $L_H \sim (\frac{\rho}{\sigma})^{-3/5} \epsilon^{-2/5}$.
- In 2D MHD we can observe similar length scale growth, but with a different exponent: $L(t) \sim t^{1/2}$.
- The PDF of concentration ψ in spinodal decomposition has peaks at ±1, while the PDF of magnetic potential A in 2D MHD has one peak at 0.
- Large enough external forcing can reverse the phase transition, and make the PDF of concentration ψ peak at 0.

Future Work

- Study the effect of memory to turbulent transport in spinodal decomposition.
- Calculate the effective diffusivity D_T and effect viscosity ν_T in 2D SD turbulence. Compare them with the physics of effect resistivity and effect viscosity in 2D MHD.
- Calculate the concentration flux in 2D SD turbulence and analyze the physics behind.
- Do a forced 2D MHD run with similar initial condition to 2D SD runs to see whether we obtain a similar length scale growth arrest.
- Study the role of the capillary wave in spectra in 2D SD turbulence.
- Find a explanation for the PDF shape change of ψ when the external forcing is present.

Appendix: Simulation Parameters

Run	Physics System	Resolution	Box size	D	ν	ξ	k_0	$F_{0\phi}$	$k_{in\phi}$	$F_{0\psi}$	$k_{in\psi}$
Run 1	SD	512^2	2π	1.00E-03	1.00E-03	0.015	512	0	0	0	0
Run 2	SD	512^2	2π	1.00E-03	1.00E-03	0.015	512	0.1	4	0	0
Run 3	SD	512^2	2π	1.00E-03	1.00E-03	0.015	512	0.2	4	0	0
Run 4	SD	1024^2	512	1	0.01	0.5	1024	0	0	0	0
Run 5	MHD	1024^2	2π	1.00E-04	1.00E-04	-	5	0	0	0	0
Run 6	MHD	1024^2	2π	1.00E-04	1.00E-04	-	1024	0	0	0	0
Run 7	SD	1024^2	2π	1.00E-03	1.00E-03	0.015	1024	0	0	0	0
Run 8	SD	1024^2	2π	1.00E-03	1.00E-03	0.015	1024	1.0	4	0	0
Run 9	SD	1024^2	2π	1.00E-03	1.00E-03	0.015	1024	0.1	4	0	0