

Term Paper Presentation, Pattern Formation Course

# Rethinking pattern formation in reaction–diffusion systems

J. Halatek and E. Frey

Vinay Kumar, 27 April 2023

Hello everyone. So I'll be speaking about the work of these two gentlemen, Halatek and Frey. They have put forward some ideas, some alternative ways to look at pattern forming reaction diffusion systems, which I'll be talking about.

## Outline

- Overview of Pattern Forming Dynamical Systems
- Limitations in current methodology
- Alternative Approach
- Mass conserving reaction diffusion equations
- Simple Illustration
- Simulation and results
- Summary

This is the outline of my talk. I'll begin by giving an overview of how we learned to approach pattern forming systems in class. I'll then tell you about some of the limitations of this method. We shall then look at an alternative approach to study pattern formation in mass conserving Reaction diffusion equations. I'll then illustrate this method with a simple example before moving on to show some results from simulations that support this idea. And then I'll end with a summary.

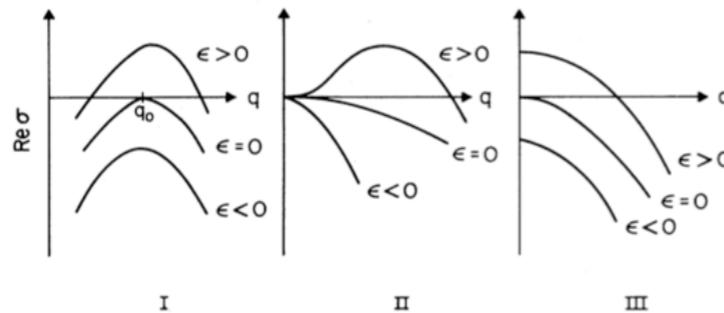
# Dynamical Systems



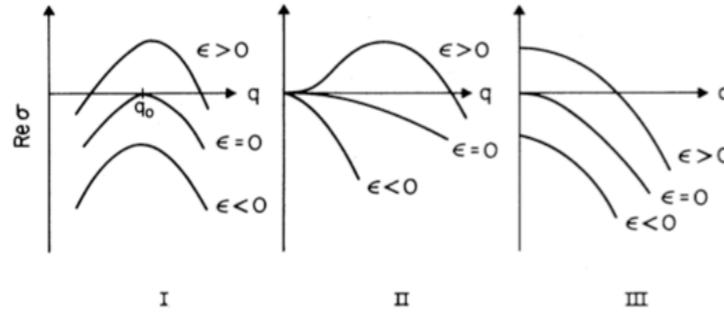
Let us recap how we study dynamical systems. We start with a system in equilibrium. The equilibrium state is obtained by setting the time derivatives of all dynamical variables to zero. Then we add perturbations to this. The perturbation can in general be decomposed in a Fourier basis. For suitable values of some parameters, known as control parameters, some of the Fourier amplitudes grow in time. We then calculate the growth rate corresponding to each Fourier mode. The dependence of this growth rate on the wave number is called the dispersion relation. The shape of the dispersion relation is then used to classify dynamical systems into Type1, Type2 or Type3 instabilities.

# Dynamical Systems

System in Equilibrium → Perturbed (Fourier Modes) → Perturbations Grow → Dispersion Relation



# Dynamical Systems



An important thing to note here is that all this is done for a system which is not just in a state of equilibrium, but in a state of GLOBAL equilibrium. That is, a state which is uniform in space. And our entire analysis is based on calculations done close to this global homogeneous equilibrium state. Whereas the final pattern is quite far from it. A natural question that arises here is this: Can we find a better way to analyze the pattern using computations done far from the homogeneous equilibrium and close to the patterned state?

## Dynamical Systems



- Analysis is valid if:
  - System is near instability threshold.
  - Non-linear effects are stabilizing.

Another constraint is that the system should be close to the threshold of the instability. That is this analysis is valid for a small subspace of the full control parameter space. Moreover, this is valid only if the system is super-critical, that is, non-linear terms have a purely stabilizing effect, keeping the system close to the uniform equilibrium.

In reality however, things are different. One may not find systems which are close to the instability threshold, but far above it. And there are many systems where the non-linear terms amplify deviations from equilibrium such as near tipping points in climatic systems.

# Dynamical Systems



- Analysis is valid if:
  - System is near instability threshold.
  - Non-linear effects are stabilizing.
- Real systems:
  - Rarely found close to threshold.
  - nonlinear interactions amplify deviations from an equilibrium position

## Alternative Approach

- For mass conserving systems, amount of conserved quantity (CQ) determines nature of equilibria.
- CQs may be inhomogeneously distributed in space.
- Different equilibria at different locations.
- Partition extended system into compartments and determine their local equilibria by local values of CQs.
- Set of all local equilibria characterize the dynamical state.

So the authors of this paper attempt to formulate an alternative approach to study pattern forming dynamical systems, trying to address some of these limitations. Their idea is based on the fact that in mass-conserving systems the available amount of each conserved quantity determines the nature of equilibria. And in general, these conserved quantities may be non-uniform in space. This means that different locations will have different equilibrium states or different LOCAL equilibria. One can then partition the full system and look the local equilibria in each compartment depending on the amount of CQ available. The full set of these local equilibria then characterize the dynamic state of the system.

# 1D Reaction Diffusion

## System Setup

$$\partial_t a(x, t) = D_a \partial_x^2 a + f(a, b)$$

$$\partial_t b(x, t) = D_b \partial_x^2 b - f(a, b)$$

Diffusion      Reaction

$$\underbrace{n_x := a(x, t) + b(x, t)}_{\substack{\text{Local Density} \\ \text{Conserved by Reactions}}}$$

For an illustration of this prescription, let us consider a simple 1D reaction diffusion system with two interconvertible components  $a$  and  $b$ , with diffusion constants  $D_a$  and  $D_b$ . The function  $f$  accounts for all the reactions leading to interconversion between  $a$  and  $b$ . The local density is given as  $n = a+b$ . If only reactions were present, it is easy to see that this local density would be conserved.

# 1D Reaction Diffusion

## Local Dynamics

$$\partial_t a(x, t) = D_a \partial_x^2 a + f(a, b)$$

$$\partial_t b(x, t) = D_b \partial_x^2 b - f(a, b)$$

Diffusion      Reaction

- Local Equilibria:  $f(a_x^*, b_x^*) = 0$ ,  $a_x^* + b_x^* = n_x$ .
- Stability depends on  $a_x^*, b_x^*$ .
- No diffusion  $\implies n_x = a_x^* + b_x^*$  is time independent.

In the absence of diffusion, Local equilibria are completely determined by solving for  $f(a,b)=0$  subject to  $n=a+b$ .  $a_{\text{star}}$  and  $b_{\text{star}}$  represent the local equilibrium states. Notice that these are not uniform in space. The stability of the local equilibria is also set by  $a_{\text{star}}$  and  $b_{\text{star}}$ . Further note, that if there is no diffusion, the local density is time independent. This also means that the local equilibria are also time independent.

## 1D Reaction Diffusion

### Add Diffusion

$$\begin{aligned}\partial_t a(x, t) &= D_a \partial_x^2 a + f(a, b) \\ \partial_t b(x, t) &= D_b \underbrace{\partial_x^2 b}_{\text{Diffusion}} - \underbrace{f(a, b)}_{\text{Reaction}}\end{aligned}\quad \left. \right\} \text{Steady, patterned state: } (\tilde{a}(x), \tilde{b}(x))$$

Steady state  $\implies D_a \partial_x \tilde{a}(x) + D_b \partial_x \tilde{b}(x) = 0$ , and  $D_a \tilde{a}(x) + D_b \tilde{b}(x) = \eta$ .

$$D_a \neq D_b \implies \left\{ \begin{array}{l} \tilde{n}_x = \tilde{a}(x) + \tilde{b}(x) \\ \text{Local equilibria } (a_x^*, b_x^*) \end{array} \right\} \text{Non Uniform}$$

We now see the effect of diffusion. Once we have a steady patterned state, the diffusive fluxes add up to zero. Which, on integrating gives  $D_a$  times  $a$  +  $D_b$  times  $b$  = some constant, eta. Eta here is an integration constant and hence is  $x$  independent. This automatically means that for unequal diffusion constants, the local densities and hence the local equilibria are Non Uniform in space. So we see that in some sense, the pattern and the local equilibria are related.

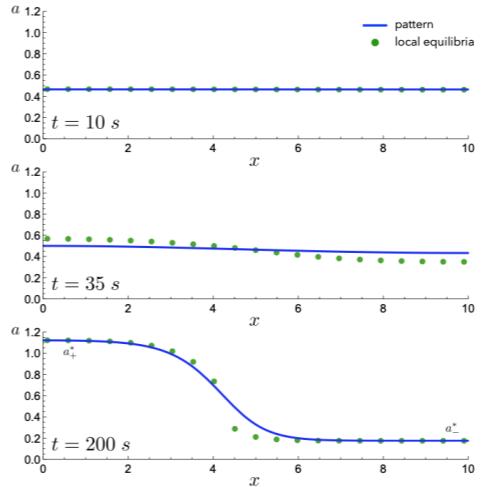
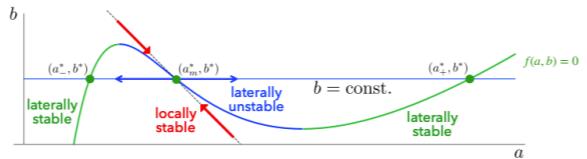
## Illustration

$$\partial_t a(x, t) = D_a \partial_x^2 a + f(a, b)$$

$$\partial_t b(x, t) = D_b \partial_x^2 b - f(a, b)$$

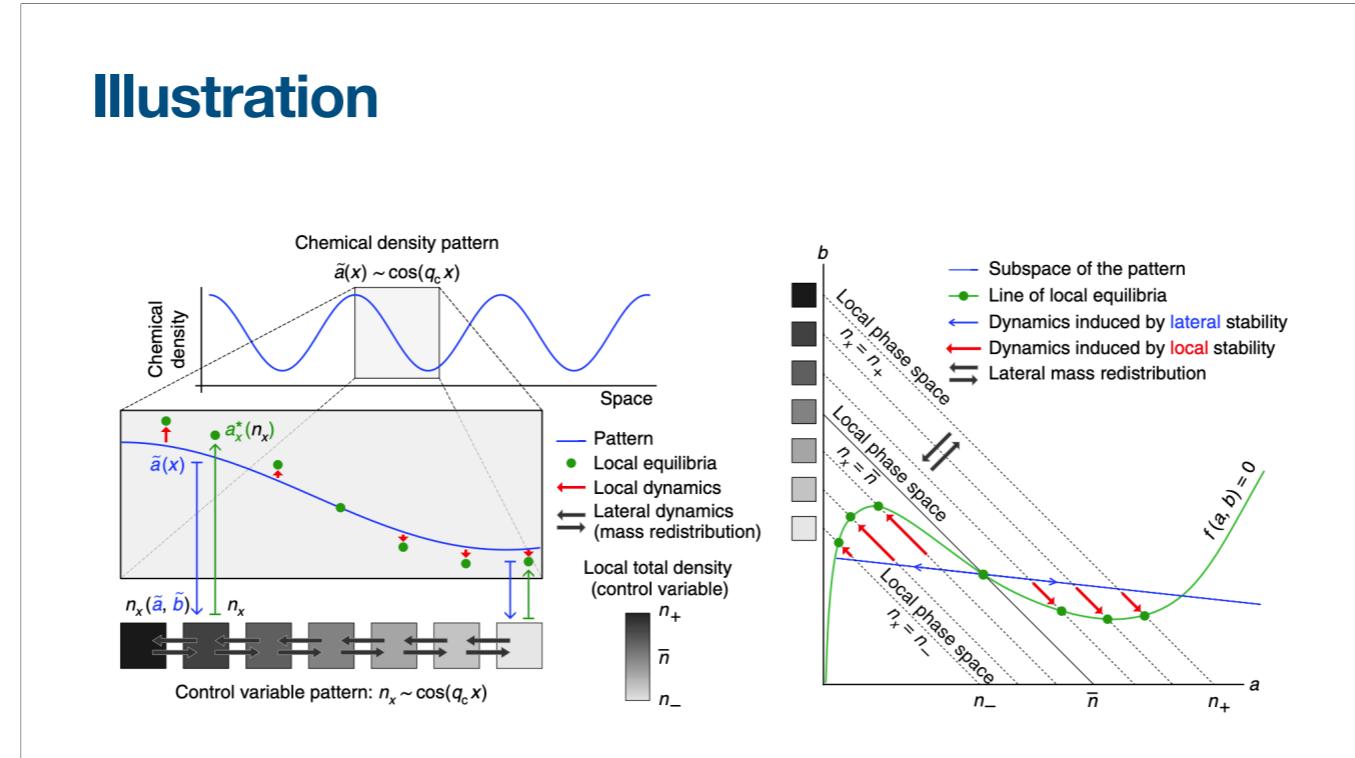
$$D_b \gg D_a \quad D_b \rightarrow \infty$$

$$f(a, b) = b \left( 0.067 + \frac{a^2}{1 + a^2} \right) - a$$



Lets look at a simple example showing this. In this simple example, we choose  $b$  to have a very large, effectively infinite diffusion constant. The reaction term has the form like so. We begin with a spatially homogeneous initial condition. Since  $D_b$  is infinite,  $b$  will be homogeneous in the steady state. So dynamics are constrained to the blue horizontal line in the phase diagram. The curvy line represents local equilibrium,  $f(a, b) = 0$ . It can be shown that the uniform state is laterally unstable in the region in blue. The figure on the right shows the result of simulating this system on a computer. It can be clearly seen that the lateral instability of the uniform state induces a dynamic displacement of local equilibria. The pattern very closely follows the movement of local equilibria. At long time, the pattern is a diffusive interface spanned between plateaus determined by the local equilibria  $a_-^*$  and  $a_+^*$ , which can be read off from the phase plot.

## Illustration



This figure shows a general schematic for this prescription. You have the patterned state. The patterned state closely follows the local equilibria. The equilibrium at a point is dependent only on the local density at that point. This local density is spatially redistributed by diffusion. And so it is indeed true that the dynamics are enslaved to moving local equilibria.

## Study of Min System

- Proteins MinD and MinE.
- Globally conserved.
- $D \equiv$  Normalized Conc. of MinD  
 $E \equiv$  Normalized Conc. of MinE.

Control Variables:

$$\Delta_x = \frac{E_x}{D_x}$$

$$\Sigma_x = \sqrt{\frac{E_x^2 + D_x^2}{2}}$$

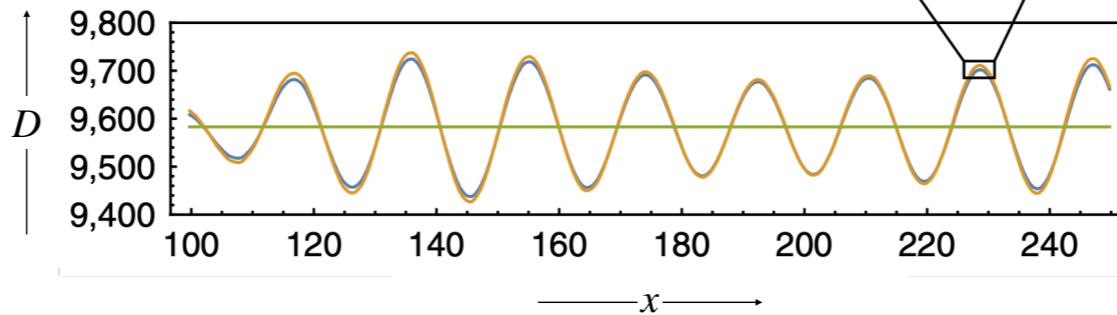
$$\vec{n}_x = (\Delta_x, \Sigma_x) \quad \bar{n} = (\bar{\Delta}, \bar{\Sigma}) = (1,1)$$

They also test this framework for a biologically motivated system, which is this system of Min proteins. MinD and MinE are two proteins which remain globally conserved. MinD leads to accumulation of both species and MinE leads to their depletion. In addition, they get spatially redistributed due to diffusion. The control variables, Delta and Sigma are constructed as shown. And any state is represented by a vector, n=Delta,Sigma. The normalization is done such that the mean of Delta and Sigma are both unity.

## Sim Results - Scaffolding

—  $u^*(x, t)$  —  $u_{\text{num}}(x, t)$  —  $\bar{u}_{\text{num}}$

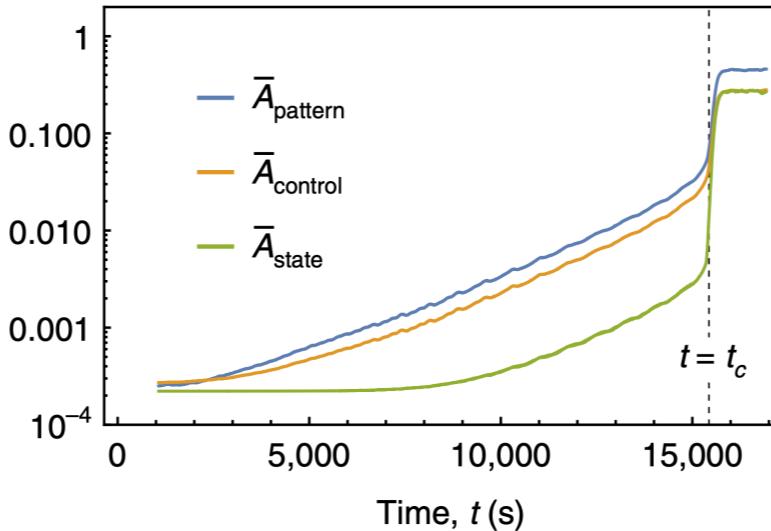
$t = 1.2 \times 10^4 \text{ s}$



The numerical simulations yield the following results.

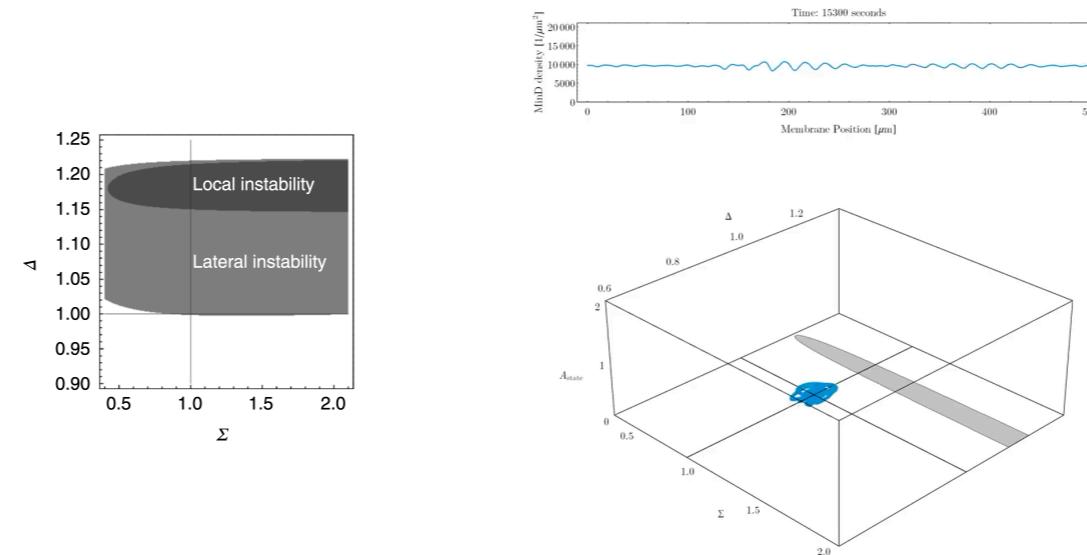
The plot here shows the distribution of MinD in space. The orange curve shows the numerically obtained distribution whereas the blue curve shows the local equilibria. One can see that the pattern and the local equilibria are very close. This is further illustrated by the zoomed panel.

## Sim Results - Scaffolding



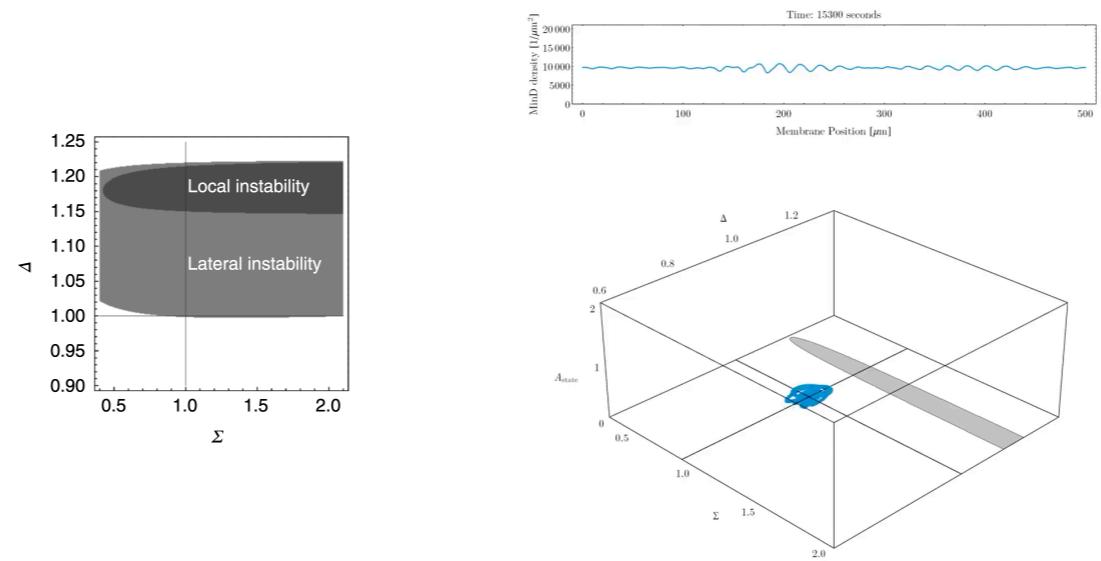
Here we see the evolution of three different amplitudes.  $A_{\text{pattern}}$  shows the root mean squared distance from the homogeneous state.  $A_{\text{control}}$  is the root MSD in the control space.  $A_{\text{state}}$  is the most interesting one. It is the RMSD between the pattern and the local equilibria. One can see that  $A_{\text{state}}$  stay very small, almost 50-60 times smaller, compared to the other curves for quite a while, again showing that the pattern is indeed scaffolded by local equilibria. Notice that at a particular time,  $t_c$ , the distance between local equilibria and the pattern suddenly shoots up by orders of magnitude. This happens when at some location, the local equilibria transition from being stable to unstable.

## Sim Results - Transition to Turbulence

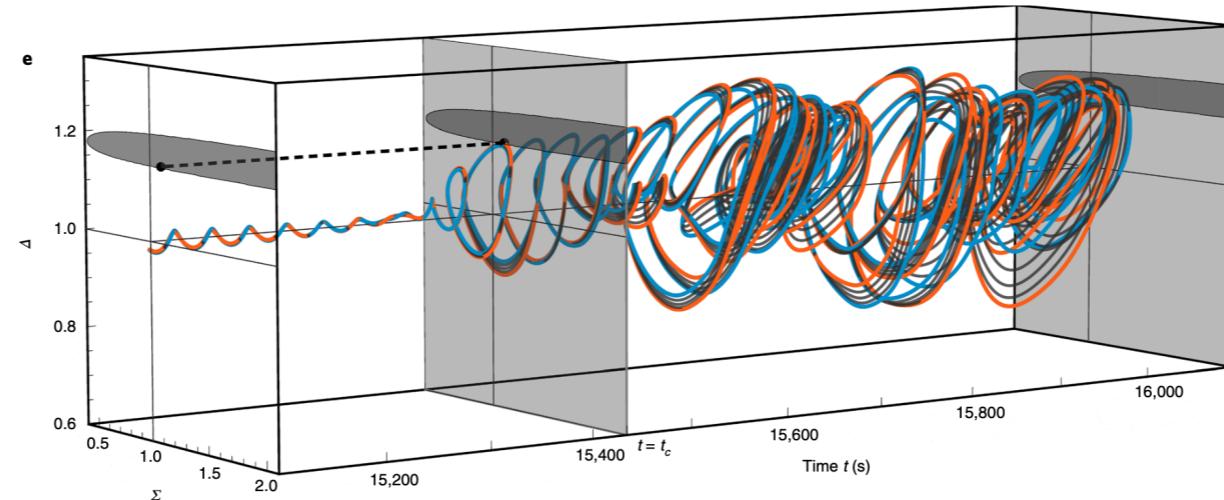


This is the stability curve in the phase space. The region of local instability is also marked in the plot alongside. The blue points correspond to the distance between the pattern and the local equilibria. When any point here enters the unstable region, it will turn to orange. The pattern is shown above and is colored in similar fashion. Points in stable local equilibrium are blue whereas points in unstable local equilibrium will be shown in orange. Let us see the dynamics and see what happens. [Play Movie](#). So you can see that these orange points form a wavefront and move along the pattern. And as they move along, they leave an increasingly disordered pattern behind them. With time, more and more such wavefronts emerge and lead to a completely disordered, turbulent state where the dynamics are spatially uncorrelated.

## Sim Results - Transition to Turbulence



## Sim Results - Transition to Turbulence



This plot also depicts the same story. It shows 5 adjacent trajectories of the control variables. Things are nice and smooth till time  $t_c$ , which is when these trajectories enter the region of local instability. After this time, the trajectories begin to diverge from each other and their amplitude becomes large and irregular.

Here also, we can see that it is indeed the nature and position of local equilibria that govern the dynamics of the system.

## Summary

- Conventional studies of pattern forming systems have limitations:
  - Computations are done near global equilibrium.
  - Valid near threshold of instability.
  - Valid for supercritical systems.
- Alternative approach - local equilibria characterize dynamics:
  - Positions of local equilibria scaffold the pattern.
  - Nature of local equilibria affect transition to turbulence.

So let me just summarise now. We have seen that conventional studies of pattern forming systems, while successful, have their limitations. This is because they involve computations performed near global equilibrium, and are valid for supercritical systems, near the threshold of instability. The alternate approach propounded by Halatek and Frey uses local equilibria to characterize the dynamics of a system. The evidence for this claim is given by the fact that the pattern closely follows the local equilibria and that the stability of the equilibria govern the transition of the system to a state of chemical turbulence.

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[Questions?](#)