riselab UC Berkeley

Chemical Reaction Noise Induced Phenomena: Change in Dynamics and Pattern Formation

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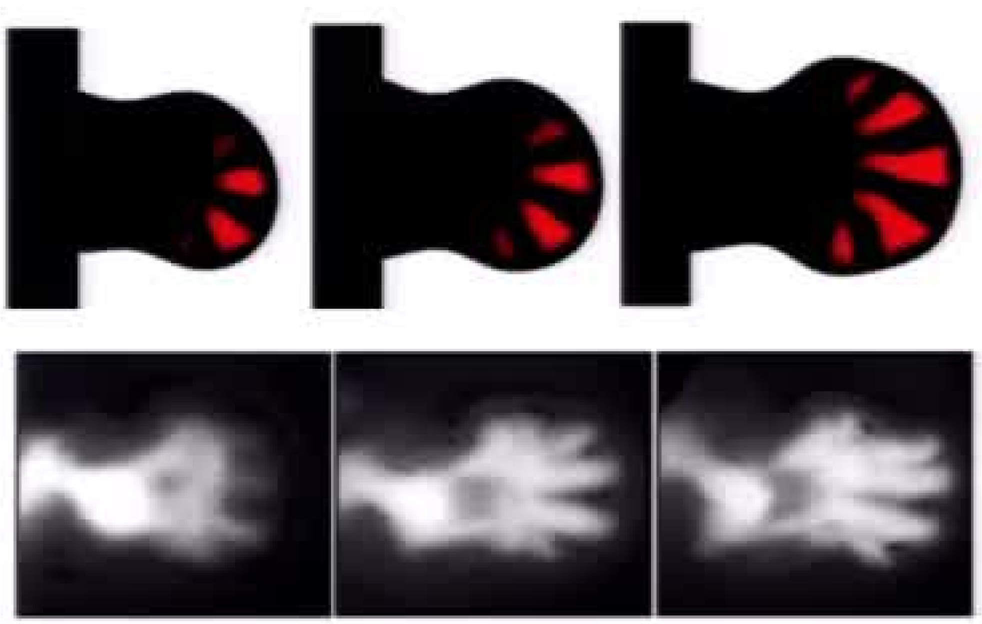
(joint work with Hong Qian, Nathan Baker)

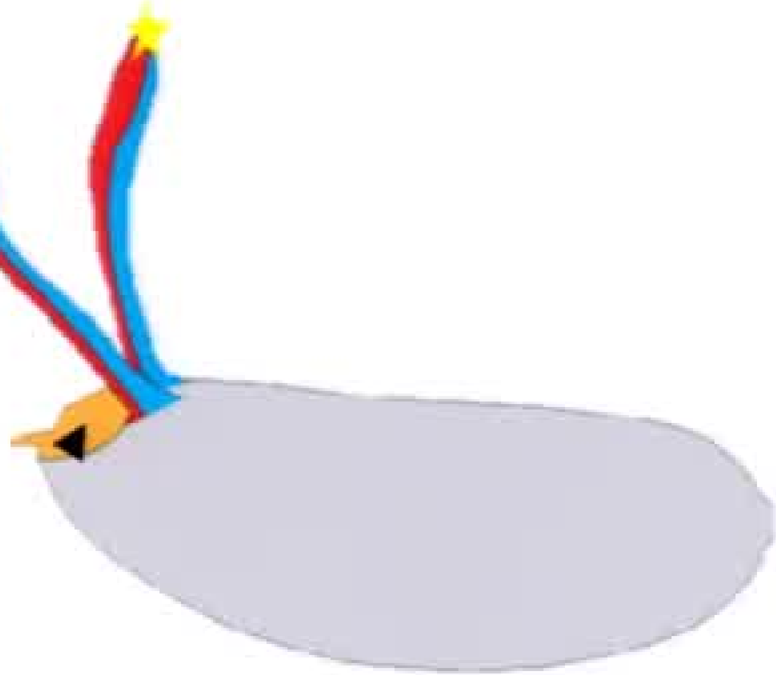
❖ Pattern formation in reaction-diffusion systems

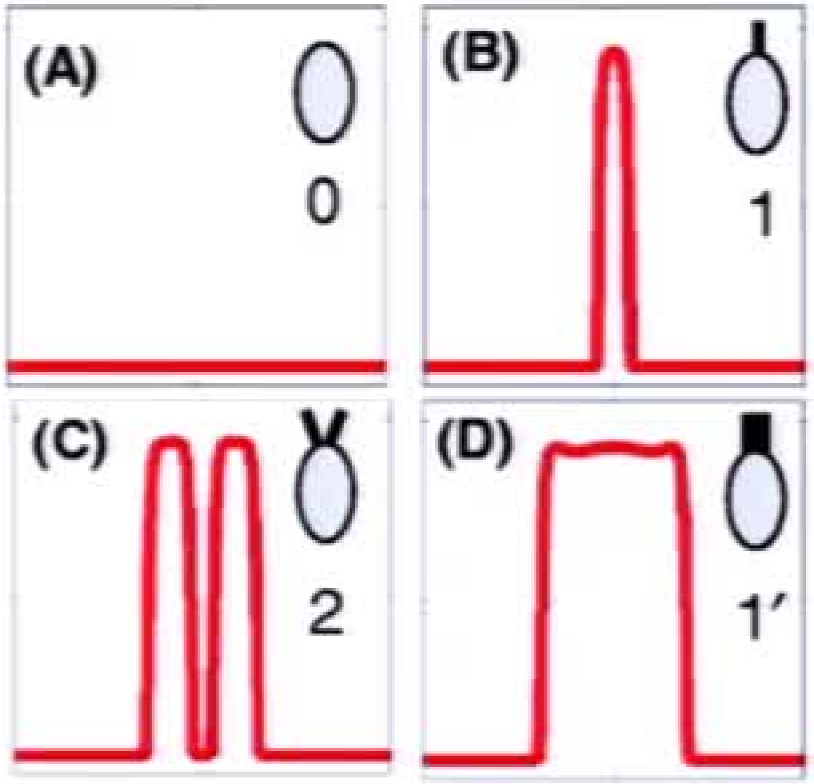
Digit patterning



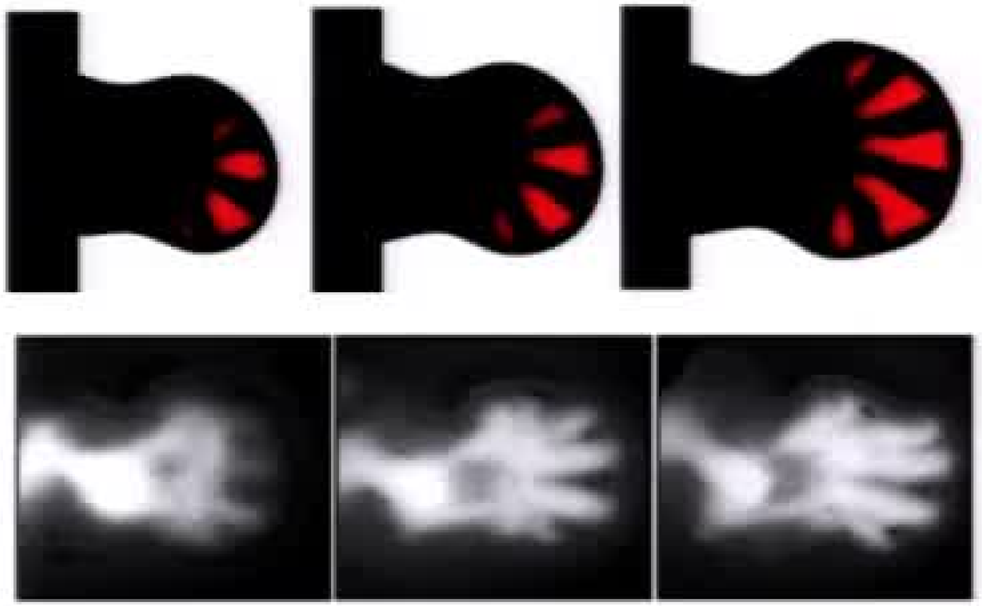
❖ Pattern formation in reaction-diffusion systems

Oogenesis





Digit patterning



❖ Gray Scott Model: Chemical Reaction Diffusion System

Chemical reaction of the Gray Scott model:

$$U + 2V \xrightarrow{1} 3V, \;\; V \xrightarrow{k} P.$$

plus spatial diffusion and input and drain:

$$\begin{pmatrix} \dfrac{\partial u(\mathbf{x},t)}{\partial t} \\ \dfrac{\partial v(\mathbf{x},t)}{\partial t} \end{pmatrix} = \mathbf{M}(u,v) + \mathbf{F}(u,v)$$

$$\mathbf{M}(u,v) = \begin{pmatrix} \mathrm{M}_u \, \Delta_{\mathbf{x}} \, u \\ \mathrm{M}_v \, \Delta_{\mathbf{x}} \, v \end{pmatrix}, \qquad \mathbf{F}(u,v) = \begin{pmatrix} -uv^2 + f(1-u) \\ uv^2 - (f+k)v \end{pmatrix}$$

❖ Chemical Reaction Noise in Gray Scott Model

With chemical reaction noise:

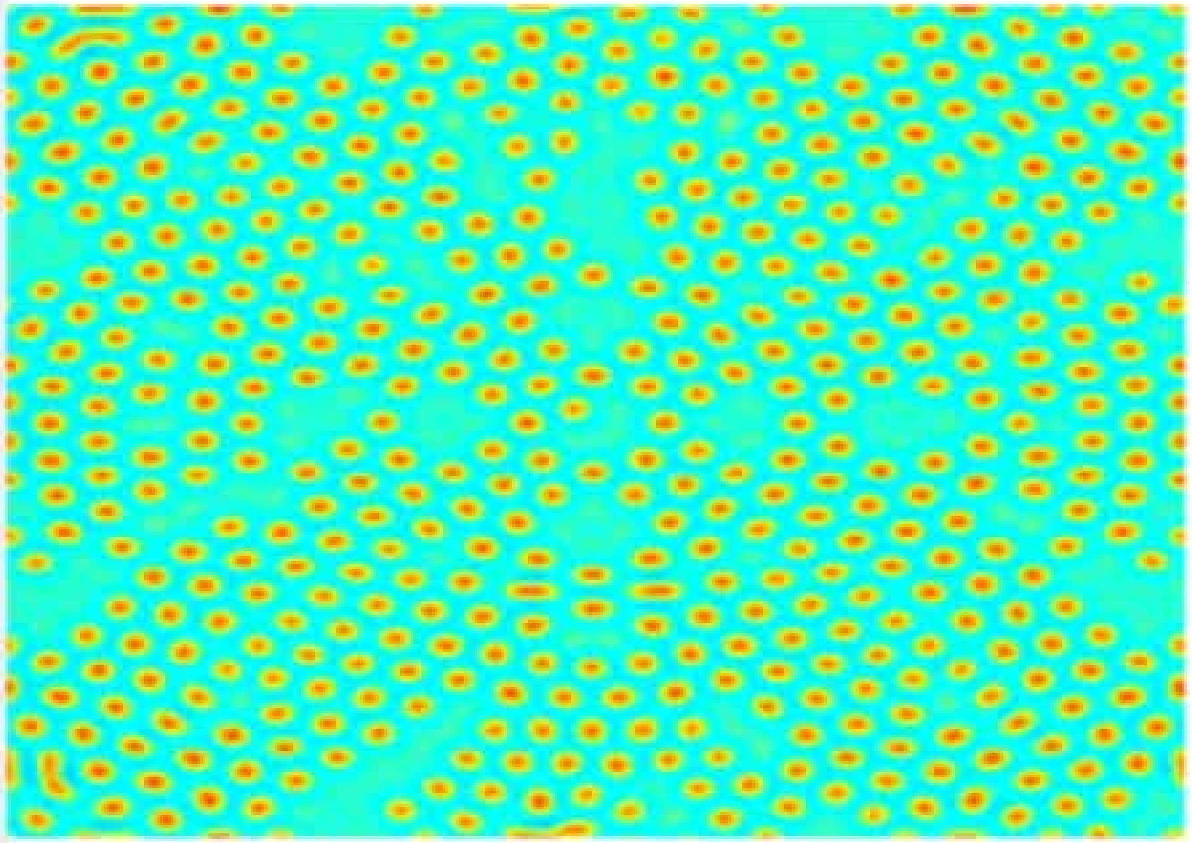
$$\begin{pmatrix} \dfrac{\partial u(\mathbf{x},t)}{\partial t} \\ \dfrac{\partial v(\mathbf{x},t)}{\partial t} \end{pmatrix} = \mathbf{M}(u,v) + \mathbf{F}(u,v) + \theta^{\frac{1}{2}}\mathbf{B}(u,v)\xi(\mathbf{x},t),$$

$$\mathbf{M}(u,v) = \begin{pmatrix} \mathrm{M}_u \ \Delta_{\mathbf{x}} \ u \\ \mathrm{M}_v \ \Delta_{\mathbf{x}} \ v \end{pmatrix}, \qquad \mathbf{F}(u,v) = \begin{pmatrix} -uv^2 + f(1-u) \\ uv^2 - (f+k)v \end{pmatrix}$$

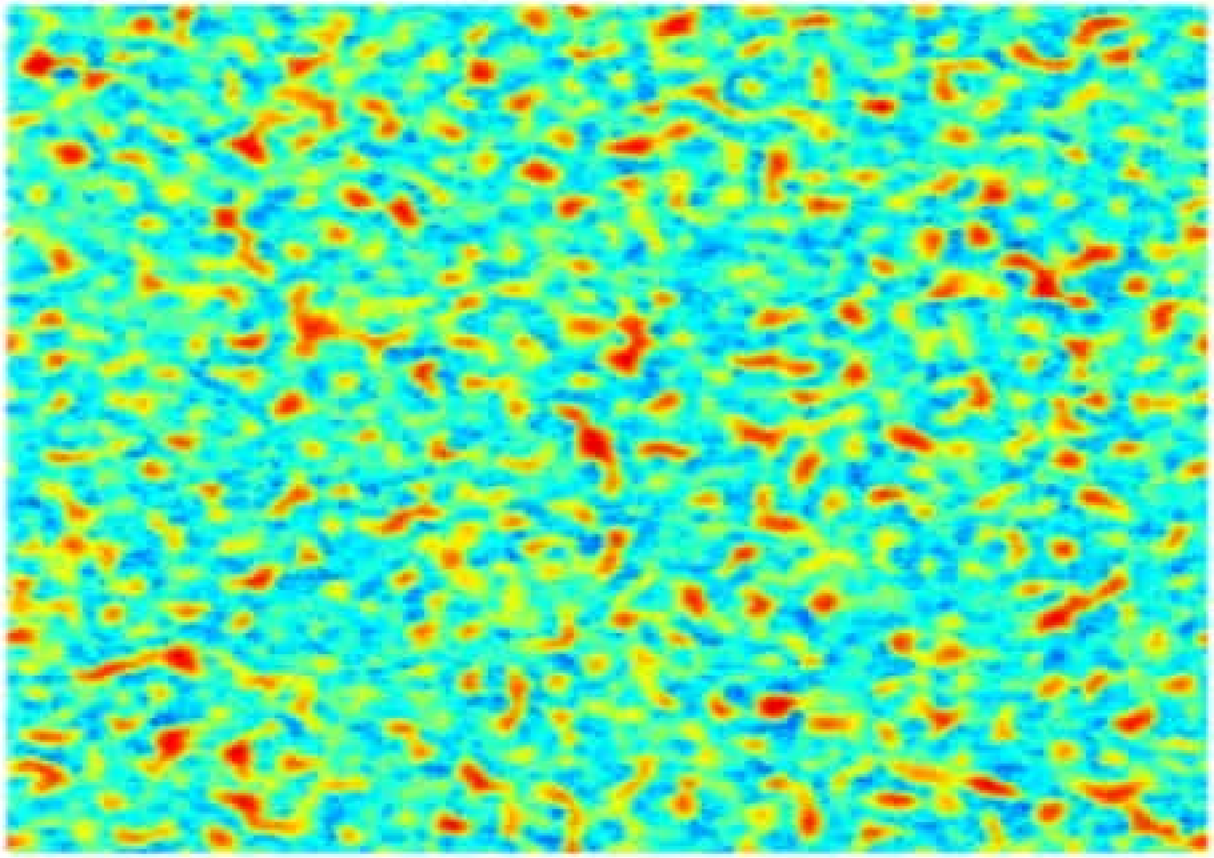
$$\mathbf{B}(u,v)\mathbf{B}(u,v)^T = \mathbf{D}(u,v) = \begin{pmatrix} uv^2 & -uv^2 \\ -uv^2 & uv^2 + kv \end{pmatrix}$$

❖ Chemical Reaction Noise Induced Pattern Change

Noise can also change the patterns formed:



Without Noise



With Noise

❖ Noise Changes Long Term Dynamics: Shift of Fixed Point

For the system:

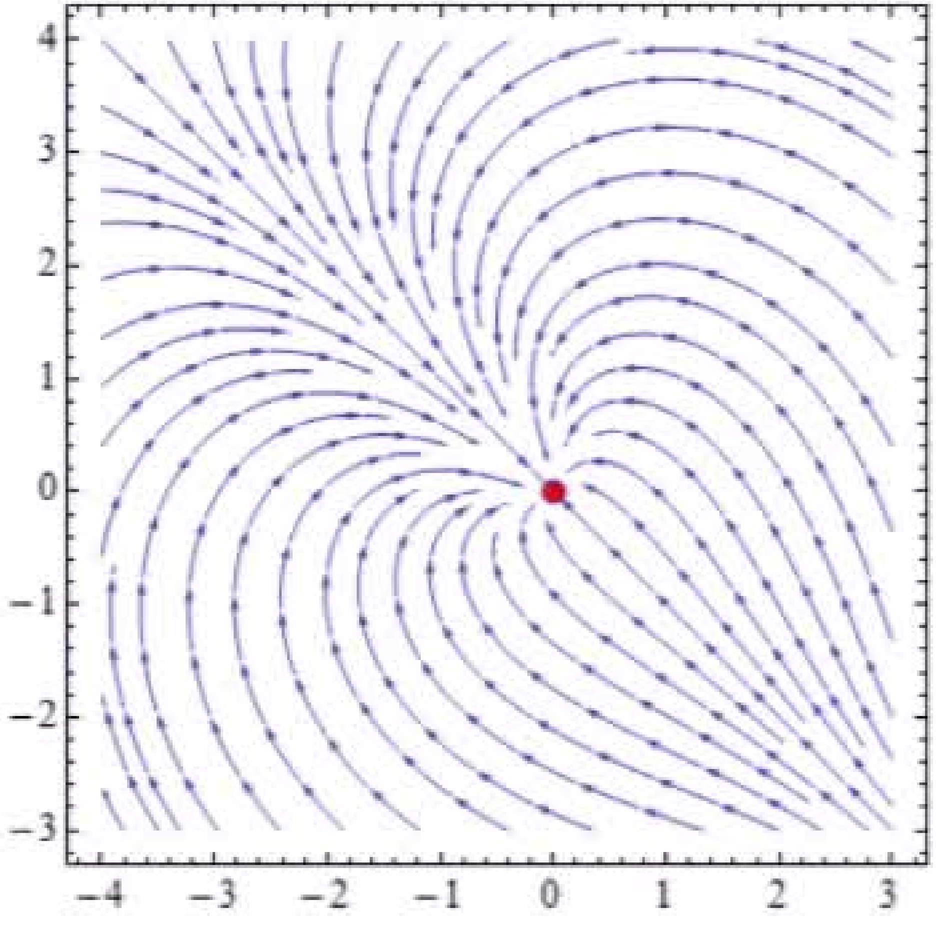
$$\mathrm{d}\mathbf{z} = \mathbf{f}(\mathbf{z}) + \mathrm{B}(\mathbf{z})\mathrm{d}\mathbf{W}(t)$$

where

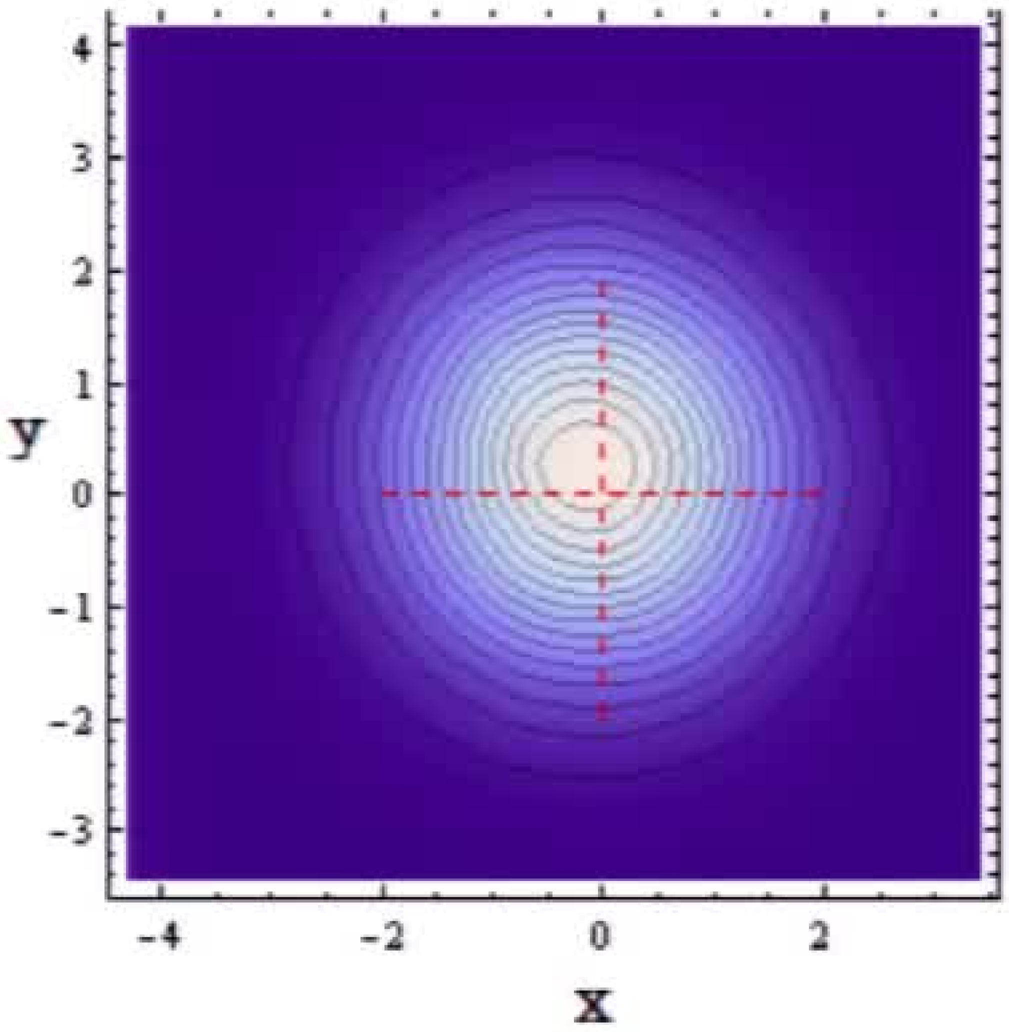
$$\mathbf{z} = \begin{pmatrix} x \\ y \end{pmatrix}; \quad \mathbf{f}(x,y) = \begin{pmatrix} -x - \dfrac{1}{4}(x+y)\,(2y-1) \\ -y + \dfrac{1}{4}(x+y)\,(2x+1) \end{pmatrix}; \quad \mathrm{B} = \mathrm{I}.$$

❖ Noise Changes Long Term Dynamics: Shift of Fixed Point

Fixed Point



Stationary Distribution

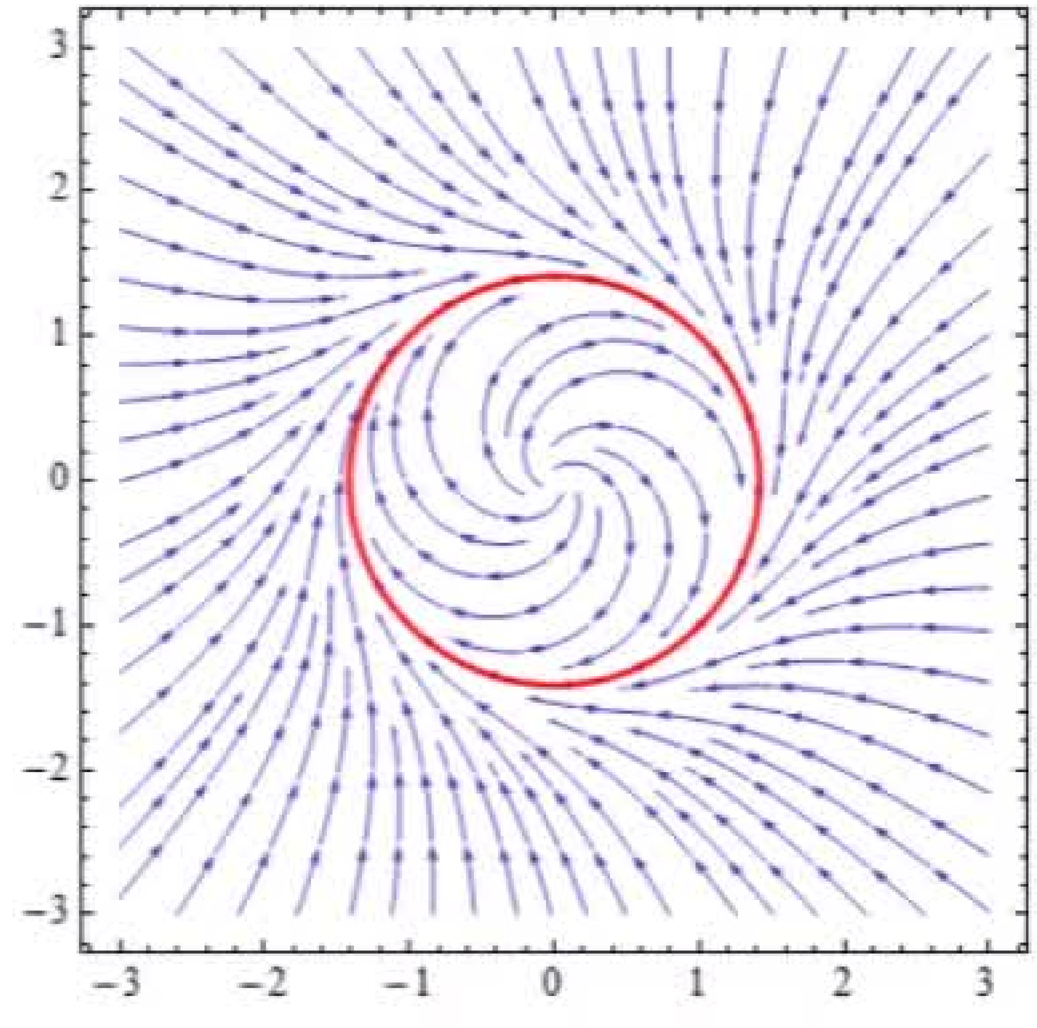


❖ Noise Changes Long Term Dynamics:

Change of Global Behavior

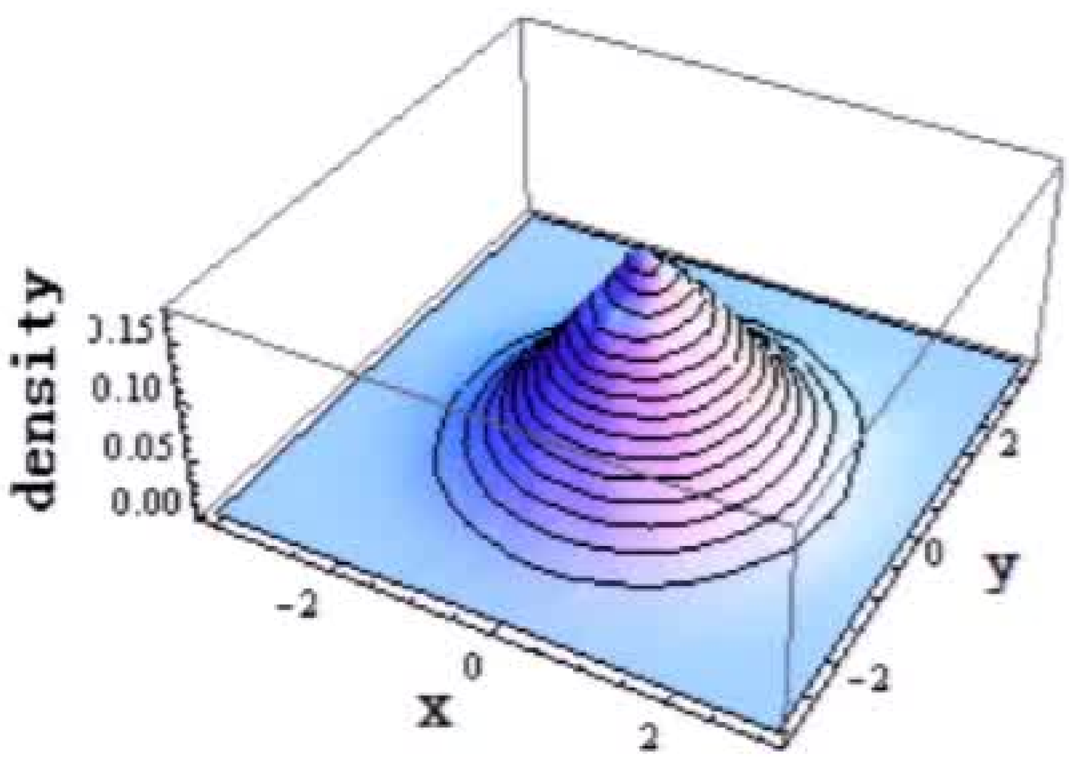
$$\mathbf{f}(x,y) = \begin{pmatrix} -\frac{1}{2}(x^2+y^2)x + x + y \\ -\frac{1}{2}(x^2+y^2)y + y - x \end{pmatrix}; \quad \mathrm{B} = \sqrt{x^2+y^2}\,\mathbf{I}.$$

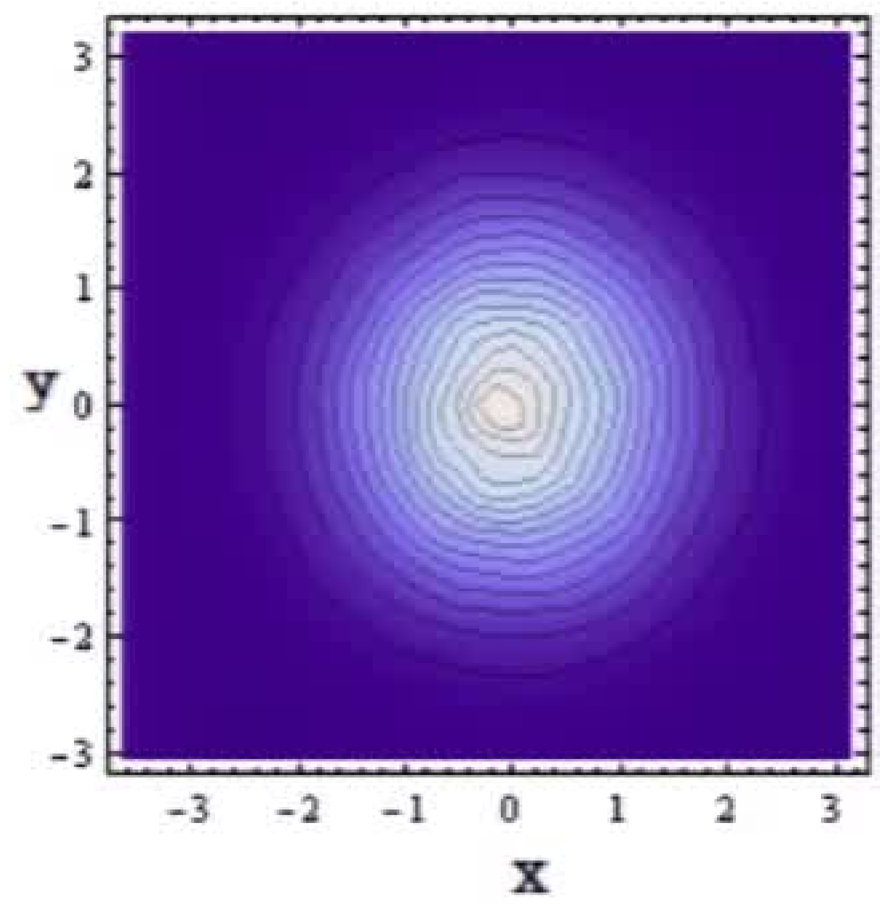
Limit Cycle Behavior



❖ Noise Changes Long Term Dynamics:
Change of Global Behavior

Stationary Distribution:
Same as Stable Fixed Point System





❖ Most Probable Path in Small Noise Limit

Consider general stochastic differential equation (SDE):

$$\mathrm{d}\mathbf{Z} = \mathbf{f}(\mathbf{Z}) + \sqrt{2\theta\mathbf{D}(\mathbf{Z})}\mathrm{d}\mathbf{W}(t)$$

Under Ito's interpretation, Fokker-Planck equation:

$$\partial_t p(\mathbf{z}, t) = \theta \sum_{i,j} \frac{\partial^2}{\partial \mathbf{z}_i \partial \mathbf{z}_j}\Big(\mathbf{D}_{ij}(\mathbf{z}) p(\mathbf{z}, t)\Big) - \sum_i \frac{\partial}{\partial \mathbf{z}_i}\Big(\mathbf{f}_i(\mathbf{z}) p(\mathbf{z}, t)\Big)$$

❖ Large Deviation Theory

For small θ, Freidlin-Wentzell theory leads to behaviors of the *most probable path*:

$$p(\mathbf{z},t) = e^{-\frac{\phi(\mathbf{z},t)}{\theta} - \psi(\mathbf{z},t) + \mathcal{O}(\theta)}$$

Implies the Hamilton-Jacobi equation:

$$\frac{\partial \phi(\mathbf{z},t)}{\partial t} = -\left(\mathbf{D}(\mathbf{z})\nabla\phi(\mathbf{z},t) + \mathbf{f}(\mathbf{z})\right)^T \nabla\phi(\mathbf{z},t)$$

In stationary:

$$0 = -\left(\mathbf{D}(\mathbf{z})\nabla\phi^s(\mathbf{z}) + \mathbf{f}(\mathbf{z})\right)^T \nabla\phi^s(\mathbf{z})$$

❖ Effective Dynamics under Large Noise

Theorem 2 **(Ma, Chen, Fox, 2015)**

Suppose SDE (**) has a unique stationary dist. $p^s(\mathbf{z}) \propto \exp(-\varphi(\mathbf{z}))$, then there exists a skew-symmetric $\mathbf{Q}(\mathbf{z}) \in W^{1,1}(p^s)$ such that

$$\mathbf{f}(\mathbf{z}) = -\left[\mathbf{D}(\mathbf{z}) + \mathbf{Q}(\mathbf{z})\right] \nabla\varphi(\mathbf{z}) + \Gamma(\mathbf{z}) \qquad \Gamma_i(\mathbf{z}) = \sum_{j=1}^{d} \frac{\partial}{\partial \mathbf{z}_j}(\mathbf{D}_{ij}(\mathbf{z}) + \mathbf{Q}_{ij}(\mathbf{z}))$$

assuming $\mathbf{f}_i(\mathbf{z})p^s(\mathbf{z}) - \sum_{j=1}^{d} \frac{\partial}{\partial \theta_j}\Big(\mathbf{D}_{ij}(\mathbf{z})p^s(\mathbf{z})\Big) \in L^1(\mathbb{R}^d)$.

Generic SDE: $\mathrm{d}\mathbf{Z} = \mathbf{f}(\mathbf{Z}) + \sqrt{2\mathbf{D}(\mathbf{Z})}\mathrm{d}\mathbf{W}(t)$ (**)

❖ Effective Dynamics under Large Noise

Decomposition along $p^s(\mathbf{z}) \propto \exp(-\varphi(\mathbf{z}))$:

$\varphi(\mathbf{z})$: Lyapunov function

Fluctuation

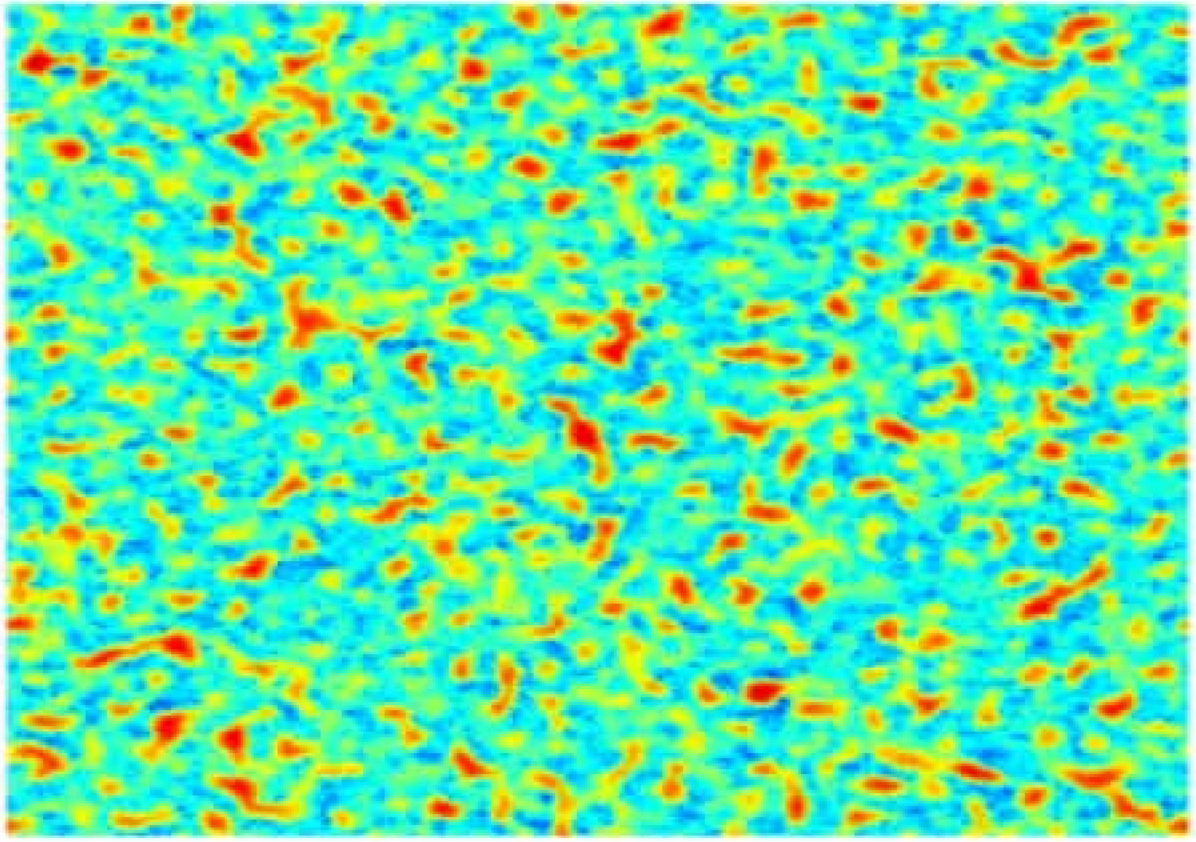
$$\mathrm{d}\mathbf{Z} = \underbrace{-(\mathbf{D}(\mathbf{Z}) + \mathbf{Q}(\mathbf{Z}))\nabla\varphi(\mathbf{Z})\mathrm{d}t}_{\text{Effective Dynamics}} + \boxed{\Gamma(\mathbf{Z})\mathrm{d}t + \sqrt{2\mathbf{D}(\mathbf{Z})}\mathrm{d}\mathbf{W}(t)}$$

Effective Dynamics

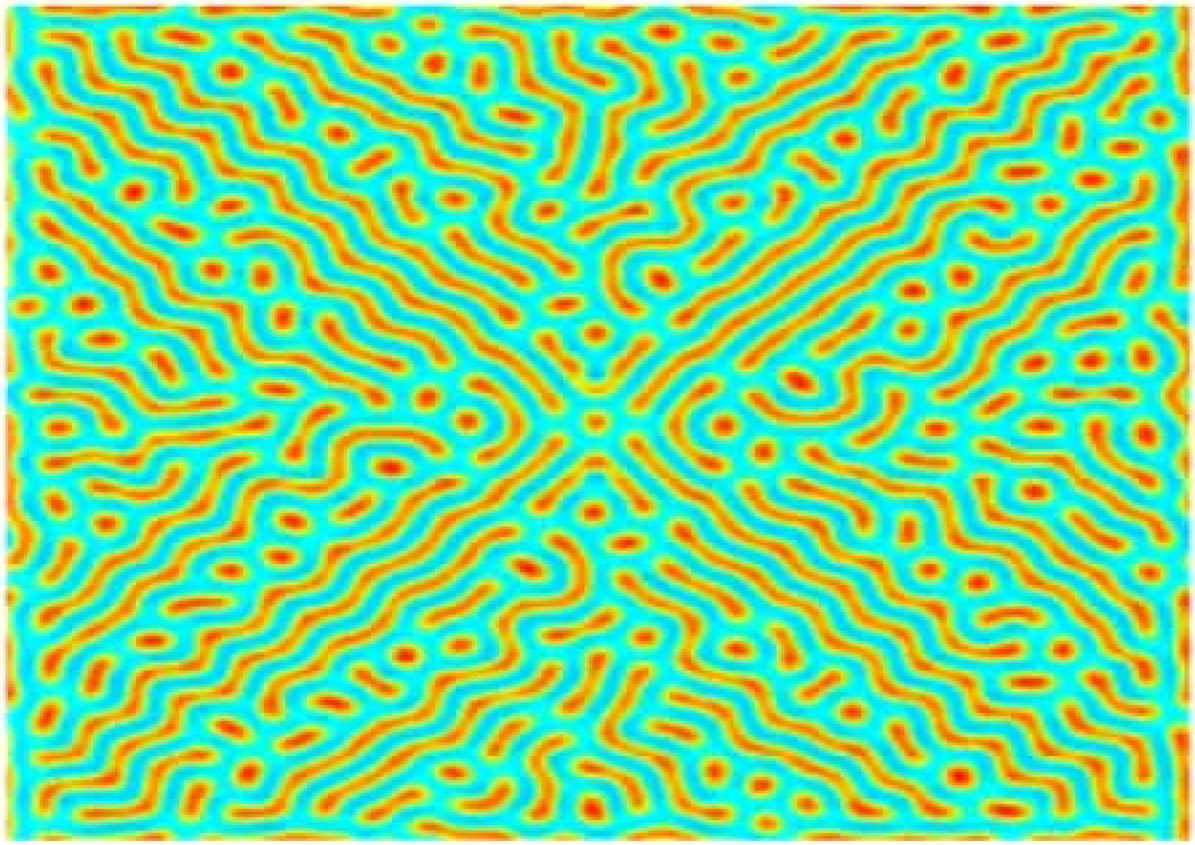
Difference w/o noise: $\Gamma_i(\mathbf{z}) = \sum_{j=1}^{d} \frac{\partial}{\partial \mathbf{z}_j}(\mathbf{D}_{ij}(\mathbf{z}) + \mathbf{Q}_{ij}(\mathbf{z}))$

❖ Effective Dynamics for Behavioral Analysis

Noisy Dynamics



Effective Dynamics



Turing Unstable

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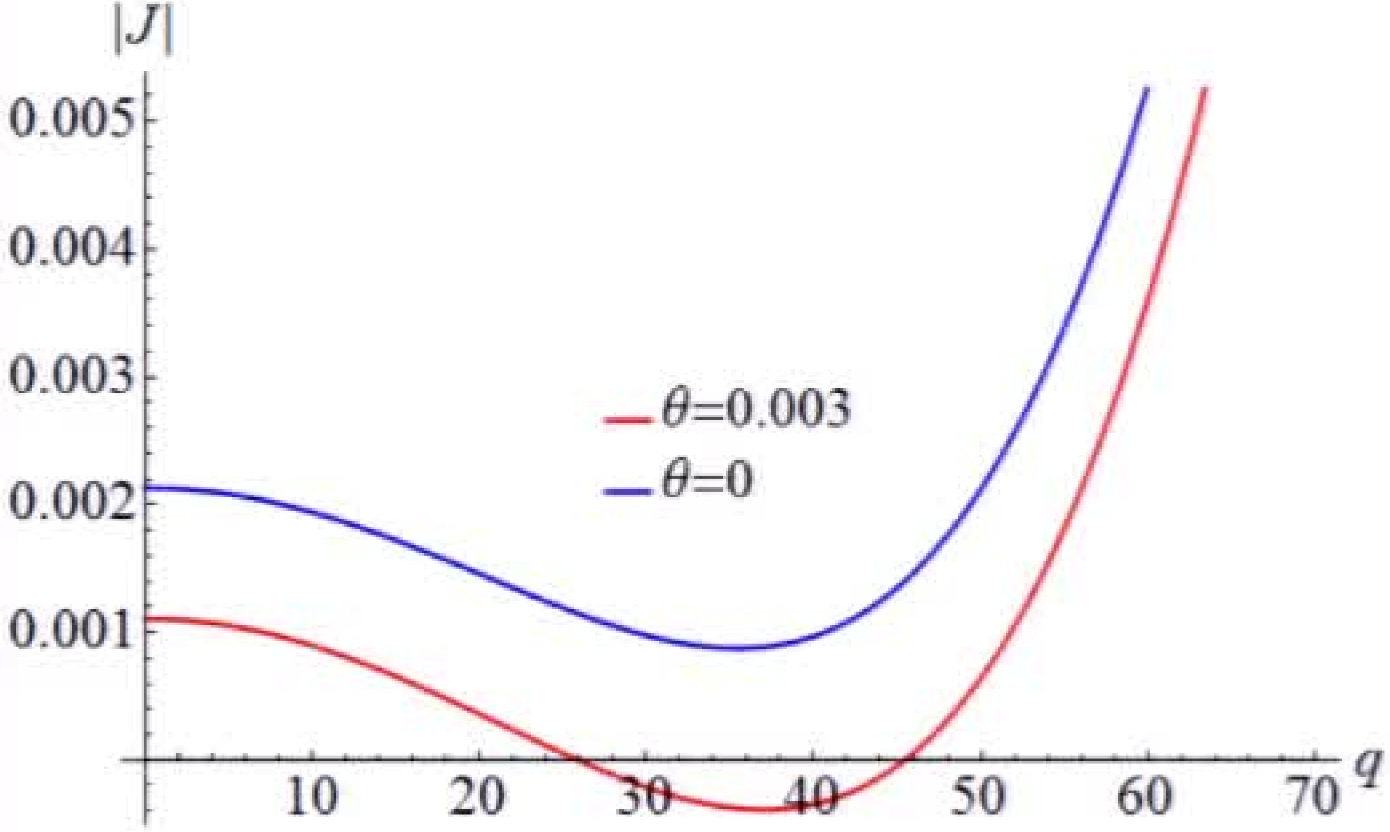

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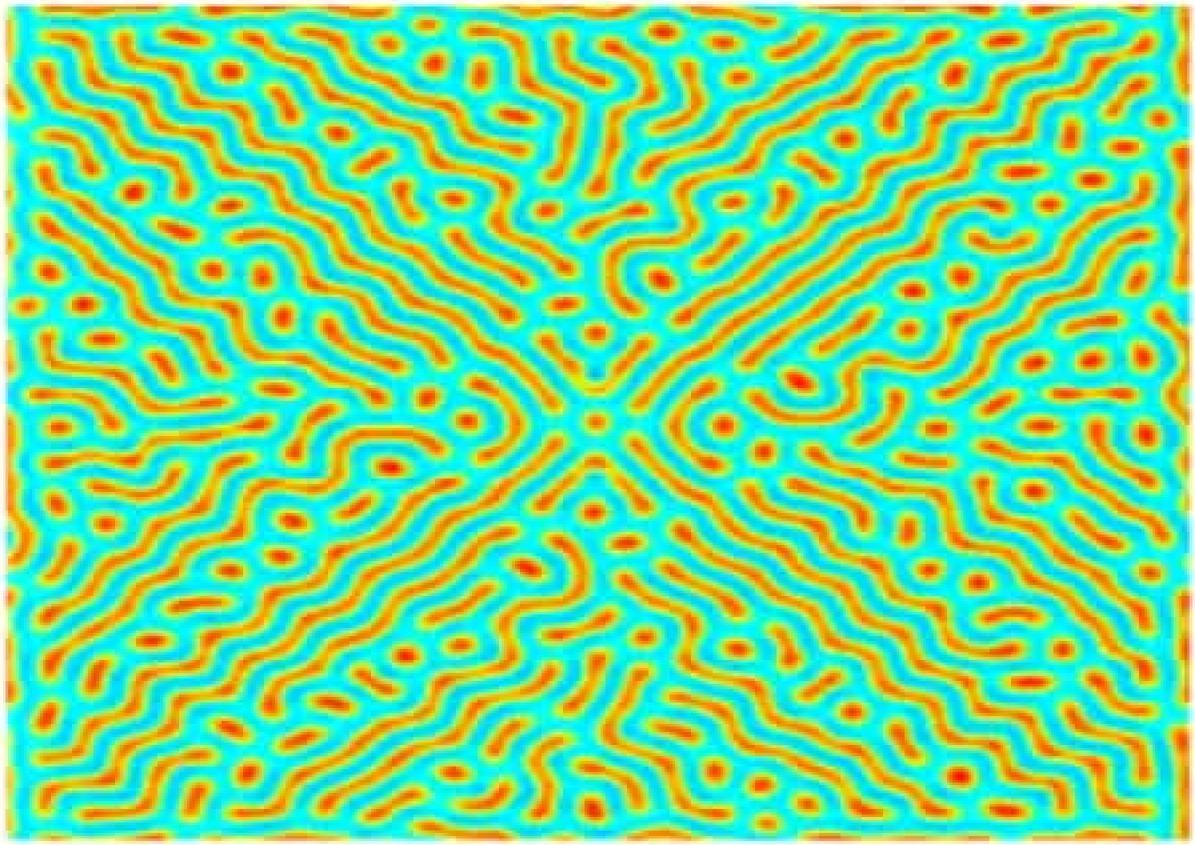
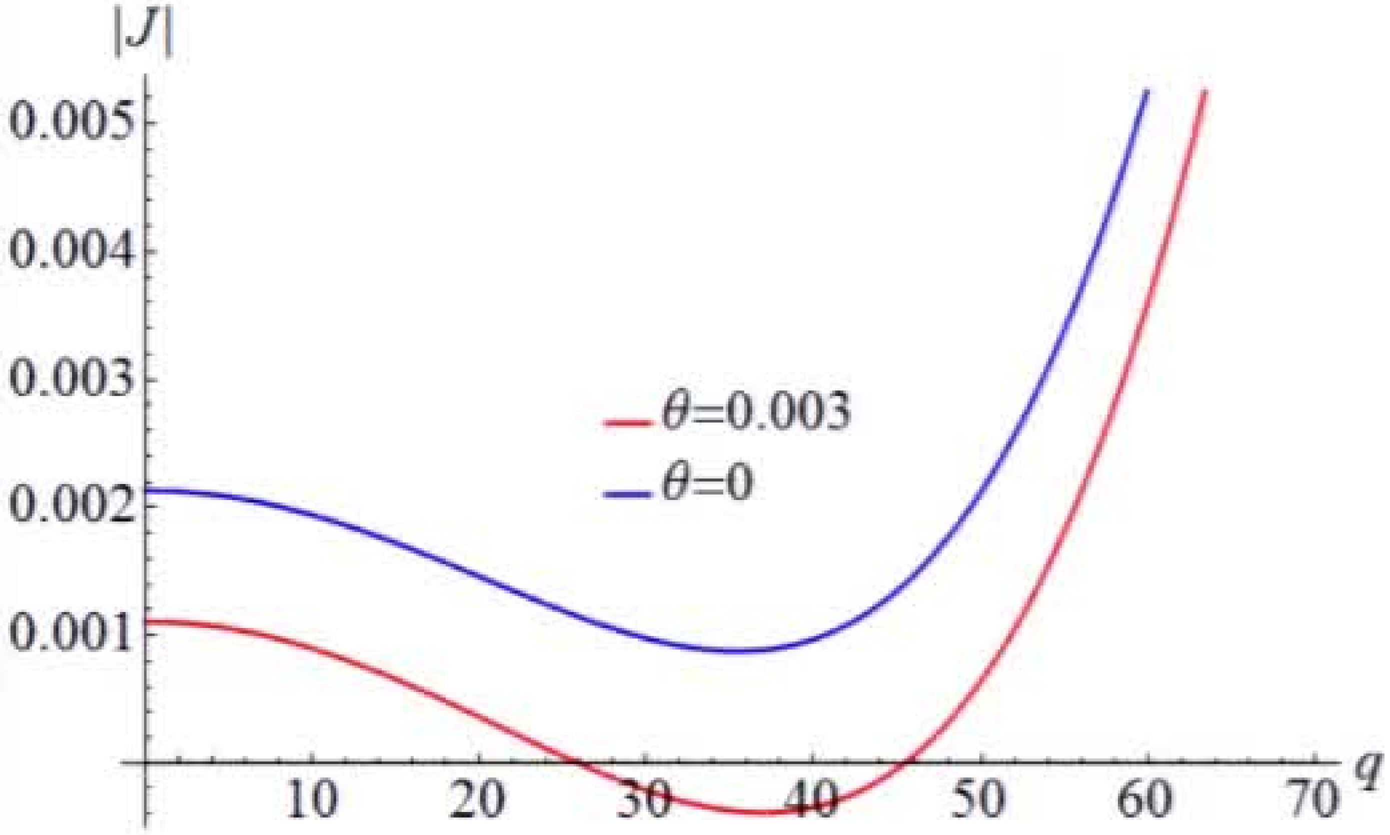


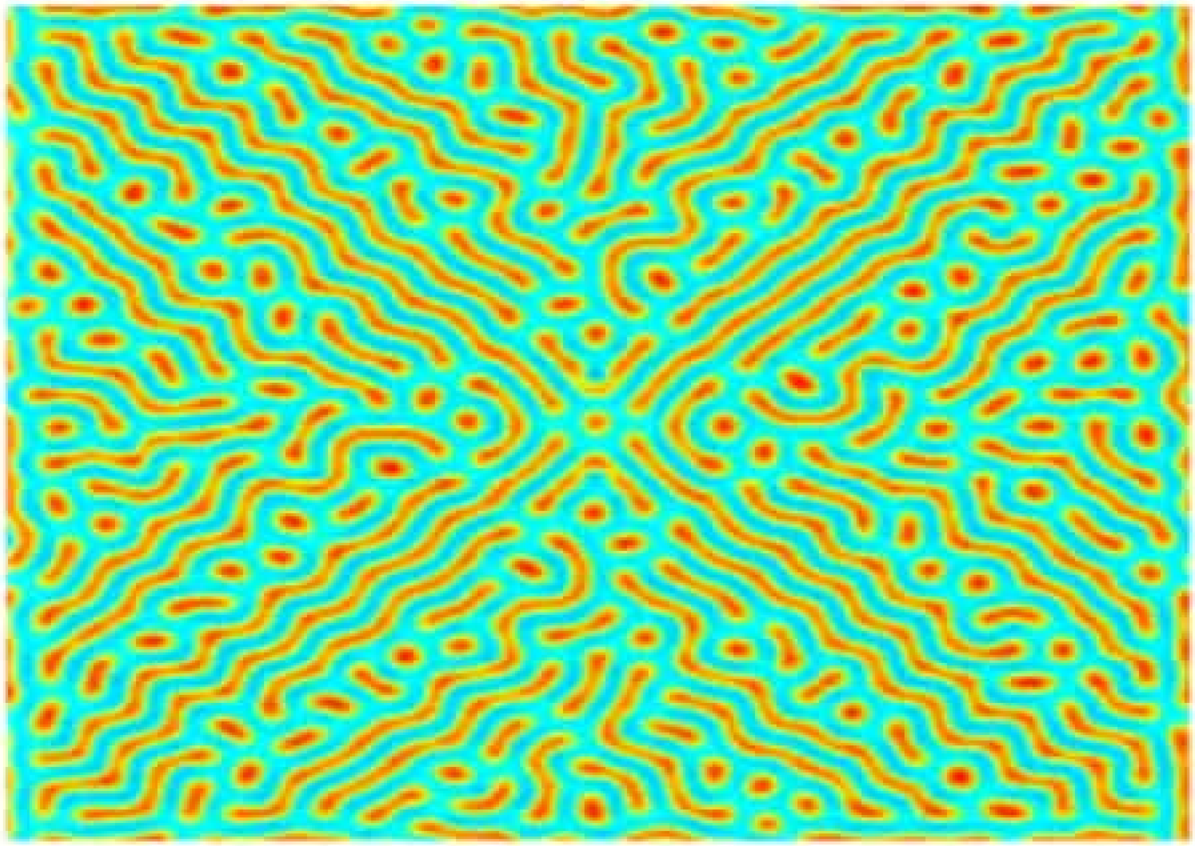
Instability after plane wave perturbation

❖ Effective Dynamics for Behavioral Analysis

Turing Unstable



Effective Dynamics



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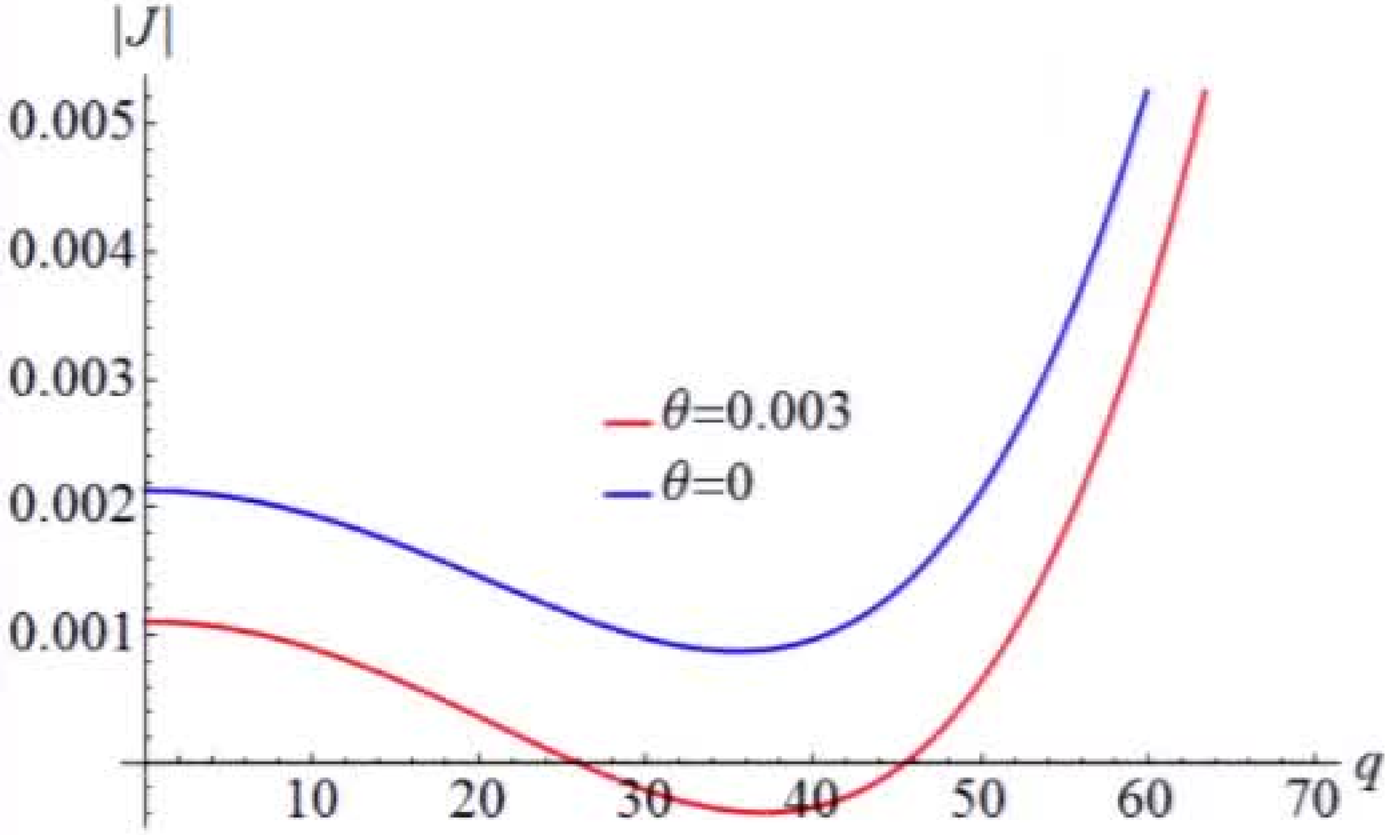

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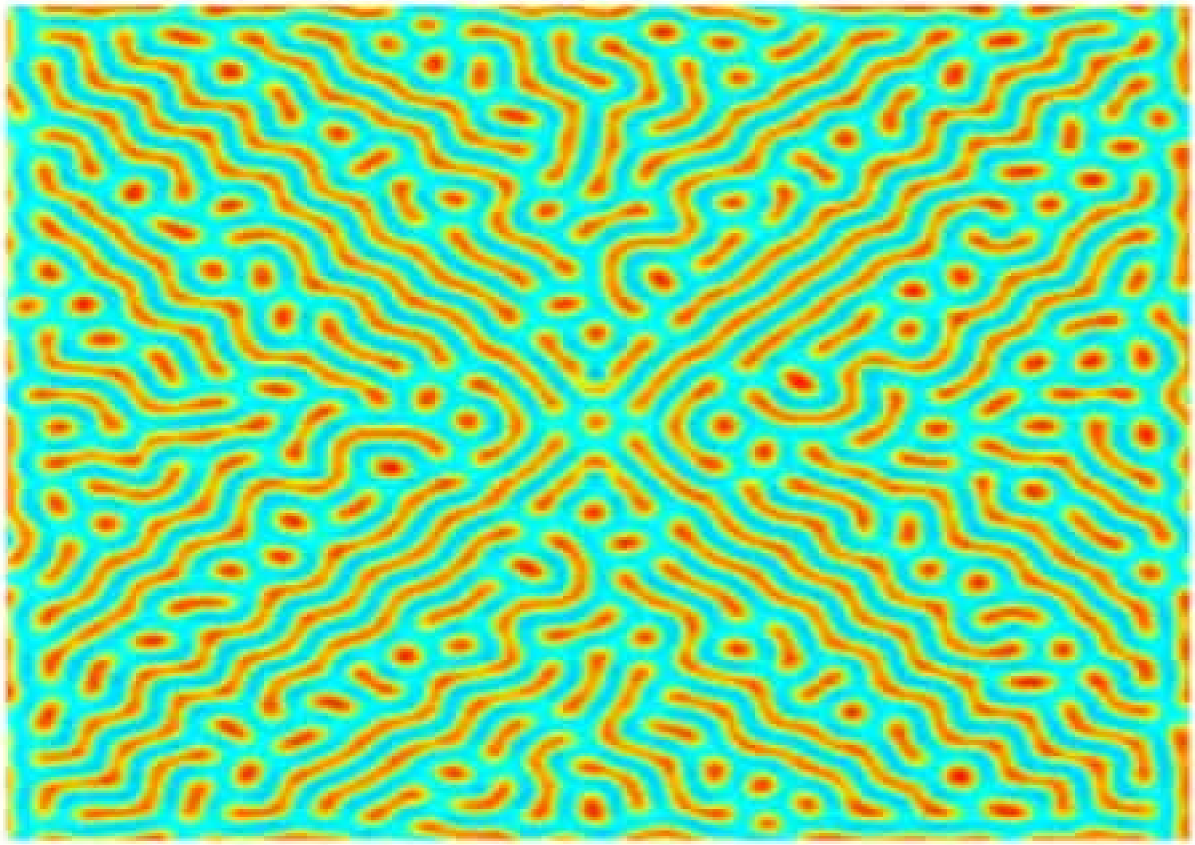

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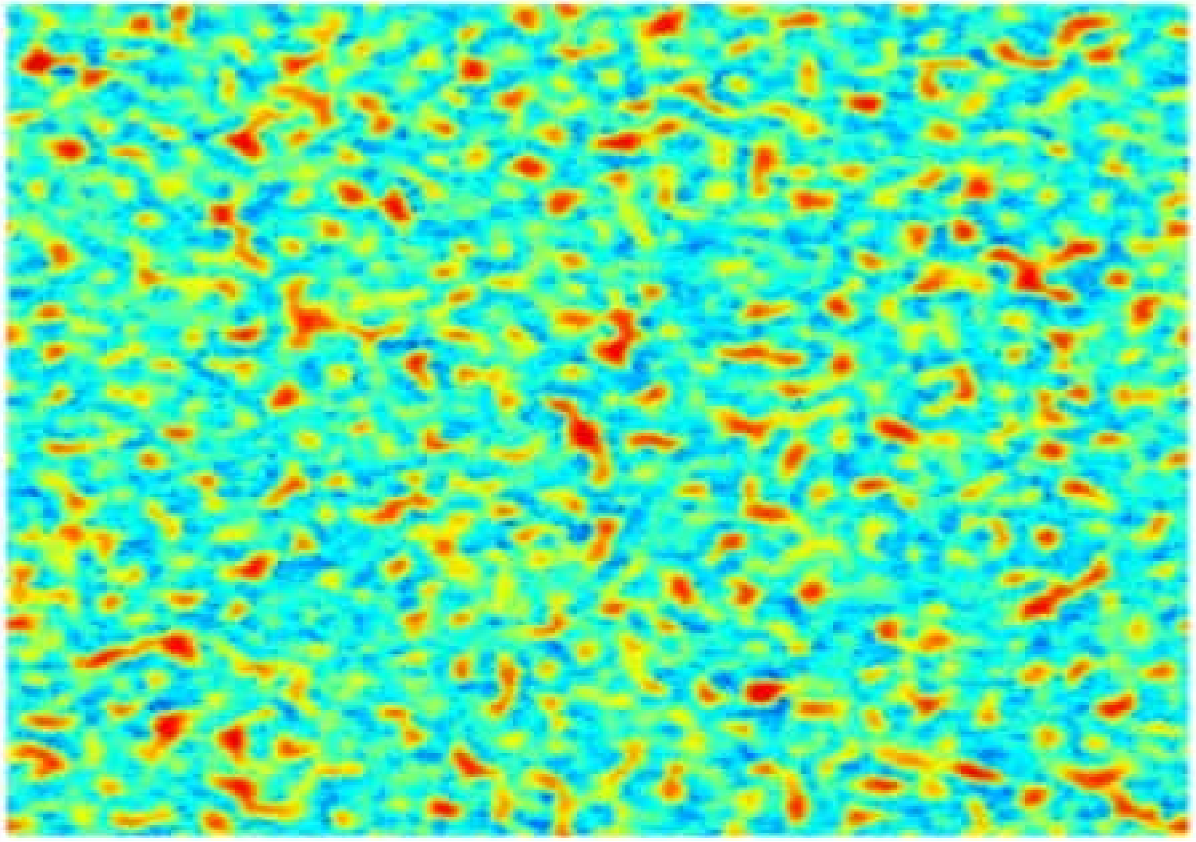
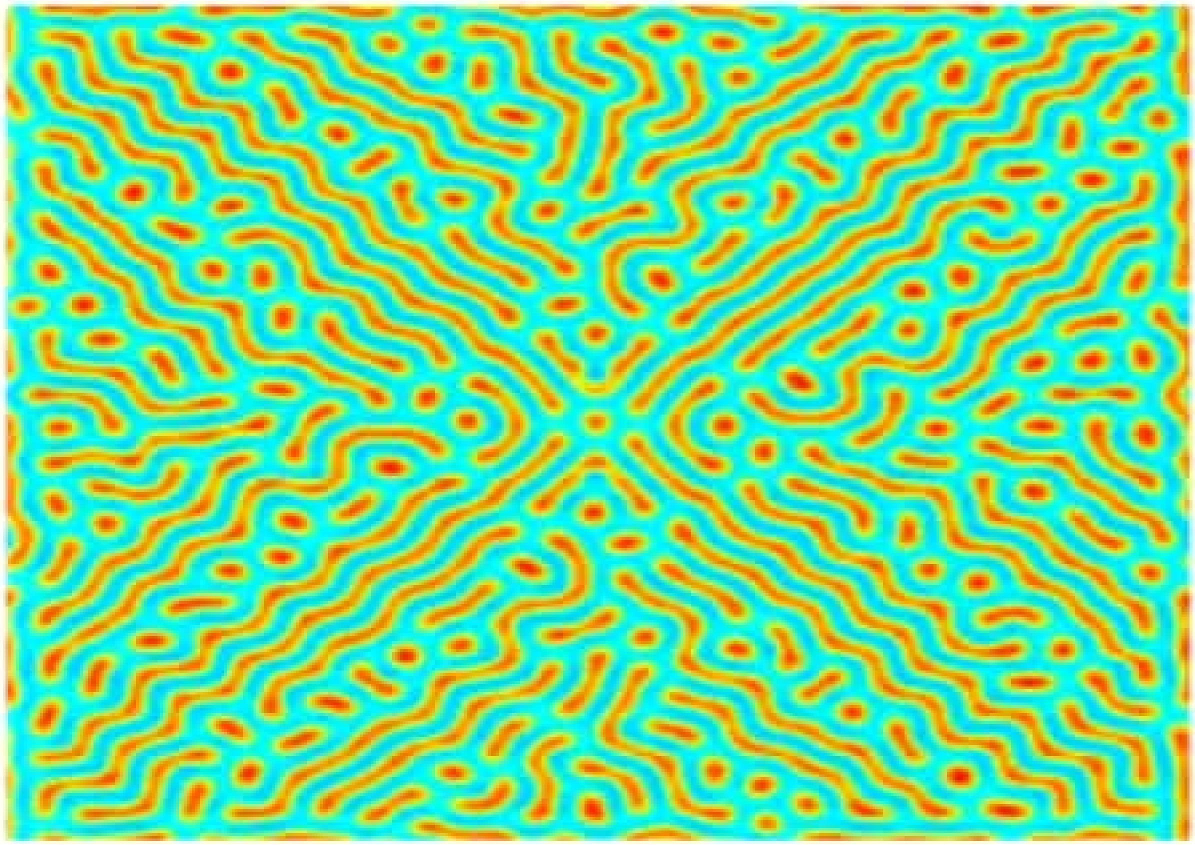
Noisy Dynamics



Effective Dynamics



Turing Unstable

❖ Dynamics of the Most Probable Path

Implies a decomposition of $\mathbf{f}(\mathbf{z})$:

$$\mathbf{f}(\mathbf{z}) = -\left(\mathbf{D}(\mathbf{z}) + \mathbf{Q}(\mathbf{z})\right) \nabla \phi^s(\mathbf{z})$$

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Change of Global Behavior

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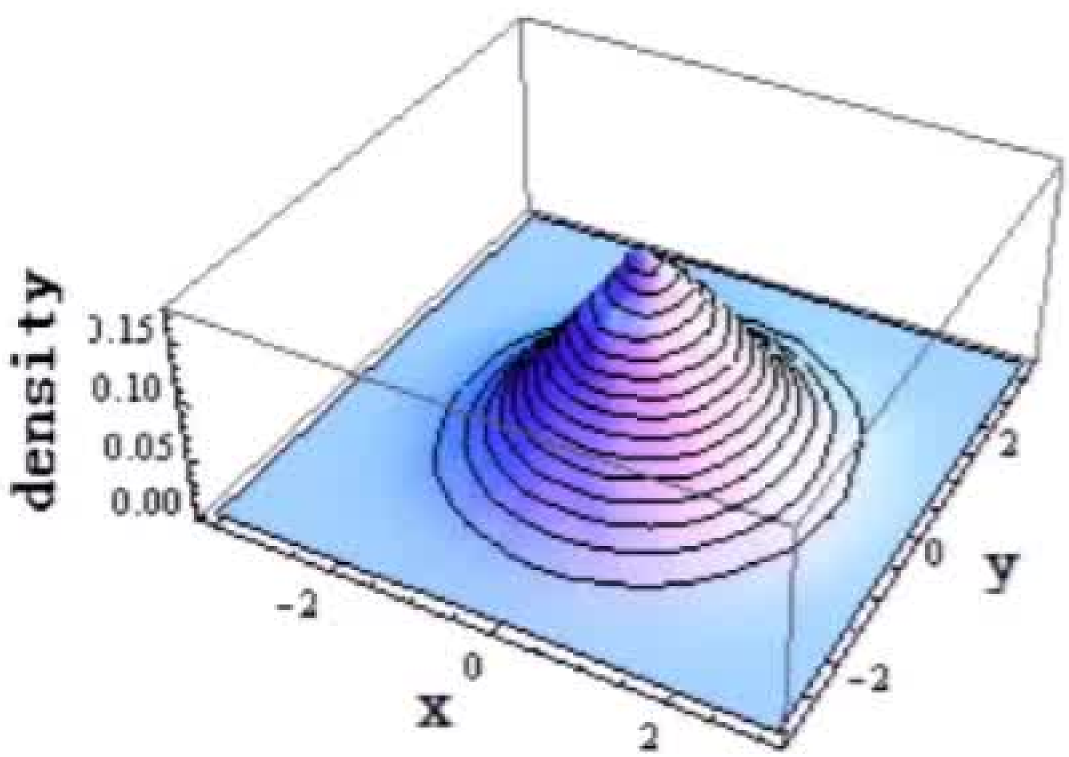

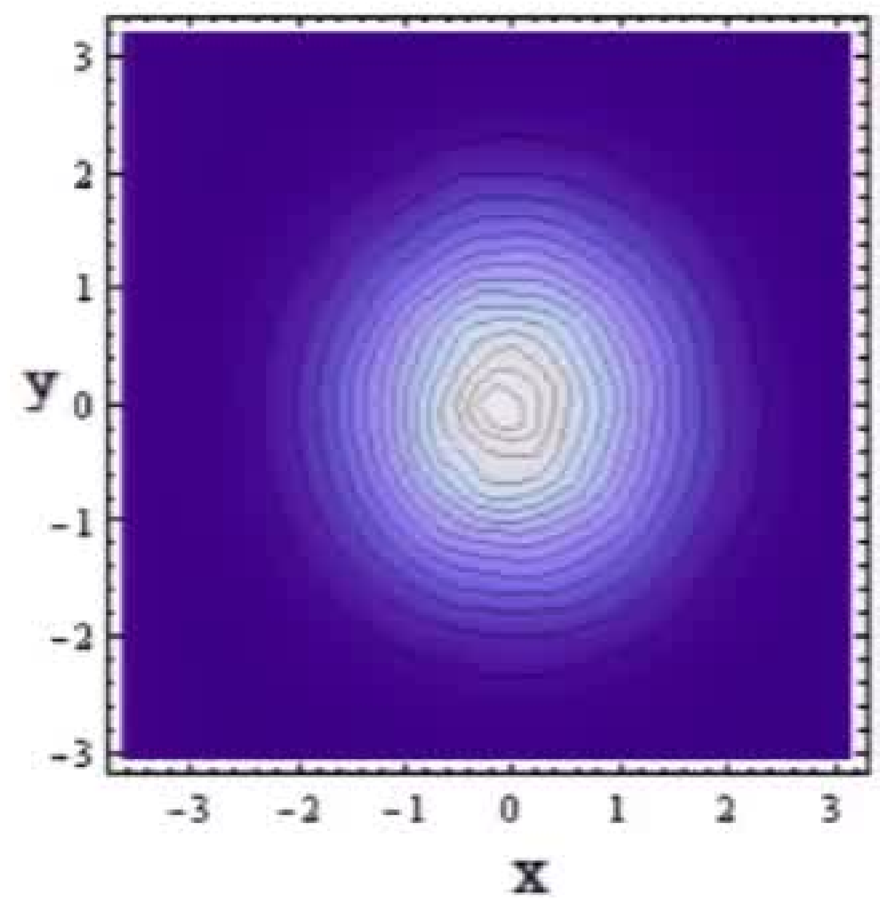

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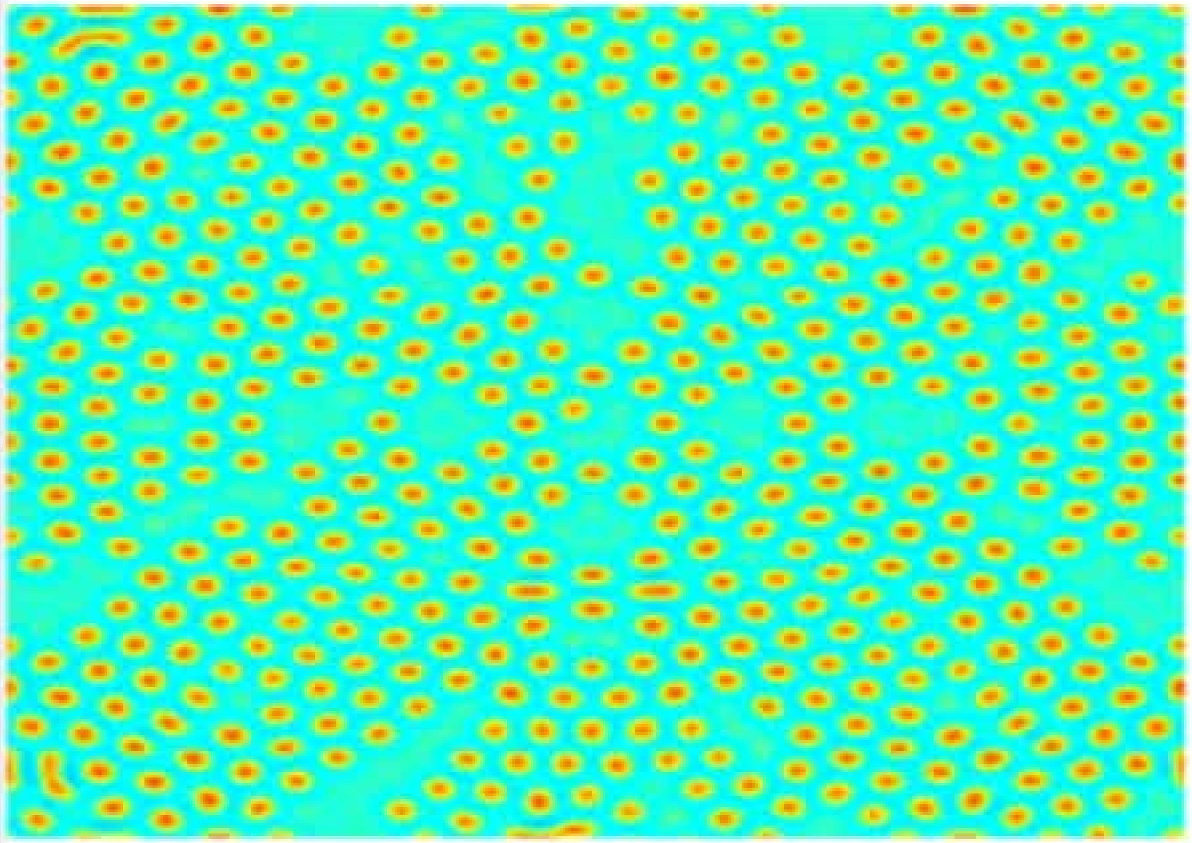
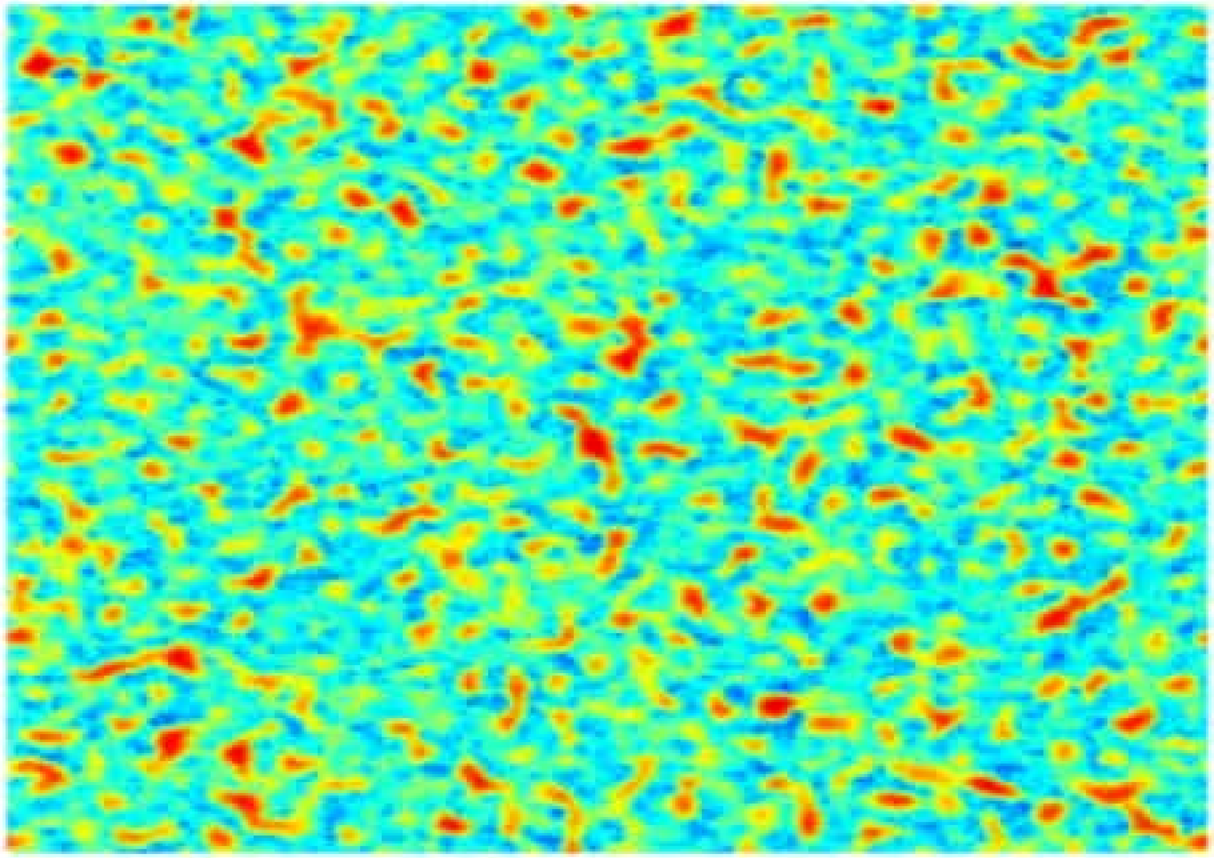


Without Noise



With Noise

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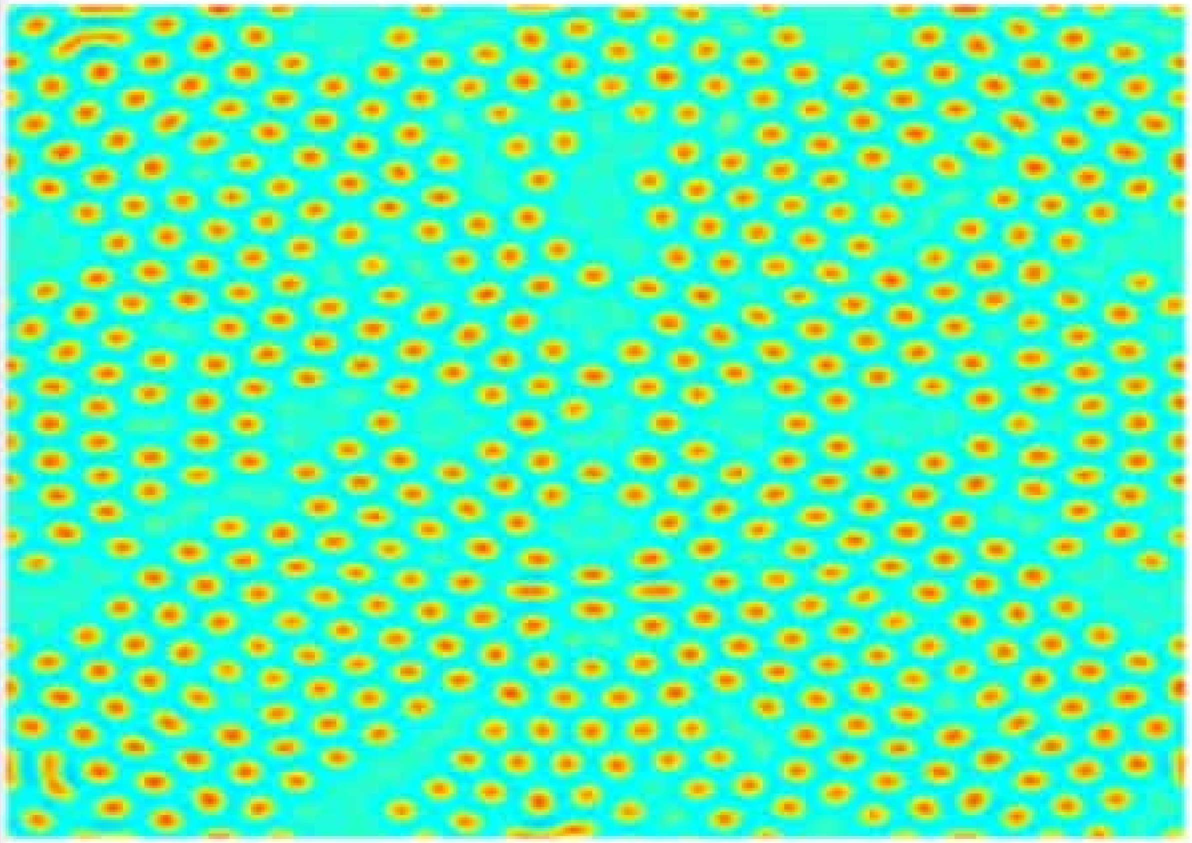
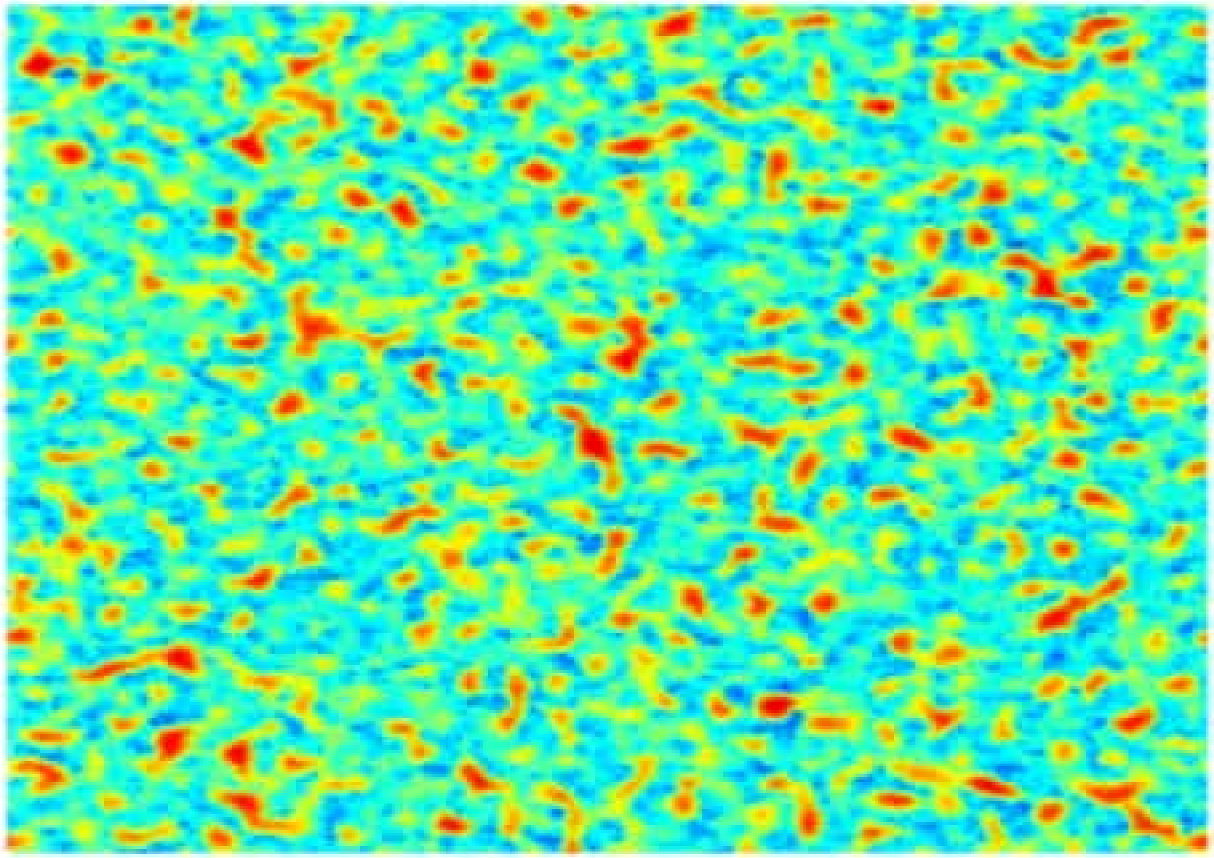


Without Noise



With Noise

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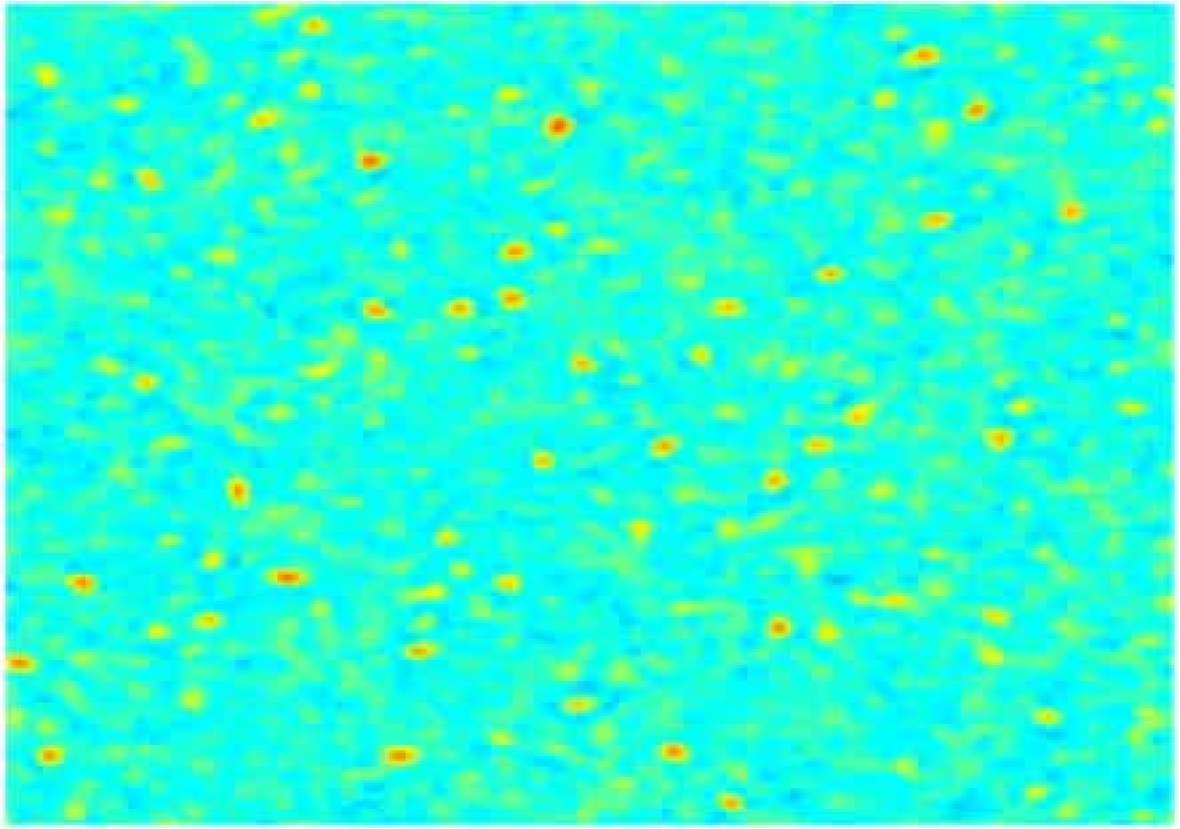
$$\mathrm{d}\mathbf{Z} = \underline{-\big(\mathbf{D}(\mathbf{Z}) + \mathbf{Q}(\mathbf{Z})\big)\nabla\varphi(\mathbf{Z})\mathrm{d}t} + \Gamma(\mathbf{Z})\mathrm{d}t + \sqrt{2\mathbf{D}(\mathbf{Z})}\mathrm{d}\mathbf{W}(t)$$

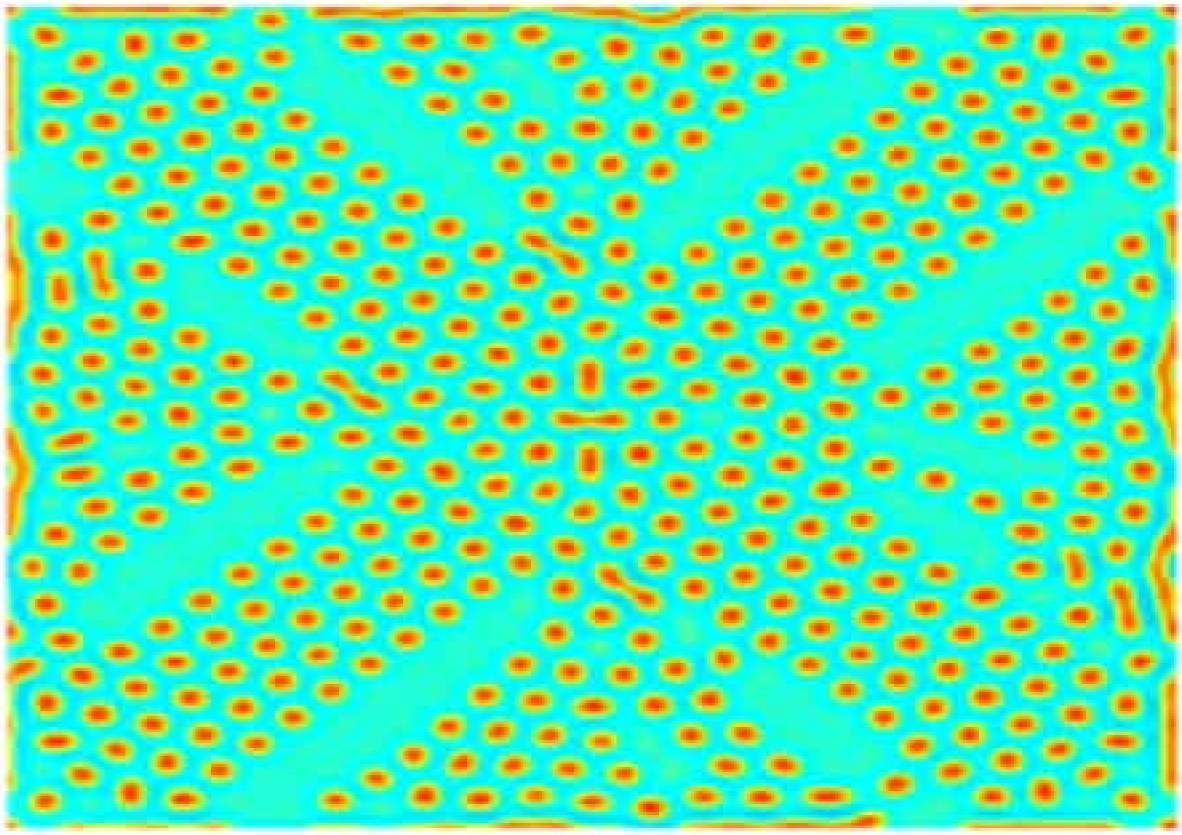
Effective Dynamics

❖ Effective Dynamics for Behavioral Analysis

Noisy Dynamics



Effective Dynamics



Nonlinear Instability