Case Study of a Reaction-Diffusion System: Brusselator Dynamics

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Outline

1. Introduction
2. Linear Stability Analysis
   - Eigenvalue problem
   - Soft and hard modes of instability
   - Characterizing the parameter space
3. Experiments
   - Method
   - Results: when inhibitor diffuse faster ($d > 1$)
   - Results: when activator diffuse faster ($d < 1$)

Nonlinear Chemical Dynamics and Belousov-Zhabotinski Reaction

Brusselator

Brusselator models the dynamics of the concentration of two chemicals in an autocatalytic reaction.

$$\frac{d}{dt}u = a - (b+1)u + u^2 v$$
$$\frac{d}{dt}v = bu - u^2 v$$

Prigogine, R. Lefever (1968) "Symmetry Breaking Instabilities in Dissipative Systems II", J. Chem. Phys. 48, 1695-1700.

Brusselator reaction-diffusion

When diffusion is added into the picture, Brusselator system captures some characteristics (qualitatively) of Belousov-Zhabotinski Reaction.

$$u_t = \gamma[a - (b+1)u + u^2 v] + u_{xx}$$
$$v_t = \gamma[bu - u^2 v] + dv_{xx}$$

u: concentration of the activator

v: concentration of the inhibitor

γ: reaction-to-diffusion ratio

d: inhibitor-to-activator ratio

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Equilibrium

$$\frac{d}{dt}u = a - (b+1)u + u^2 v$$
$$\frac{d}{dt}v = bu - u^2 v$$

The equilibrium point of the original ODE system is $(u^*, v^*) = (a, \frac{b}{a})$.

We can linearize the system near this point $(\xi, \eta) = (u - u^*, v - v^*)$

$$\begin{pmatrix} \frac{d}{dt}\xi \\ \frac{d}{dt}\eta \end{pmatrix} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

Linearized system with diffusion

When diffusion is taken into account, we have

$$\begin{pmatrix} \frac{d}{dt}\xi \\ \frac{d}{dt}\eta \end{pmatrix} = \gamma \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} \frac{d^2}{dx^2}\xi \\ \frac{d^2}{dx^2}\eta \end{pmatrix}$$

Assume the solution takes the form of $\sum c_k e^{\lambda_k t} e^{ikx}$. e^{ikx} are time-invariant spatial modes of spatial frequency k.

Considering each mode individually, we have

$$\lambda_k \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix} = \gamma \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix} \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix} - k^2 \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix}$$

(k is subscript not partial)

Jacobian

Eventually we have our linearized reaction-diffusion system

$$\lambda_k \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix} = \begin{pmatrix} \gamma(b-1)-k^2 & \gamma a^2 \\ -\gamma b & -\gamma a^2 - dk^2 \end{pmatrix} \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix}$$

λ_k is the eigenvalue of the Jacobian matrix

$$\mathbf{J} = \begin{pmatrix} \gamma(b-1)-k^2 & \gamma a^2 \\ -\gamma b & -\gamma a^2 - dk^2 \end{pmatrix}$$

The system is stable near equilibrium point if $\lambda_k < 0$ or $\Re\lambda_k < 0$, unstable if $\lambda_k > 0$ or $\Re\lambda_k > 0$.

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Terms are borrowed from Hermann Haken in "Synergetics. An Introduction. Nonequilibrium Phase Trasitions and Self-organization in Physics, Chemistry, and Biology."(Berlin, 1977).

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What will happen?
First, we need to do the parameter treasure hunt...

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The eigenvalues

The eigenvalues of

$$\mathbf{J} = \begin{pmatrix} \gamma(b-1)-k^2 & \gamma a^2 \\ -\gamma b & -\gamma a^2 - dk^2 \end{pmatrix}$$

are

$$\lambda_{k1,2} = \frac{1}{2}\{\mathcal{tr} \pm \sqrt{\mathcal{tr}^2 - 4\mathcal{D}et}\}$$

with

$$\mathcal{tr} = \gamma(b-1-a^2)-(1+d)k^2,$$
$$\mathcal{D}et = d(k^2)^2 + \gamma(a^2-bd+d)k^2 + \gamma^2 a^2$$

Let

$h(k^2) = tr^2 - 4\mathcal{D}et$

$= (1-d)^2(k^2)^2 - 2\gamma(1-d)(b-1+a^2)k^2 + \gamma^2[(b-1-a^2)^2 - 4a^2]$

Parameters that ensure hard-mode instability

. It is necessary that (1) for some k^2, tr is positive

$$\lambda_{k1,2} = \frac{1}{2}\{tr \pm \sqrt{h(k^2)}\}$$

$$tr = \gamma(b - 1 - a^2) - (1 + d)k^2 > 0$$

We need $b > a^2 + 1 > 1$

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We need $b > a^2 + 1 > 1$ and (2) for some k^2 that $h(k^2)$ is negative

$h(k^2) =$

$$(1-d)^2(k^2)^2 - 2\gamma(1-d)(b-1+a^2)k^2 + \gamma^2[(b-1-a^2)^2 - 4a^2] < 0$$

And the range of k^2's that satisfy (1) and (2) must overlap.

Closer look at h(k^2)

To have

$h(k^2) =$

$(1-d)^2(k^2)^2-2\gamma(1-d)(b-1+a^2)k^2+\gamma^2[(b-1-a^2)^2-4a^2] < 0$

$h(k^2)$ must cross horizontal axis.

The minimum of $h(k^2)$ is

$$h_{min} = h({k^2}_{h_{min}}) = -4\gamma^2 a^2 b < 0$$

at

$${k^2}_{h_{min}} = \frac{(b-1+a^2)\gamma}{1-d}$$

meaning $h(k^2)$ must have two roots, which is good news, but we also need to make sure the k^2's bounded by the two roots overlap with the region where tr is positive. That is when

$$k^2 \in [0, \frac{\gamma(b-1-a^2)}{1+d})$$

Closer look at h(k^2)

Let us look at the roots of $h(k^2) = 0$:

$$k^2{}_{h1,2} = \frac{\gamma}{1-d}(b - 1 + a^2 \pm 2a\sqrt{b})$$

When $d < 1$, $k^2{}_{h_{min}} > 0$. All we need is the smaller root to be less than the intersection between tr and horizontal axis. With $d < 1$, the smaller root is the one with minus sign; we need

$$\frac{\gamma}{1-d}(b - 1 + a^2 - 2a\sqrt{b}) < \frac{\gamma(b - 1 - a^2)}{1+d}$$

$$\Rightarrow (b - 1 - a\sqrt{b})d < a\sqrt{b} - a^2$$

This sets a more restrictive upper bound of d if $a < \sqrt{b} - 1/\sqrt{b}$.

Closer look at h(k^2)

$$h(k^2) = (1-d)^2(k^2)^2 - 2\gamma(1-d)(b-1+a^2)k^2 + \gamma^2[(b-1-a^2)^2 - 4a^2]$$

When $d > 1$, ${k^2}_{h_{min}} < 0$. We will be fine if $h(k^2 = 0) < 0$:

$$\gamma^2[(b-1-a^2)^2 - 4a^2] < 0$$

$$\Rightarrow b < (a+1)^2$$

Coexistence of soft-mode instability

Now we need to check when soft-mode instability also exists, i.e. λ needs to be real and positive for some k^2. It would be sufficient if we have $\mathscr{D}et < 0$. We notice that $\mathscr{D}et(k^2 = 0) = \gamma^2 a^2 > 0$. This means if the minimum of $\mathscr{D}et$ is to the left of $k^2 = 0$, $\mathscr{D}et(k^2)$ will always be greater than 0. We want the opposite – that is

$$a^2 - bd + d < 0 \tag{2}$$

At the same time, we want $\mathscr{D}et(k^2) = 0$ to have roots, which requires

$$\gamma^2(a^2 - bd + d)^2 - 4d\gamma^2 a^2 > 0 \quad \Rightarrow b > (\frac{a}{\sqrt{d}} + 1)^2$$

Coexistence of soft-mode instability

If for all k, $\mathscr{Det} > 0$, we can still have soft-mode instability if the range of k's corresponding to $\mathscr{tr} > 0$ does not entirely overlap with those corresponding to $h(k^2) < 0$. Particularly, we want a root of $h(k^2)$ to be bounded:

$$d < 1 \Rightarrow 0 < \frac{\gamma}{1-d}(b - 1 + a^2 - 2a\sqrt{b})$$

$$d > 1 \Rightarrow \frac{\gamma}{1-d}(b - 1 + a^2 - 2a\sqrt{b}) < \frac{\gamma(b-1-a^2)}{1+d}$$

In addition to the criteria that guarantees the existence of hard-mode instability.

Outline

Boundary conditions and intial conditions

Explored both 1-D (straight line) and 2-D domains (circular disk). For 1-D domain, used Dirichlet Boundary Conditions

$$u(0,t) = u(L,t) = a, \quad v(0,t) = v(L,t) = b/a$$

where $L = 30$ is the length of the 1-D domain.

For 2-D domain (radius 15), used Neumann Boundary Conditions

$$\nabla u = \nabla v = \mathbf{0}$$

(zero-flux)

Parameter choices

Fix $a = 2$, and consider two conditions

- $d < 1, \quad b > (a+1)^2$: here hard modes associate with smaller k^2 and soft modes associate with greater ones.
- $d > 1, \quad b < (a+1)^2$: here soft modes occupy the lower end of the k^2 spectrum.

Tuning γ for aesthetics.

Variational Formulation in 1D

Considering the dynamics of u, with f as the reaction term

$$u_t = \gamma f + u_{xx}$$

The variational formulation of the problem with respect to the space of test functions $\phi(x)$ (compactly supported):

$$\int_0^L u_t \phi dx = \gamma \int_0^L f \phi dx + \int_0^L u_{xx} \phi dx$$

$$\int_0^L u_{xx} \phi dx = u_x \phi|_0^L - \int_0^L u_x \phi' dx$$

If we use zero-flux boundary conditions $u_x(0) = u_x(L) = 0$, or ϕ vanishes at the boundary, $u_x \phi|_0^L = 0$. We have

$$\int_0^L u_t \phi dx = \gamma \int_0^L f \phi dx - \int_0^L u_x \phi' dx$$

Variational Formulation in 2D (circular disk)

$$u_t = \gamma f + \Delta u$$

$$\iint\limits_{\Omega} u_t \phi dxdy = \gamma \iint\limits_{\Omega} f \phi dxdy + \iint\limits_{\Omega} u_{xx} \phi dxdy + \iint\limits_{\Omega} u_{yy} \phi dydx$$

Similary to 1-D case, the rightmost two terms:

$$\iint\limits_{\Omega} u_{xx} \phi dxdy = \int_{-r}^{r} [u_x \phi|_{-\sqrt{r^2-y^2}}^{\sqrt{r^2-y^2}} - \int_{-\sqrt{r^2-y^2}}^{\sqrt{r^2-y^2}} u_x \phi_x dx] dy$$

$$= -\iint\limits_{\Omega} u_x \phi_x dxdy$$

$$\iint\limits_{\Omega} u_{yy} \phi dxdy = -\iint\limits_{\Omega} u_y \phi_y dxdy$$

Eventually we have

$$\iint\limits_{\Omega} u_t \phi dxdy = \gamma \iint\limits_{\Omega} f \phi dxdy - \iint\limits_{\Omega} (u_x \phi_x + u_y \phi_y) dxdy$$

Galerkin approximation

Now we approximate the variational formulation in finite dimensional space.
Test functions $\phi_j \quad (j = 1, 2, ...N)$ are piecewise continuous, and form a basis for approximate solution $u = u_h$, $v = v_h$:

$$u = \sum_{j=1}^{N} c_j^{(u)} \phi_j \qquad u_x = \sum_{j=1}^{N} c_j^{(u)} \phi_j'$$

$$v = \sum_{j=1}^{N} c_j^{(v)} \phi_j \qquad v_x = \sum_{j=1}^{N} c_j^{(v)} \phi_j'$$

Galerkin approximation of u in 1-D and 2-D

In 1-D

$$\frac{d}{dt}\sum_{j=1}^{N} c_j \int_0^L \phi_j\phi_i dx = \gamma \int_0^L f\phi_i dx - \sum_{j=1}^{N} c_j \int_0^L \phi_j'\phi_i' dx$$

In 2-D

$$\frac{d}{dt}\sum_{j=1}^{N} c_j \iint_{\Omega} \phi_j\phi_i dA = \gamma \iint_{\Omega} f\phi_i dA - \sum_{j=1}^{N} c_j \iint_{\Omega} \{\phi_{j_x}\phi_{i_x} + \phi_{j_y}\phi_{i_y}\} dA$$

Galerkin Approximation in matrix form

Putting the approximated reaction-diffusion system into matrix form,

$$\mathbf{M}\frac{d}{dt}\mathbf{c}^{(\mathbf{u})} = \gamma\mathbf{b}^{(\mathbf{f})} - \mathbf{\Psi}\mathbf{c}^{(\mathbf{u})}$$
$$\mathbf{M}\frac{d}{dt}\mathbf{c}^{(\mathbf{v})} = \gamma\mathbf{b}^{(\mathbf{g})} - d\mathbf{\Psi}\mathbf{c}^{(\mathbf{v})}$$

- $\mathbf{c}_j = c_j$
- $\mathbf{M}_{ij} = \int_0^L \phi_i\phi_j dx$, or $\mathbf{M}_{ij} = \iint_\Omega \phi_j\phi_i dA$
- $\mathbf{b}_i^{(f)} = \int_0^L f\phi_i dx$, or $\mathbf{b}_i^{(f)} = \iint_\Omega f\phi_i dA$
- $\mathbf{b}_i^{(g)} = \int_0^L g\phi_i dx$, or $\mathbf{b}_i^{(g)} = \iint_\Omega g\phi_i dA$
- $\mathbf{\Psi}_{ij} = \int_0^L \phi_i'\phi_j' dx$, or $\mathbf{\Psi}_{ij} = \iint_\Omega \{\phi_{j_x}\phi_{i_x} + \phi_{j_y}\phi_{i_y}\} dA$

Numerical Integration

Combine Crank-Nicolson Method and Adams-Bashforth Method:

$$\mathbf{M}\frac{\mathbf{U^{k+1}}-\mathbf{U^k}}{\Delta t} = \gamma(\frac{3}{2}\mathbf{F^k}-\frac{1}{2}\mathbf{F^{k-1}}) - \mathbf{\Psi}\frac{\mathbf{U^{k+1}}+\mathbf{U^k}}{2} \tag{3}$$

$$\mathbf{M}\frac{\mathbf{V^{k+1}}-\mathbf{V^k}}{\Delta t} = \gamma(\frac{3}{2}\mathbf{G^k}-\frac{1}{2}\mathbf{G^{k-1}}) - d\mathbf{\Psi}\frac{\mathbf{V^{k+1}}+\mathbf{V^k}}{2} \tag{4}$$

k is the index of iteration and Δt denotes the time step. The matrices $\mathbf{M}$ and $\mathbf{\Psi}$ are computed using 3-point Gaussian Quadrature.

By rearranging (3) and (4), we can solve $\mathbf{U^{k+1}}$ and $\mathbf{V^{k+1}}$ for each iteration in Matlab. ☺

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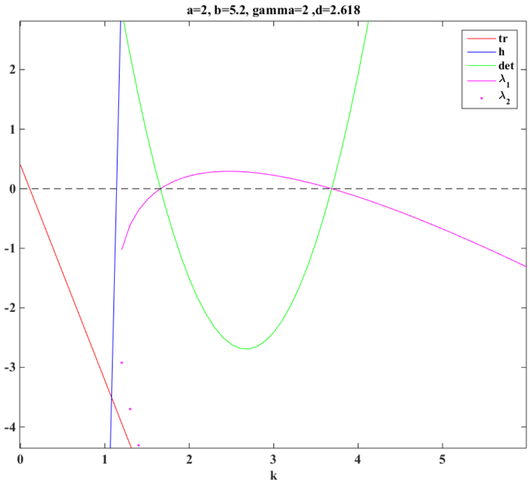
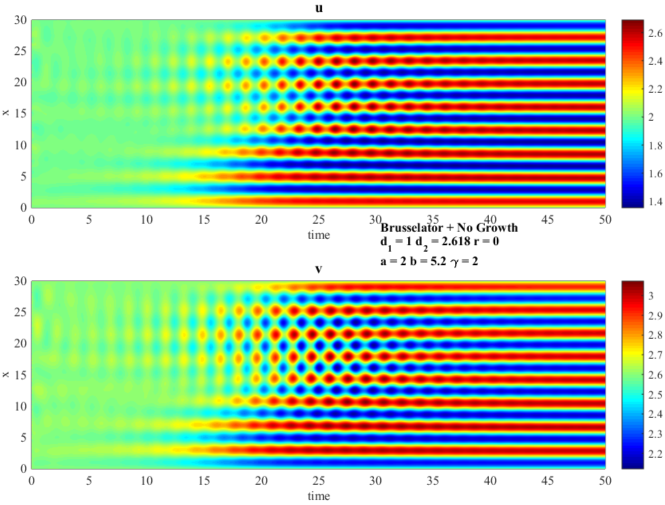
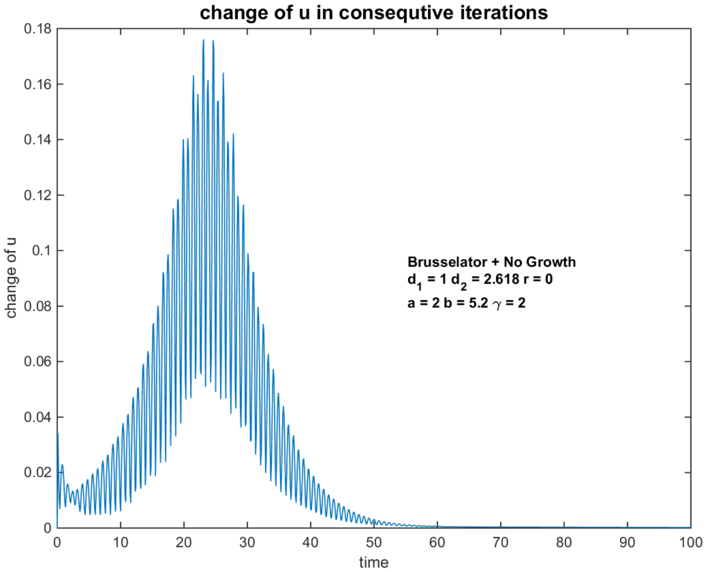
Damped oscillation: parameters



Damped oscillation



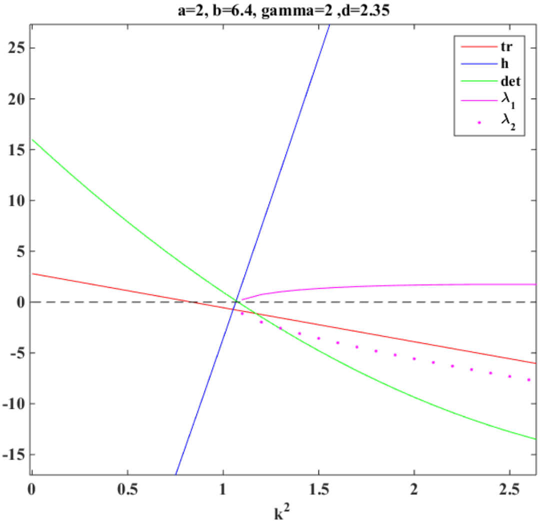
L_1 norm of du/dt



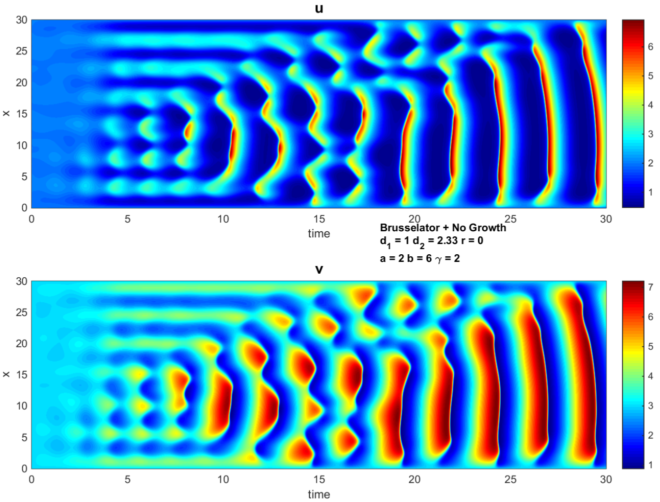
Growth of soft modes modulates hard modes.
Oscillations are damped more rapidly if the real part of all the oscillatory modes are made positive with certain choice of b, keeping d fixed (not shown).

Damped oscillation in 2-D

Transient coexitence: parameter neighborhood

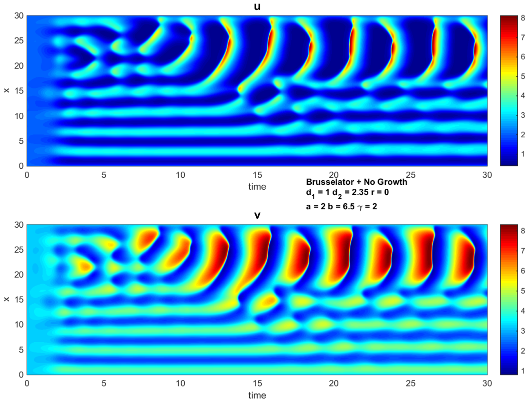


Transient coexitence: oscillation takes over in 1-D



Transient coexitence: oscillation takes over in 2-D

Sort of coexist



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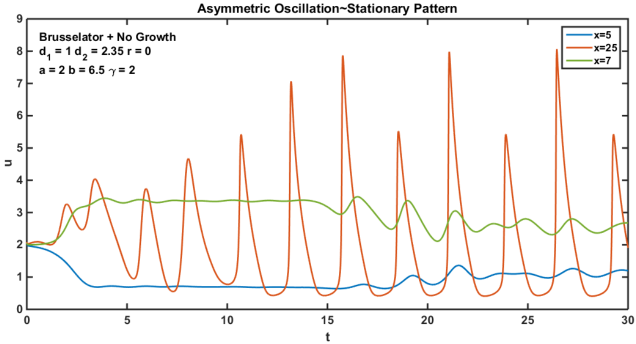
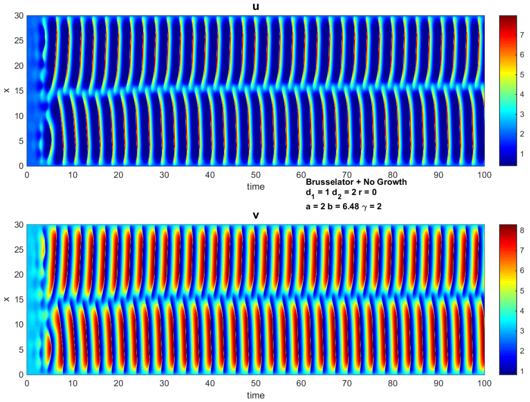
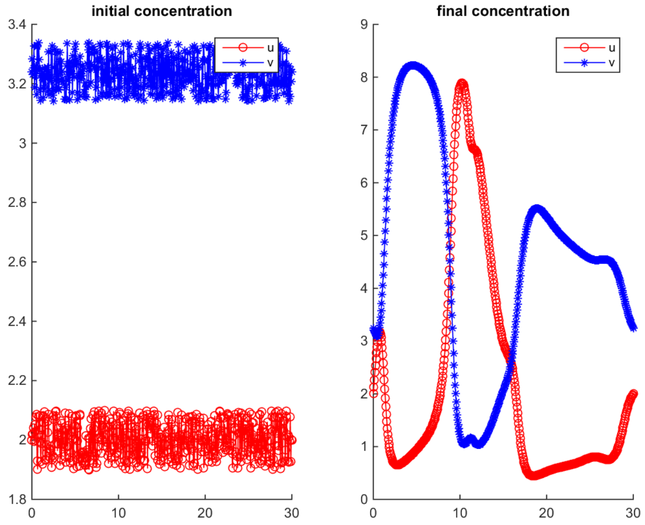


Sort of coexist



Sort of coexist



In this region of parameter space ($b \in [6, 6.5]$, $d \in [2, 2.35]$), the solutions seem to be sensitive to small changes in parameter and initial conditions.

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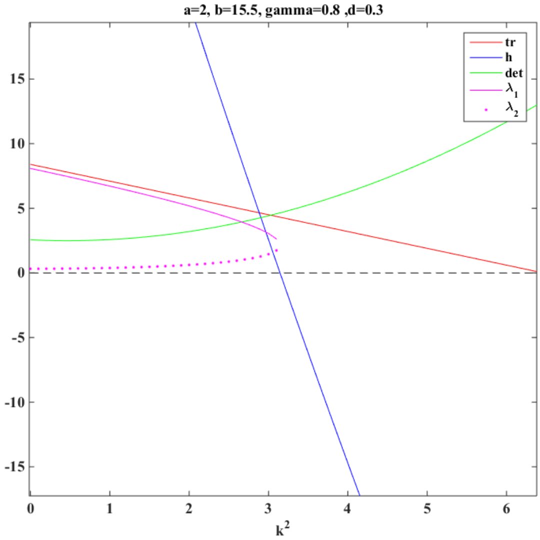
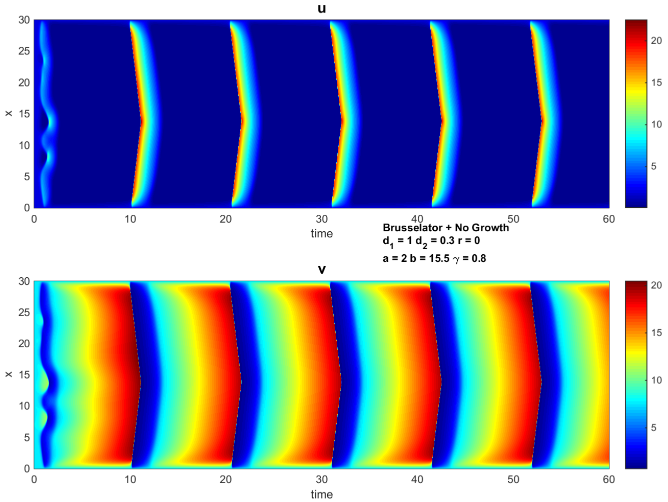
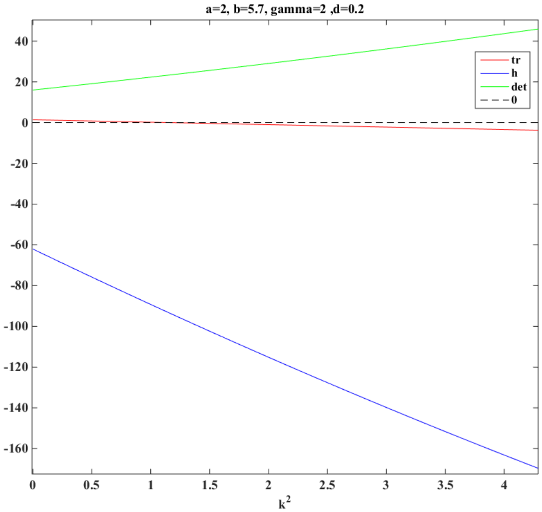
Mixed-mode instability: parameters



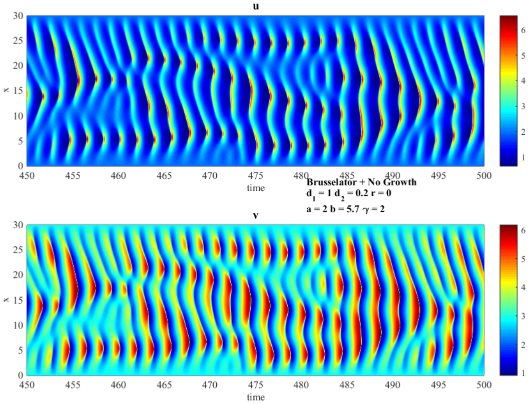
Mixed-mode instability



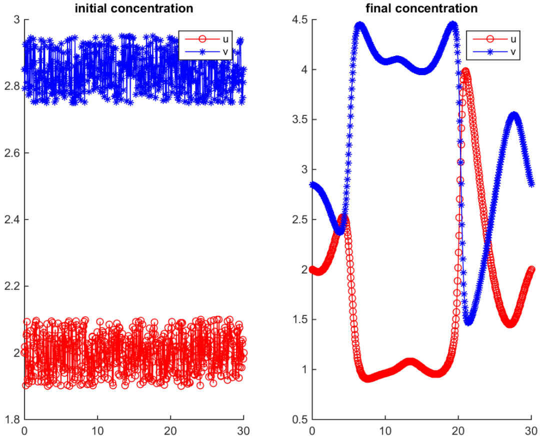
Purely hard-mode: parameters



Purely hard-mode



Purely hard-mode: final moment



Purely oscillatory mode for 2-D domain

Summary

- 1-D dynamics is analogous to 2-D dynamics for the same parameters, even when different boundary conditions have been used.
- With the current integration method, coexistence of hard- and soft-mode instability does not easily settled to a regular spatial temporal pattern, as has been observed when more traditional integration methods are used. The reasons could be
  - variational formulation impose less constraints.
  - insufficient spatial and temporal resolution. Error analysis and/or more experiments should be done.
- certain parameter setting gives interesting purely oscillatory pattern.
- nonlinear analysis is desired to have a better grasp of the dynamics