Mixed mode instability in Brusselator reaction-diffusion system

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Outline

1. Introduction

2. Linear Stability Analysis
   - Eigenvalue problem
   - Mixed mode instability
   - Characterizing the parameter space

3. Experiments
   - Method
   - Results: damped and sustained oscillations
   - Error Analysis

Nonlinear Chemical Dynamics and Belousov-Zhabotinski Reaction

Brusselator

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}v = bu - u^2 v$$

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.

$$u_t = \gamma[a - (b+1)u + u^2 v] + u_{xx}$$
$$v_t = \gamma[bu - u^2 v] + dv_{xx}$$
$$x \in (0, L),\ t > 0,\ BCs$$

u: concentration of the activator
v: concentration of the inhibitor
γ: reaction-to-diffusion ratio
d: inhibitor-to-activator ratio

Outline

Equilibrium

$$\frac{\mathrm{d}}{\mathrm{d}t}u = f(u,v) = a - (b+1)u + u^2 v$$
$$\frac{\mathrm{d}}{\mathrm{d}t}v = g(u,v) = bu - u^2 v$$

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

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

$$\begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t}\xi \\ \frac{\mathrm{d}}{\mathrm{d}t}\eta \end{pmatrix} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

Linearized system with diffusion

When diffusion is taken into account, we have

$$\begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t}\xi \\ \frac{\mathrm{d}}{\mathrm{d}t}\eta \end{pmatrix} = \gamma \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} \frac{d^2}{dx^2}\xi \\ \frac{d^2}{dx^2}\eta \end{pmatrix}$$

Assume the solution takes the form of $\sum c_k e^{\lambda_k t} e^{ik\pi x/L}$. $e^{ik\pi x/L}$ are time-invariant spatial modes of spatial frequency k. Considering each mode individually, we have

$$\lambda_k \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix} = \gamma \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix} - \left(\frac{k\pi}{L} \right)^2 \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \begin{pmatrix} \xi_k \\ \eta_k \end{pmatrix}$$

(k is subscript not partial)

Jacobian

λ_k is the eigenvalue of the Jacobian matrix

$$\mathbf{J} = \begin{pmatrix} \gamma f_u - (k\pi/L)^2 & \gamma f_v \\ -\gamma g_u & -\gamma g_v - d(k\pi/L)^2 \end{pmatrix}$$

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

Outline

Modes of instability

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Modes of instability

- soft-mode instability: eigenvalue of the linearized system, λ_k, is real, and $\lambda_k \geq 0$, leads to stationary spatial pattern.
- hard-mode instability: λ_k is complex, and $\Re\lambda_k > 0$, leads to oscillatory pattern.
- For certain parameter regimes, soft and hard instabilities can coexist, taken on by different spatial modes.

Outline

The eigenvalues

The eigenvalues of

$$\mathbf{J} = \begin{pmatrix} \gamma f_u - (k\pi/L)^2 & \gamma f_v \\ -\gamma g_u & -\gamma g_v - d(k\pi/L)^2 \end{pmatrix}$$

are

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

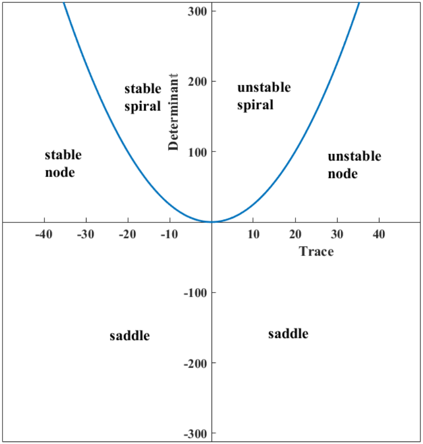
with

$$\mathcal{tr} = \gamma(f_u + g_v) - (1+d)\omega, \quad \omega = (k\pi/L)^2$$

$$\mathcal{D}et = d\omega^2 - \gamma(df_u + g_v)\omega + \gamma^2(f_u g_v - f_v g_u)$$

Stability in terms of $\mathscr{tr}$ and $\mathscr{Det}$

$$\lambda_{k1,2} = \frac{1}{2}\{\mathscr{tr} \pm \sqrt{\mathscr{tr}^2 - 4\mathscr{Det}}\}$$



Parameters that ensure hard-mode instability

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

$$tr = \gamma(f_u + g_v) - (1+d)\omega, \quad \omega = (k\pi/L)^2$$

We need $f_u + g_v > 0$.

In particular, $tr(k=1) > 0$, we need

$$f_u + g_v > \frac{d+1}{\gamma}\left(\frac{\pi}{L}\right)^2$$

Parameters that ensure soft-mode instability

As long as we have $\mathscr{D}et < 0$, we have soft-mode instability for some k

$$\mathscr{D}et = d\omega^2 - \gamma(df_u + g_v)\omega + \gamma^2(f_u g_v - f_v g_u)$$

We need the minimum of $\mathscr{D}et(\omega_0) < 0$ and $\omega_0 = \dfrac{\gamma(df_u + g_v)}{2d} > 0$. That requires

$$df_u + g_v > 0$$

$$f_u g_v - f_v g_u < \frac{(df_u + g_v)^2}{4d}$$

Evalue Jacobian at $(u^*, v^*) = (a, b/a)$, we

- to ensure oscillation (hard-mode instability)

$$b > a^2 + 1 \quad \text{or} \quad b > a^2 + 1 + \frac{d+1}{\gamma}\left(\frac{\pi}{L}\right)^2$$

- to ensure spatial pattern (soft-mode instability)

$$b > \left(\frac{a}{\sqrt{d}} + 1\right)^2$$

For convenience, we set

$$a^2 + 1 = \left(\frac{a}{\sqrt{d}} + 1\right)^2 \quad \Rightarrow d = \left(\frac{a}{\sqrt{a^2+1} - 1}\right)^2$$

Outline

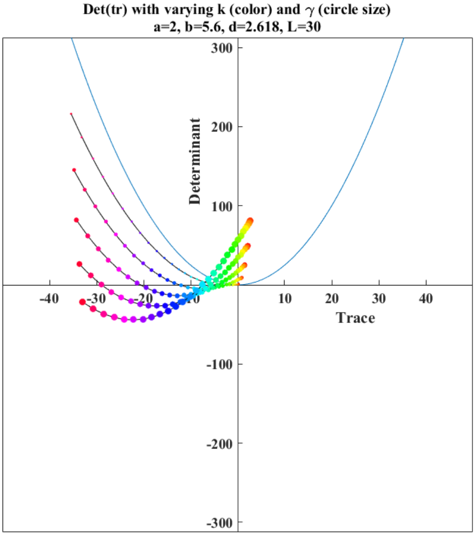
Boundary conditions and intial conditions

1-D domain, Dirichlet Boundary Conditions

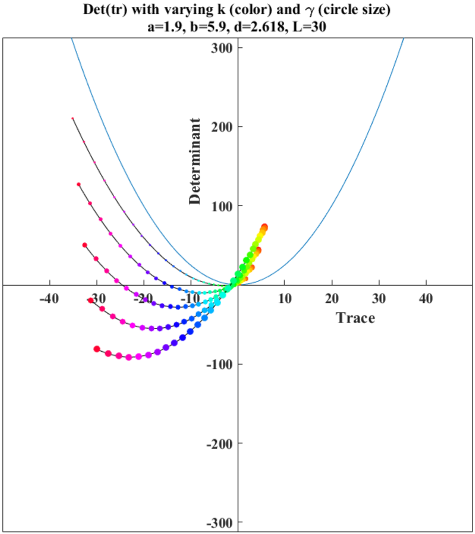
$$u(0,t) = u(L,t) = a, \quad v(0,t) = v(L,t) = b/a$$

where $L = 30$ is the length of the domain.

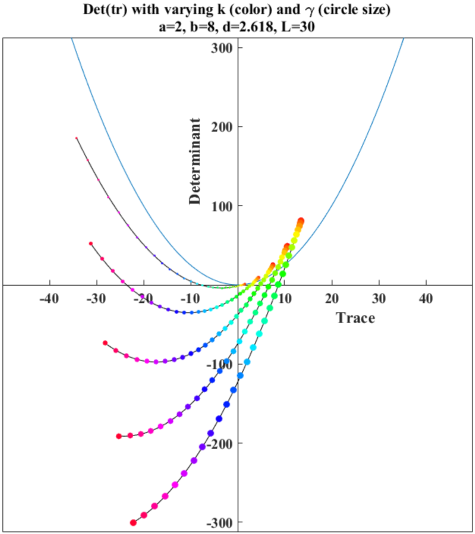
Parameter choices: $b = 5.6$



Parameter choices: $b = 5.9$



Parameter choices: $b = 8$



Variational Formulation

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

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

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 $u = u_h$, $v = v_h$:

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{j=1}^{N} c_j \int_0^L \phi_j \phi_i dx = \gamma \int_0^L f \phi_i dx - \sum_{j=1}^{N} c_j \int_0^L \phi_j' \phi_i' dx$$

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:

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

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

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

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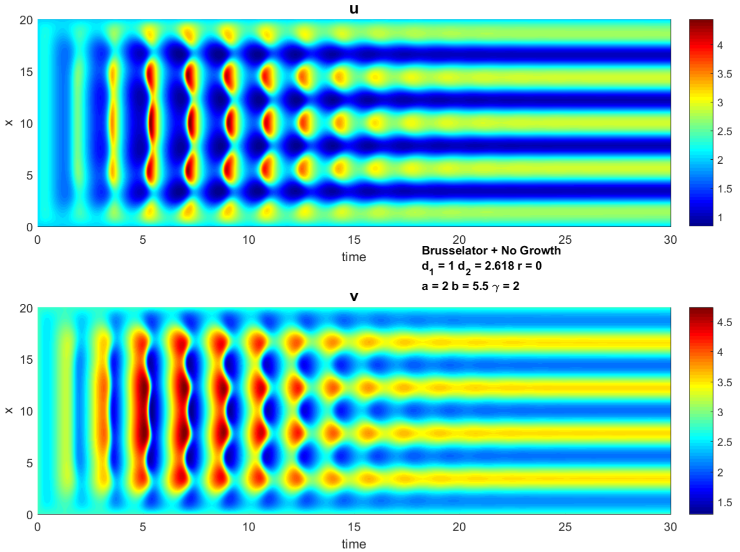
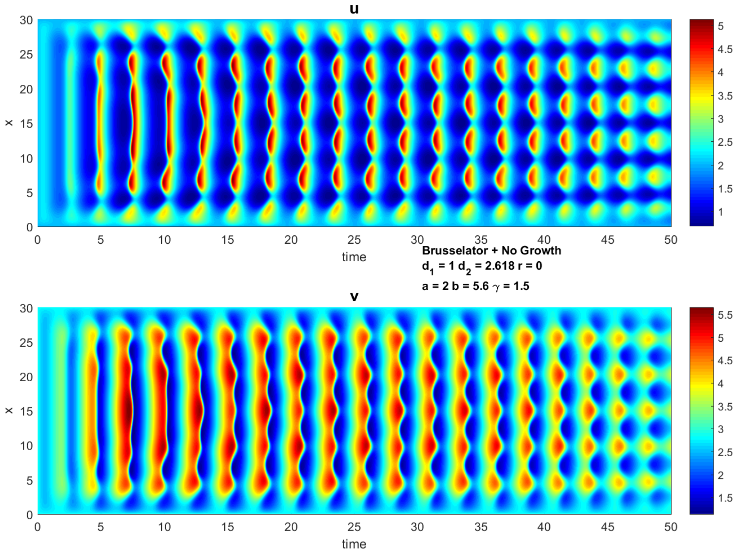
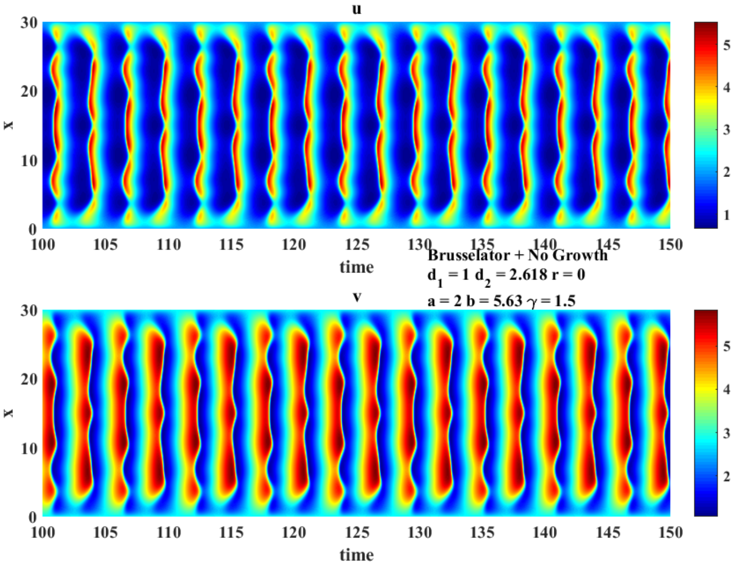
Damped oscillation: $b = 5.5$



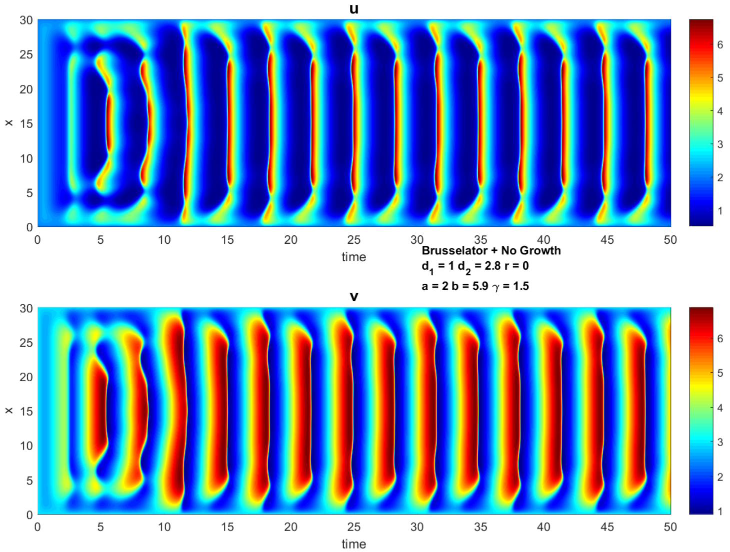
Damped oscillation: $b = 5.6$



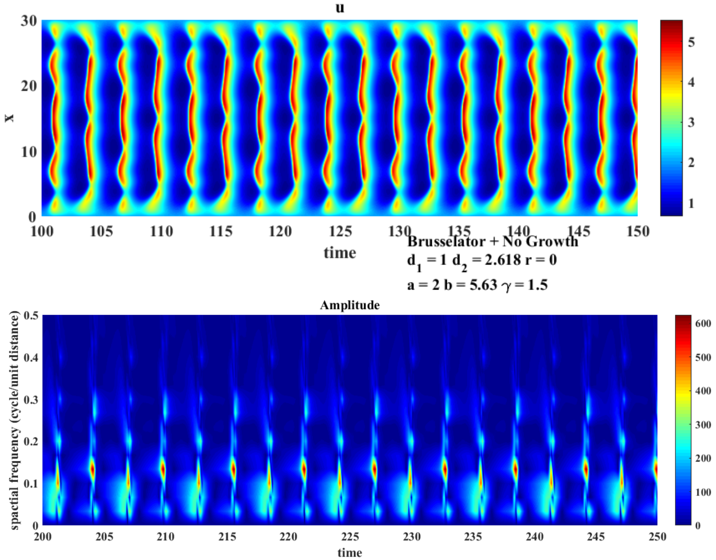
Sustained oscillation: $b = 5.63$



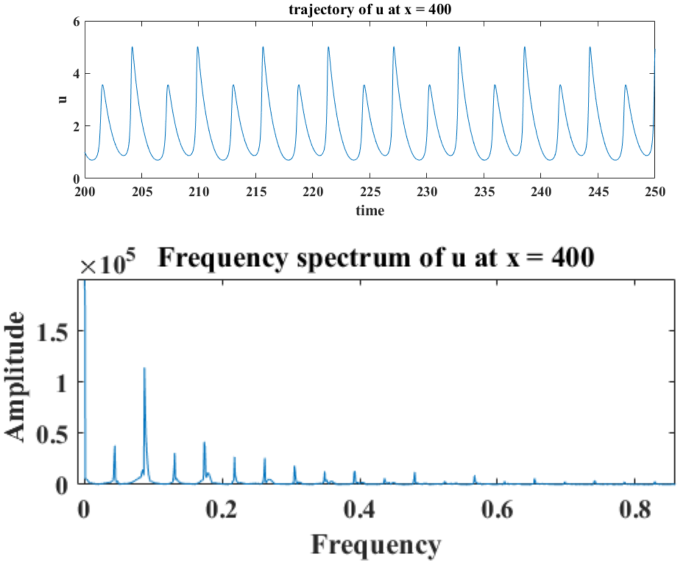
Oscillation rules: $b = 5.9$



Spatial frequency changes in sustained oscillation

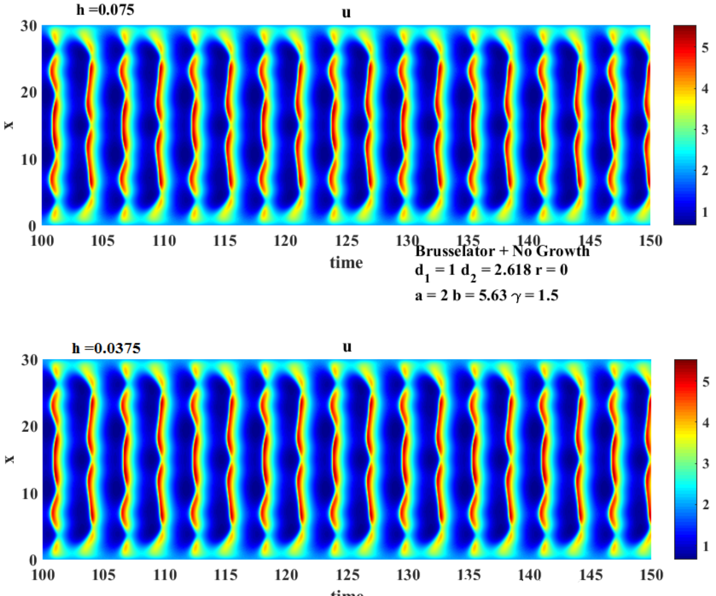


Oscillation at a single location

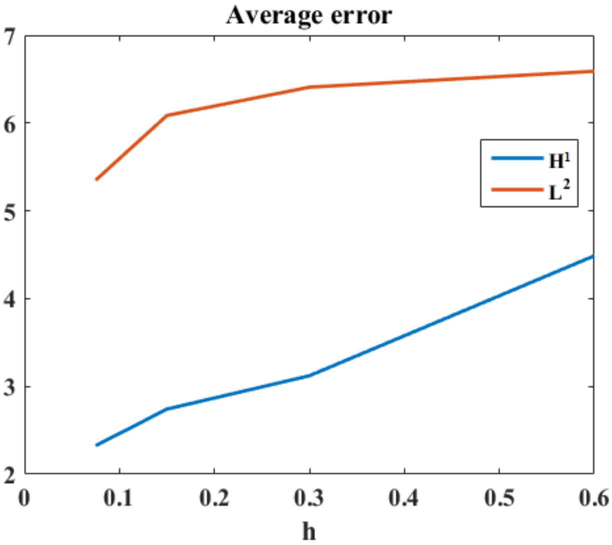


Outline

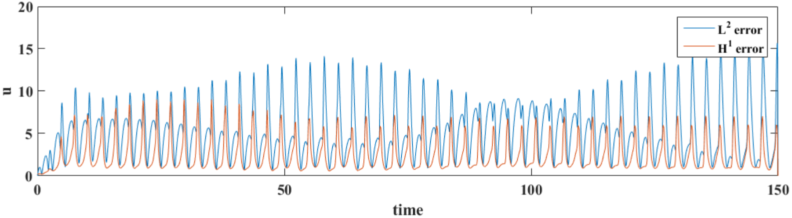
Comparing results at different resolutions



Convergence with respect to mesh size h

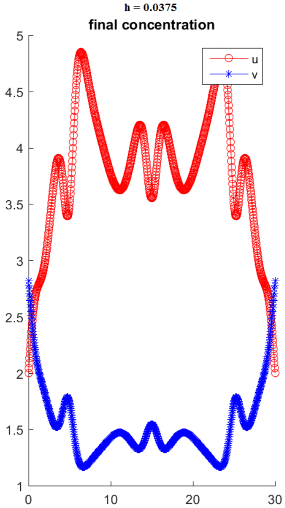


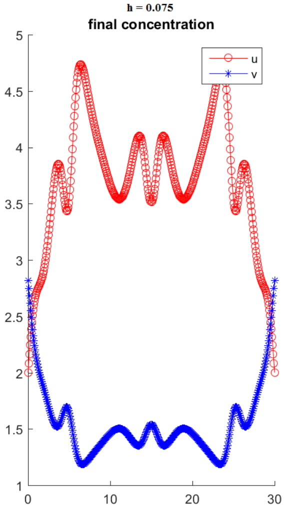
Time series of errors



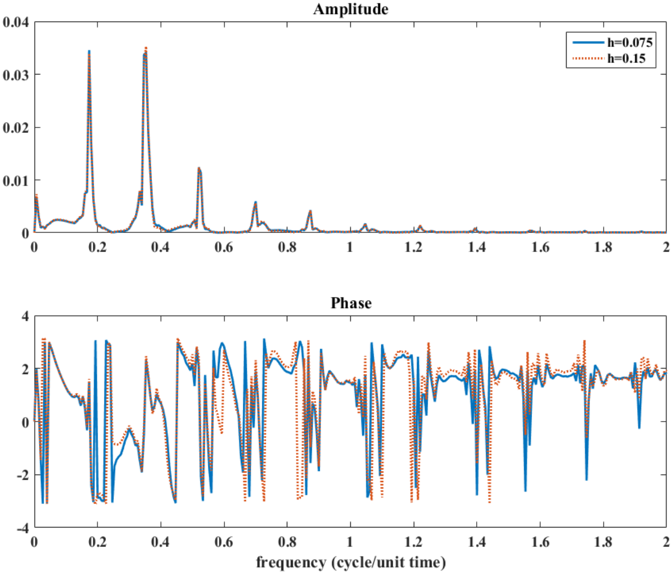
Errors surely depend on amplitude. A more important question is: whether there was accumulative phase shift as time went on.

Comparing results at final time





Yes, phase shift



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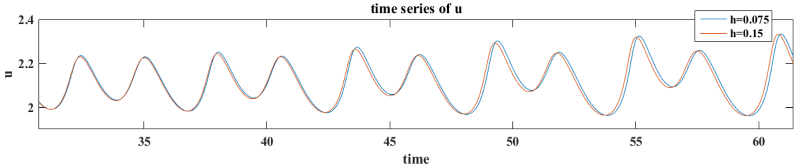

Summary

- There is a narrow band where oscillation and spatial can actually coexist.
  - The spatiotemporal pattern can be complicated.
  - It remains a question how spatial and temporal frequency interact
- Error estimate could make more sense if done in the frequency domain, and considered separately for amplitude and phase.