Finite Element Error Analysis and Numerical Simulations for Moving-Boundary Wave-Pinning Model

(One-Dimensional Error Estimates and Two-Dimensional Cell-Motion Simulations)

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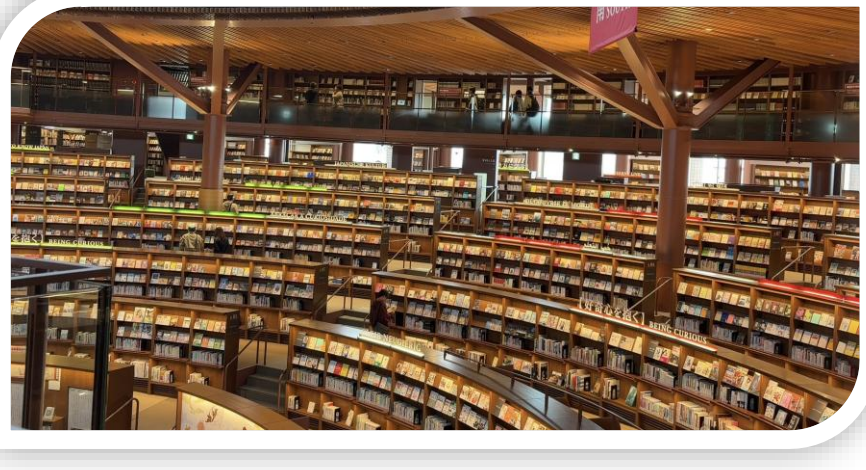
自己紹介 (Self Introduction)



- Name: Ayumu Masaki
- Major: Numerical Analysis
  (Finite Element Method)
- MBTI:INTJ-T(**建築家**)
- From: Funabashi, Chiba Prefecture
- University: Musashino Uni.(Sasaki Lab.)→Kanazawa Uni.
- Hobby: Cooking, Drinking, Reading…







導入 (Introduction)

Wave-Pinning model

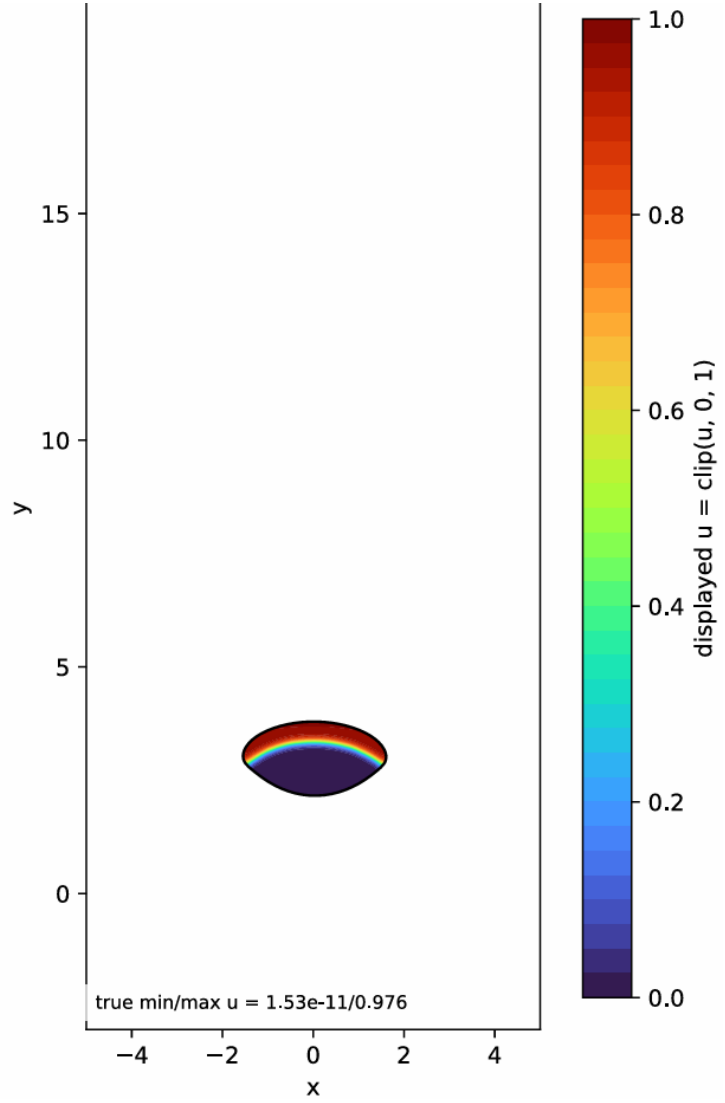
A reaction-diffusion system describing the interactio between active and inactive forms, which generates an intracellular concentration gradient.

Cf:Y. Mori, A. Jilkine and L. Edelstein-Keshet (2008)

Objective

- Extend the WP model to a moving boundary.
- Construct Finite element schemes,
- Perform numerical simulations.
- Establish error estimate from theoretical and numerical perspective.

Cell morphology



1次元WPモデル (Wave-Pinning Model in 1-D)

Domain: $\Omega(t) = (a(t), b(t))$

V :Outward normal velocity

$f(u, v)$:Nonlinear (Bisetable type)

$\alpha, \beta, D_u, D_v > 0$:Constants



Partial Differential Equations

$$\begin{cases} \partial_t u = D_u \partial_x^2 u + f(u, v) & \text{in } \Omega(t), \\ \partial_t v = D_v \partial_x^2 v - f(u, v) & \text{in } \Omega(t), \end{cases}$$

Domain Dynamics

$$\begin{cases} V(a(t), t) = -\dot{a}(t) = \alpha u(a(t), t) - \beta, \\ V(b(t), t) = \dot{b}(t) = \alpha u(b(t), t) - \beta. \end{cases}$$

Boundary Conditions

$$\begin{cases} -D_u \partial_x u + uV = 0 & \text{on } a(t), \\ D_u \partial_x u + uV = 0 & \text{on } b(t), \\ -D_v \partial_x u + vV = 0 & \text{on } a(t), \\ D_v \partial_x v + vV = 0 & \text{on } b(t). \end{cases}$$

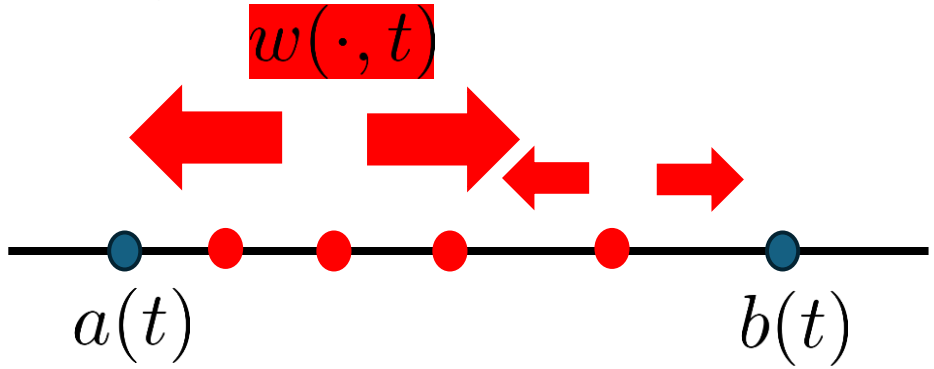
(Natural Neumann B.C. on Moving Domain)

ALE-型弱形式 (ALE-Weak Formulation)

Introducing an artificial velocity field w :

$$\begin{cases} \partial_x^2 w(\cdot,t) = 0 \quad \text{in } \Omega(t), \\ w(a(t),t) = \dot{a}(t) = -V(a(t),t) = -(\alpha u(a(t),t) - \beta), \\ w(b(t),t) = \dot{b}(t) = V(b(t),t) = \alpha u(b(t),t) - \beta. \end{cases}$$

Material derivative: $\partial^{\bullet(w)} u = \partial_t u + w\partial_x u.$



ALE-Weak Formulation

Find $u(\cdot,t), v(\cdot,t) \in L^2(0,T;H^1(\Omega(t)))$ for all $t \in (0,T]$, s.t.

$$\begin{cases} \dfrac{d}{dt}\left(\displaystyle\int_{\Omega(t)} u\xi\,dx\right) + \displaystyle\int_{\Omega(t)} \left[-u\partial^{\bullet(w)}\xi + uw\partial_x\xi + D_u(\partial_x u)(\partial_x\xi) - f(u,v)\xi\right] dx = 0 \quad \text{for } \forall \xi \in H^1(\Omega(t)), \\ \dfrac{d}{dt}\left(\displaystyle\int_{\Omega(t)} v\varphi\,dx\right) + \displaystyle\int_{\Omega(t)} \left[-v\partial^{\bullet(w)}\varphi + vw\partial_x\varphi + D_v(\partial_x v)(\partial_x\varphi) + f(u,v)\varphi\right] dx = 0 \quad \text{for } \forall \varphi \in H^1(\Omega(t)). \end{cases}$$

参照領域へ移す (Transfer to Reference Domain)

◎Key concepts

Reformulated on fixed Reference Domain $\hat{\Omega} = (0, 1)$.

Using the map $x = q(\hat{x}, t) := a(t)(1 - \hat{x}) + b(t)\hat{x}$

ALE-Weak Formulation on Reference Domain

Find $\hat{u} \in L^2(0, T; H^1(\hat{\Omega}))$ with $\partial_t \hat{u} \in L^2(0, T; L^2(\hat{\Omega}))$ for all $t \in (0, T]$ s.t.

$$\int_{\hat{\Omega}} \left[(\partial_t \hat{u})\hat{\xi} l(t) + \hat{u}\hat{\xi}\dot{l}(t) + \hat{u}\hat{w}\partial_{\hat{x}}\hat{\xi} + \frac{D_u}{l(t)}(\partial_{\hat{x}}\hat{u})(\partial_{\hat{x}}\hat{\xi}) - f(\hat{u}, \hat{v})\hat{\xi} l(t) \right] d\hat{x} = 0 \quad \text{for } \forall \hat{\xi} \in H^1(\hat{\Omega}).$$

– (1)

Spatially discretized Weak Formulation on Reference Domain

Find $\hat{u}_h \in L^2(0, T; \hat{\Psi}_h)$ with $\partial_t \hat{u}_h \in L^2(0, T; L^2(\hat{\Omega}))$ for all $t \in (0, T]$, s.t.

$$\int_{\hat{\Omega}} \left[(\partial_t \hat{u}_h)\hat{\xi}_h l_h + \hat{u}_h \hat{\xi}_h \dot{l}_h(t) + \hat{u}_h \hat{w}_h (\partial_{\hat{x}}\hat{\xi}_h) + \frac{D_u}{l_h}(\partial_{\hat{x}}\hat{u}_h)(\partial_{\hat{x}}\hat{\xi}_h) - f(\hat{u}_h, \hat{v}_h)\hat{\xi}_h l_h \right] d\hat{x} = 0$$

$$\text{for } \forall \hat{\xi}_h \in \hat{\Psi}_h \quad \text{with} \quad \partial^{(\bullet w_h)} \hat{\xi}_h = 0.$$

– (2)

※Same applies to v

誤差評価の概要 (Overview of Error-Analysis)

1. Subtracting Semi-discrete formulation (2) from Continuous formulation (1)
2. Deriving the energy inequality
3. Using Gronwall's inequality

※Full discrete error analysis can be carried out in the same manner (Skip this as short of time)

This part was very hard… !

L^2-inner product:

$$(a,b) := \int_{\hat{\Omega}} a(\hat{x})b(\hat{x})\,d\hat{x}.$$

$$I_1 + I_2 + I_3 + I_4 + I_5 = 0,$$

$$I_1 := ((\partial_t \hat{u})l(t) - (\partial_t \hat{u}_h)l_h(t), \theta_u)\,,$$

$$I_2 := \left(\hat{u}\dot{l}(t) - \hat{u}_h\dot{l}_h(t), \theta_u\right),$$

$$I_3 := (\hat{u}\hat{w} - \hat{u}_h\hat{w}_h, \partial_{\hat{x}}\theta_u)\,,$$

$$I_4 := D_u\left(\frac{\partial_{\hat{x}}\hat{u}}{l(t)} - \frac{\partial_{\hat{x}}\hat{u}_h}{l_h(t)}, \partial_{\hat{x}}\theta_u\right),$$

$$I_5 := -\left(f(\hat{u},\hat{v})l(t) - f(\hat{u}_h,\hat{v}_h)l_h(t), \theta_u\right).$$

誤差評価の結果 (Conclusion of Error-Analysis)

Assuming that there is sufficient regularity, reaction term is Lipschitz, and the mesh size h and time step τ are sufficiently small,
Then following holds:

Spatial Semi-Discrete Error Estimation

$$\sup_{t\in[0,T]} \left(\|\hat{u}(t) - \hat{u}_h(t)\|_{L^2(\hat{\Omega})} + \|\hat{v}(t) - \hat{v}_h(t)\|_{L^2(\hat{\Omega})} + |\dot{\ell}(t) - \dot{\ell}_h(t)| \right) \leq Ch^2,$$

$$\left(\int_0^T \|\hat{u}(t) - \hat{u}_h(t)\|^2_{H^1(\hat{\Omega})}\, dt \right)^{1/2} + \left(\int_0^T \|\hat{v}(t) - \hat{v}_h(t)\|^2_{H^1(\hat{\Omega})}\, dt \right)^{1/2} \leq Ch.$$

Full-Discrete Error Estimation

$$\max_{1\leq n\leq N_T} \left(\|\hat{u}^n - \hat{u}_h^n\|_{L^2(\hat{\Omega})} + \|\hat{v}^n - \hat{v}_h^n\|_{L^2(\hat{\Omega})} + |\ell^n - \ell_h^n| \right) \leq C(h^2 + \tau).$$

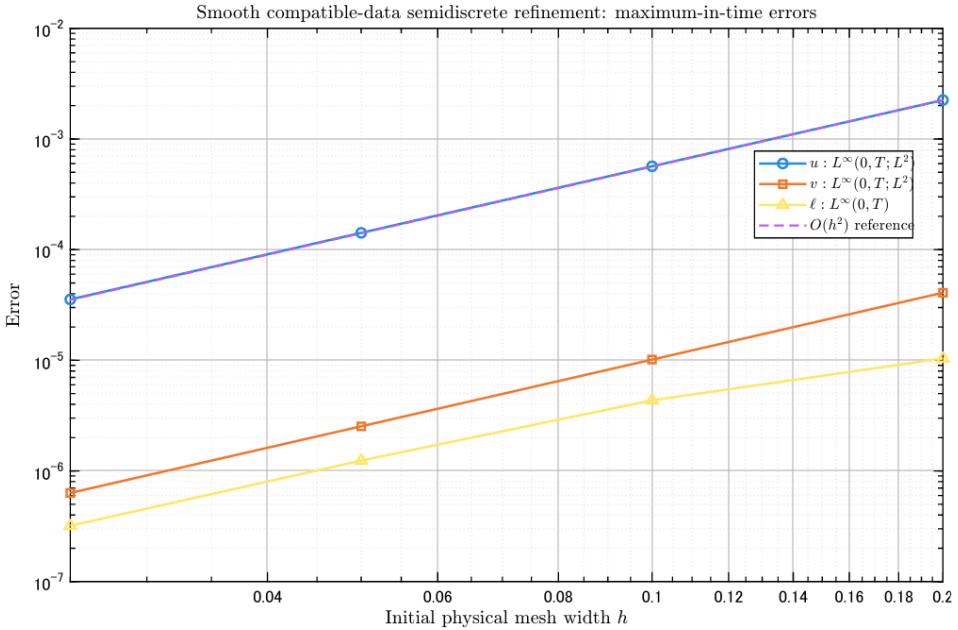
$$\left(\tau \sum_{n=1}^{N_T} \|(\hat{u}^n - \hat{u}_h^n)\|^2_{H^1(\hat{\Omega})} \right)^{1/2} + \left(\tau \sum_{n=1}^{N_T} \|(\hat{v}^n - \hat{v}_h^n)\|^2_{H^1(\hat{\Omega})} \right)^{1/2} \leq C(h + \tau).$$

数値実験 (Numerical Experiments)

Spatial Semi-Discrete Error Estimation

(※Self-Convergence Test)

$$L^\infty(0,T;L^2(\hat{\Omega})) \quad \sup_{t\in[0,T]} \left(\|\hat{u}(t)-\hat{u}_h(t)\|_{L^2(\hat{\Omega})} + \|\hat{v}(t)-\hat{v}_h(t)\|_{L^2(\hat{\Omega})} + |\dot{\ell}(t)-\dot{\ell}_h(t)| \right) \le Ch^2$$



$N_c \to N_f$	$u : L^\infty(0,T;L^2)$		$v : L^\infty(0,T;L^2)$		$\ell : L^\infty(0,T;L^2)$	
	Error	EOC	Error	EOC	Error	EOC
$51 \to 101$	2.2483×10^{-3}	1.99	4.0791×10^{-5}	2.01	1.0401×10^{-5}	1.26
$101 \to 201$	5.6648×10^{-4}	2.00	1.0143×10^{-5}	2.00	4.3497×10^{-6}	1.81
$201 \to 401$	1.4190×10^{-4}	2.00	2.5314×10^{-6}	2.00	1.2409×10^{-6}	1.96
$401 \to 801$	3.5492×10^{-5}	–	6.3264×10^{-7}	–	3.1999×10^{-7}	–

$$L^2(0,T;H^1(\hat{\Omega}))$$

$$\left(\int_0^T \|\hat{u}(t)-\hat{u}_h(t)\|^2_{H^1(\hat{\Omega})}\,dt \right)^{1/2} + \left(\int_0^T \|\hat{v}(t)-\hat{v}_h(t)\|^2_{H^1(\hat{\Omega})}\,dt \right)^{1/2} \le Ch.$$

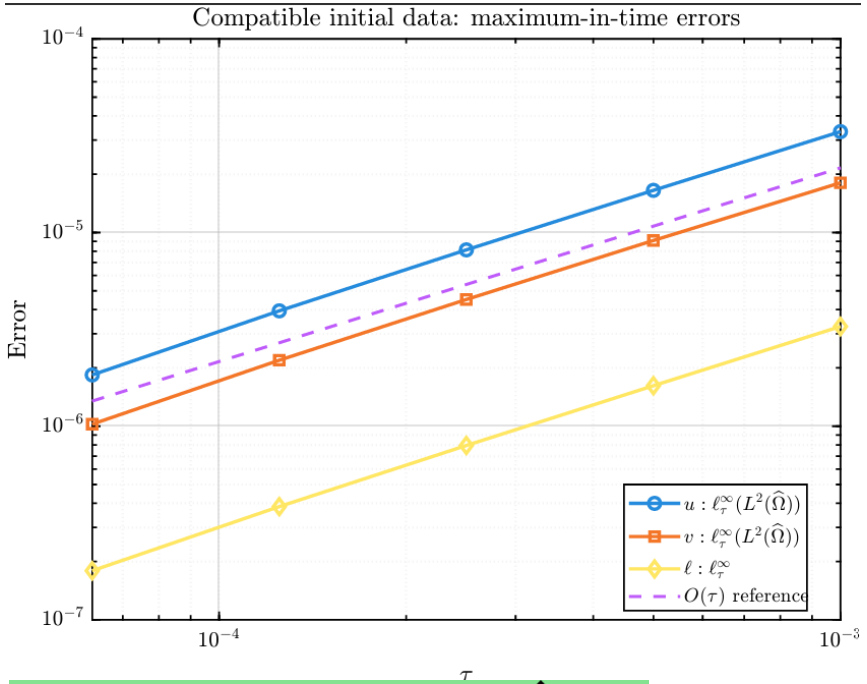
$N_c \to N_f$	$u : L^2(0,T;H^1)$		$v : L^2(0,T;H^1)$	
	Error	EOC	Error	EOC
$51 \to 101$	8.5243×10^{-2}	0.99	8.2186×10^{-4}	0.99
$101 \to 201$	4.2908×10^{-2}	1.00	4.1237×10^{-4}	1.00
$201 \to 401$	2.1491×10^{-2}	1.00	2.0636×10^{-4}	1.00
$401 \to 801$	1.0750×10^{-2}	–	1.0320×10^{-4}	–

数値実験 (Numerical Experiments)

Full-Discrete Error Estimation

$\ell_\tau^\infty(0,T;L^2(\hat{\Omega}))$

$$\max_{1\le n\le N_T}\left(\|\hat{u}^n-\hat{u}_h^n\|_{L^2(\hat{\Omega})}+\|\hat{v}^n-\hat{v}_h^n\|_{L^2(\hat{\Omega})}+|\ell^n-\ell_h^n|\right)\le C(h^2+\tau).$$



τ	$u:\ell_\tau^\infty(L^2)$ Error	EOC	$v:\ell_\tau^\infty(L^2)$ Error	EOC	$\ell:\ell_\tau^\infty$ Error	EOC
1.000×10^{-3}	3.318×10^{-5}	1.01	1.807×10^{-5}	0.99	3.272×10^{-6}	1.02
5.000×10^{-4}	1.651×10^{-5}	1.02	9.098×10^{-6}	1.01	1.618×10^{-6}	1.03
2.500×10^{-4}	8.138×10^{-6}	1.05	4.511×10^{-6}	1.04	7.952×10^{-7}	1.05
1.250×10^{-4}	3.941×10^{-6}	1.10	2.191×10^{-6}	1.10	3.845×10^{-7}	1.10
6.250×10^{-5}	1.840×10^{-6}	–	1.024×10^{-6}	–	1.794×10^{-7}	–

$l_\tau^2(0,T;L^2(\hat{\Omega}))$

$$\left(\tau\sum_{n=1}^{N_T}\|(\hat{u}^n-\hat{u}_h^n)\|_{H^1(\hat{\Omega})}^2\right)^{1/2}+\left(\tau\sum_{n=1}^{N_T}\|(\hat{v}^n-\hat{v}_h^n)\|_{H^1(\hat{\Omega})}^2\right)^{1/2}\le C(h+\tau).$$

τ	$u:\ell_\tau^2(H^1)$ Error	EOC	$v:\ell_\tau^2(H^1)$ Error	EOC
1.000×10^{-3}	1.379×10^{-3}	0.99	8.240×10^{-5}	0.99
5.000×10^{-4}	6.920×10^{-4}	1.01	4.146×10^{-5}	1.01
2.500×10^{-4}	3.426×10^{-4}	1.04	2.056×10^{-5}	1.04
1.250×10^{-4}	1.663×10^{-4}	1.10	9.988×10^{-6}	1.10
6.250×10^{-5}	7.775×10^{-5}	–	4.671×10^{-6}	–

動く様子 (How moves)

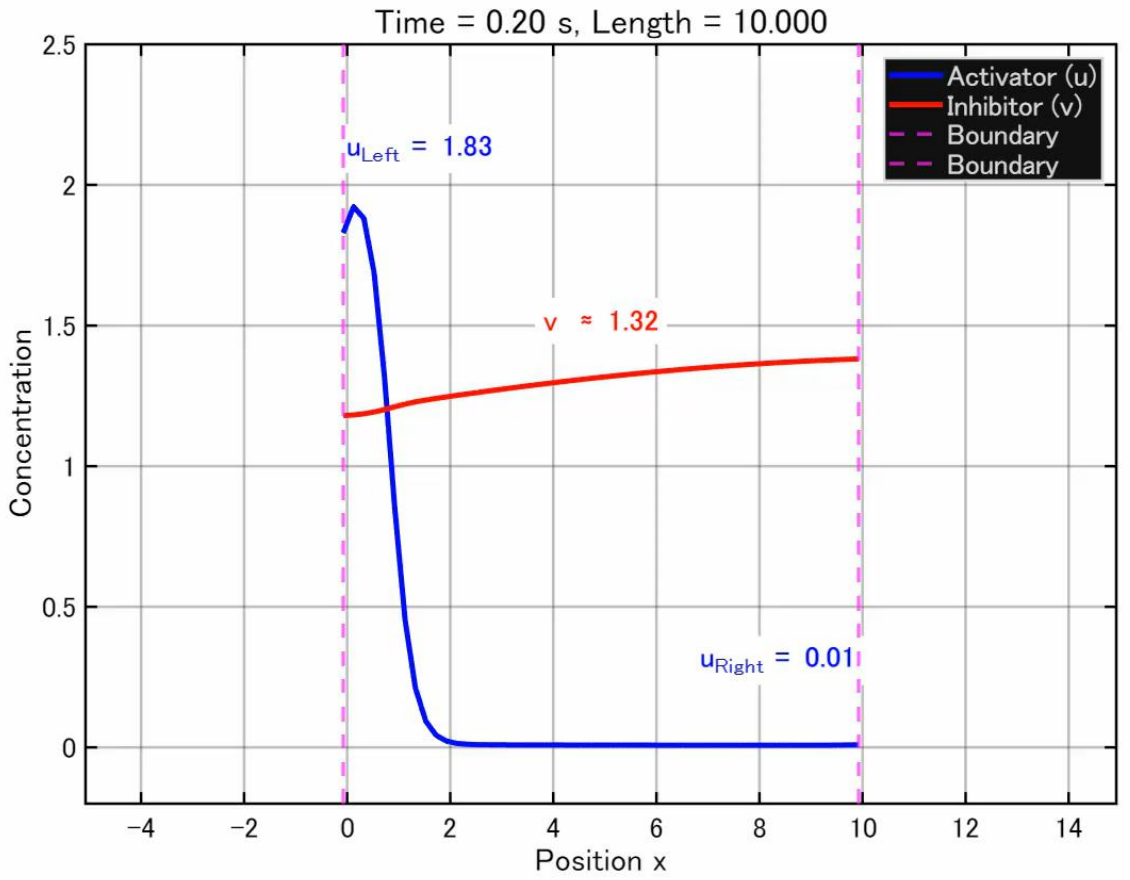
Initial Condition: $\Omega(0) = (0, 10),\ u(x,0) = \begin{cases} 1.5, & (x \le 1), \\ 0.4, & (x > 1), \end{cases} \quad v(x,0) = 1.0,$

Parameters: $D_u = 0.1, \quad D_v = 10, \quad \alpha = 0.5, \quad \beta = 0.398,$

$$\begin{cases} \partial_t u = D_u \partial_x^2 u + f(u,v) & \text{in } \Omega(t), \\ \partial_t v = D_v \partial_x^2 v - f(u,v) & \text{in } \Omega(t), \\ -D_u \partial_x u + uV = 0 & \text{on } a(t), \\ D_u \partial_x u + uV = 0 & \text{on } b(t), \\ -D_v \partial_x u + vV = 0 & \text{on } a(t), \\ D_v \partial_x v + vV = 0 & \text{on } b(t). \end{cases}$$

$$f(u,v) = u(1-u)(u-1-v),$$

$$\begin{cases} V(a(t),t) = -\dot{a}(t) = \alpha u(a(t),t) - \beta, \\ V(b(t),t) = \dot{b}(t) = \alpha u(b(t),t) - \beta. \end{cases}$$



2次元WPモデル (Wave-Pinning Model in 2-D)

Cell Domain: $\Omega(t) \subset \mathbb{R}^2$, Cell Boundary: $\Gamma(t) = \partial\Omega(t)$

Active form: $u = u(\mathbf{x}, t)$, Inactive form: $v = v(\mathbf{x}, t) \quad \mathbf{x} \in \Omega(t)$

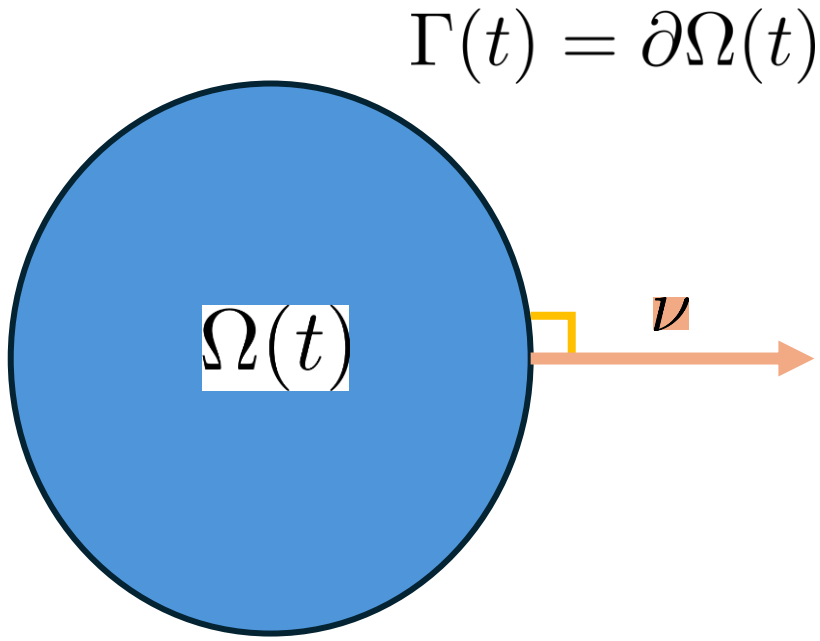
Outward normal vector: ν

Differentiation along the normal direction: ∂_ν

Friction: $\tau_{\text{fric}} > 0$ Inward pressure: $a > 0$

Surface tension: $\gamma > 0$ Restraining force: $b > 0$

$$
\begin{cases}
\tau_{\text{fric}} V = au - b - \gamma\kappa & \text{on } \Gamma(t), \\
\partial_t u = D_u \Delta u + f(u, v) & \text{in } \Omega(t), \\
\partial_t v = D_v \Delta v - f(u, v) & \text{in } \Omega(t), \\
D_u \partial_\nu u + uV = 0 & \text{on } \Gamma(t), \\
D_v \partial_\nu v + vV = 0 & \text{on } \Gamma(t).
\end{cases}
$$



境界のパラメータ表示と接線速度 (Display of Boundary Parameters and Tangential Velocity)

$$\mathbf{p} : \mathbb{S}^1 \times [0,T] \longrightarrow \mathbb{R}^2, \quad (\rho, t) \mapsto \mathbf{p}(\rho, t)$$

$$\Gamma(t) = \{\mathbf{p} : \rho \in \mathbb{S}^1\}$$

Arc length differential: ∂_s

$$\tau_{\text{fric}} \partial_t \mathbf{p} = g(u)\nu + \gamma \partial_p^2 \mathbf{p}$$
$$\Leftrightarrow \partial_t \mathbf{p} = V\nu$$

→ Determine only the laws of motion in the Normal direction

$+W\tau$ → Add movement in the tangential direction

Tangential velocity that makes the arc length distribution uniform

$$\partial_s W = -\kappa V + \langle \kappa V \rangle_\Gamma \omega \left(\frac{L}{2\pi G} - 1 \right)$$

- $\omega > 0$: Parameters for Tangent Repositioning
- Boundary average $\langle \kappa V \rangle_\Gamma := \frac{1}{L} \int_{\gamma(t)} \kappa V \, ds$
- Average arc-length density: $G := \frac{L(t)}{2\pi}$

cf. :K. Mikula, D. Ševčovič, and M. Balažovjech (2010)

数值计算算法(Numerical Computation Algorithms)

Given Ω_h^n, Γ_h^n, $\{\mathbf{p}_i^n\}_{i=0}^{N_\Gamma-1}$, u_h^n, v_h^n. on t^n

① Applying the reaction term to the old domain:

$$u_R^n = u_h^n + \Delta t f(u_h^n, v_h^n), \qquad v_R^n = v_h^n - \Delta t f(u_h^n, v_h^n).$$

(Operator Splitting Method)

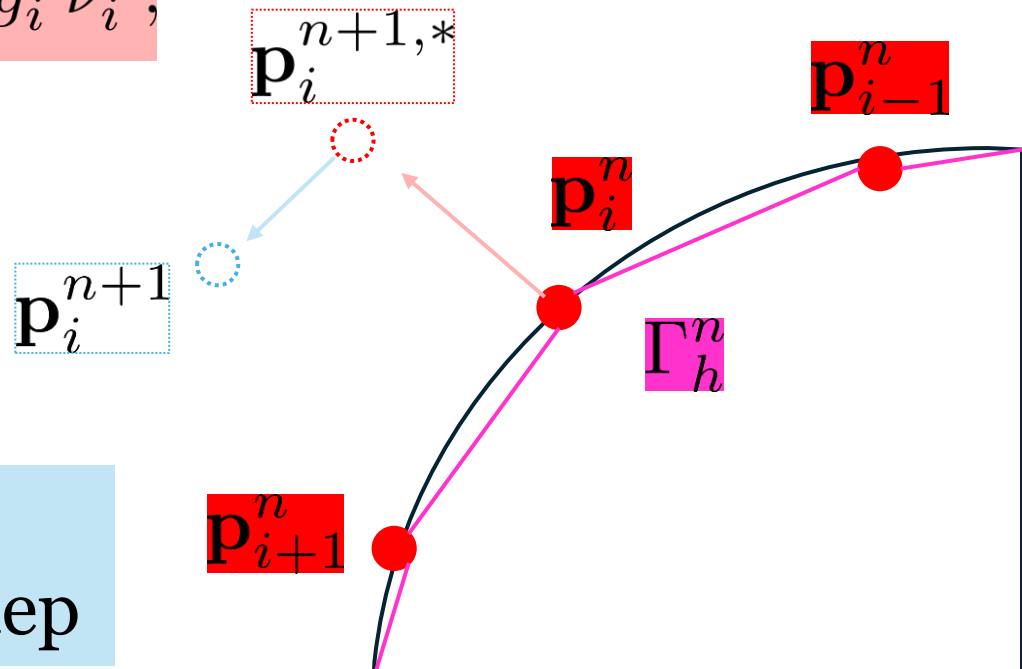
② Move the boundary to obtain new boundary points:

$$\frac{\tau_{\text{fric}}}{\Delta t} m_i^n \left(\mathbf{p}_i^{n+1,*} - \mathbf{p}_i^n\right) + \gamma (K_\Gamma^n \mathbf{p}^{n+1,*})_i = m_i^n g_i^n \nu_i^n,$$

→Move only in the normal direction to find a temporary point

$$\mathbf{p}_i^{n+1} = \mathbf{p}_i^{n+1,*} + \Delta t W_i^n \tau_i^n$$

→Move along the tangent direction to determine the point for the next step



③Harmonically extend the boundary displacement $\mathbf{d}_{\Gamma,i}^{n+1} := \mathbf{p}_i^{n+1} - \mathbf{p}_i^n$ inwards to obtain a new region Ω_h^{n+1} :

$$\mathbf{d}_h^{n+1} := (d_{x,h}^{n+1}, d_{y,h}^{n+1}) \quad \begin{cases} -\Delta d_{x,h}^{n+1} = 0 & \text{in } \Omega_h^n, \\ d_{x,h}^{n+1} = d_{\Gamma,x}^{n+1} & \text{on } \Gamma_h^n, \end{cases} \quad \begin{cases} -\Delta d_{y,h}^{n+1} = 0 & \text{in } \Omega_h^n, \\ d_{y,h}^{n+1} = d_{\Gamma,y}^{n+1} & \text{on } \Gamma_h^n, \end{cases}$$

Using Discrete ALE map: $A_h^{n+1,n} : \Omega_h^n \to \Omega_h^{n+1}, \quad A_h^{n+1,n}(\mathbf{x}) := \mathbf{x} + \mathbf{d}_h^{n+1}(\mathbf{x})$

We obtain $\Omega_h^{n+1}, \quad \Gamma_h^{n+1}$.

④ Solve the scheme to obtain a new concentration

Find u_h^{n+1} s.t.

$$\int_{\Omega_h^{n+1}} u_h^{n+1}\varphi_h^{n+1}dx + \Delta t D_u \int_{\Omega_h^{n+1}} \nabla u_h^{n+1} \cdot \nabla \varphi_h^{n+1} dx = \int_{\Omega_h^n} u_R^n \varphi_h^n dx$$

We obtained

$$\Omega_h^{n+1}, \quad \Gamma_h^{n+1}, \quad \{\mathbf{p}_i^{n+1}\}_{i=0}^{N_\Gamma - 1}, \quad u_h^{n+1}, \quad v_h^{n+1}.$$

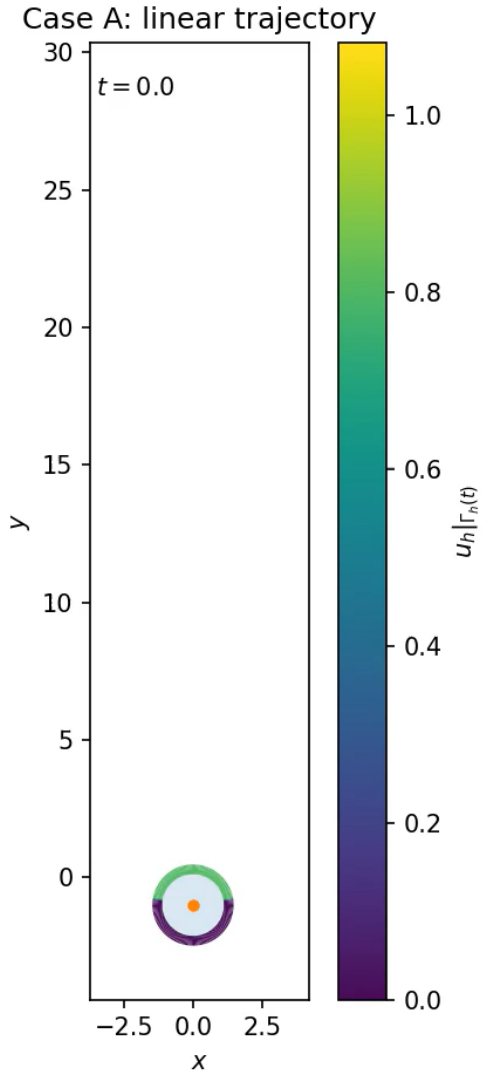
動く様子 (How moves)

Common Initial Condition: $\Omega(0) = \{(x, y) \in \mathbb{R}^2 : x^2 + (y+1)^2 < 1.3^2\}$

①Linear trajectory Parameters

$$\tau = 1 \quad D_u = 0.1, \quad D_v = 10, \quad b = 0.4, \quad \gamma = 0.1.$$

$$\begin{cases} \tau V = au - b - \gamma\kappa & \text{on } \Gamma(t), \\ \partial_t u = D_u \Delta u + f(u, v) & \text{in } \Omega(t), \\ \partial_t v = D_v \Delta v - f(u, v) & \text{in } \Omega(t), \\ D_u \partial_\nu u + uV = 0 & \text{on } \Gamma(t), \\ D_v \partial_\nu v + vV = 0 & \text{on } \Gamma(t). \end{cases}$$



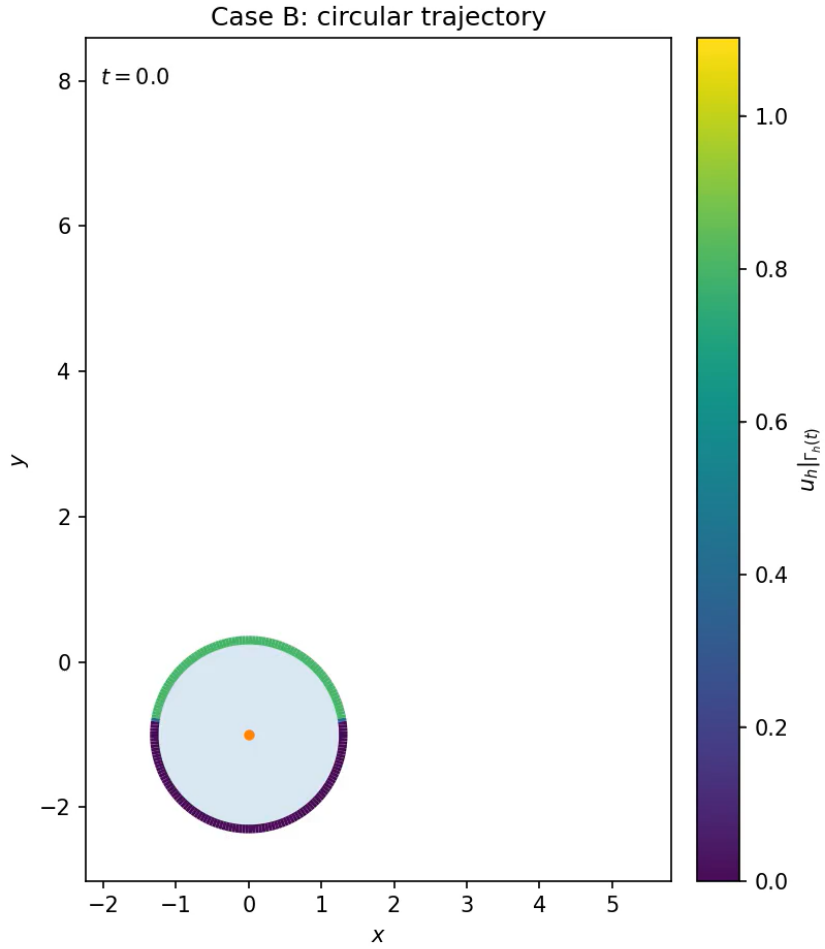
動く様子 (How moves)

②Circular trajectory Parameters

$$\tau = 1 \quad D_u = 0.2, \quad D_v = 20, \quad b = 0.4, \quad \gamma = 0.1.$$

Change Concentrations ×2

$$\begin{cases} \tau V = au - b - \gamma\kappa & \text{on } \Gamma(t), \\ \partial_t u = D_u \Delta u + f(u,v) & \text{in } \Omega(t), \\ \partial_t v = D_v \Delta v - f(u,v) & \text{in } \Omega(t), \\ D_u \partial_\nu u + uV = 0 & \text{on } \Gamma(t), \\ D_v \partial_\nu v + vV = 0 & \text{on } \Gamma(t). \end{cases}$$



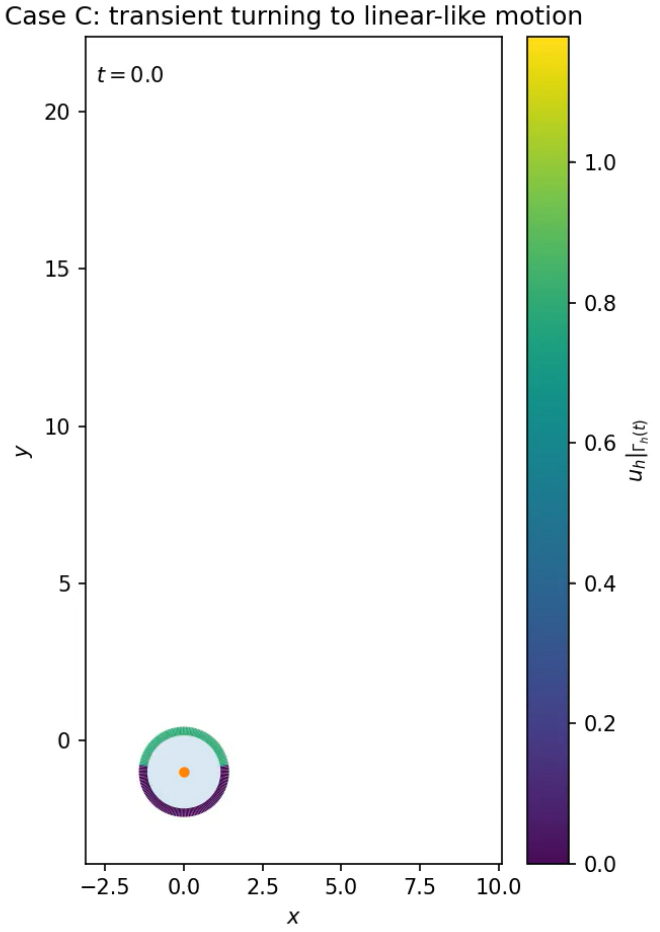
動く様子 (How moves)

③Circular→Linear-like trajectory Parameters

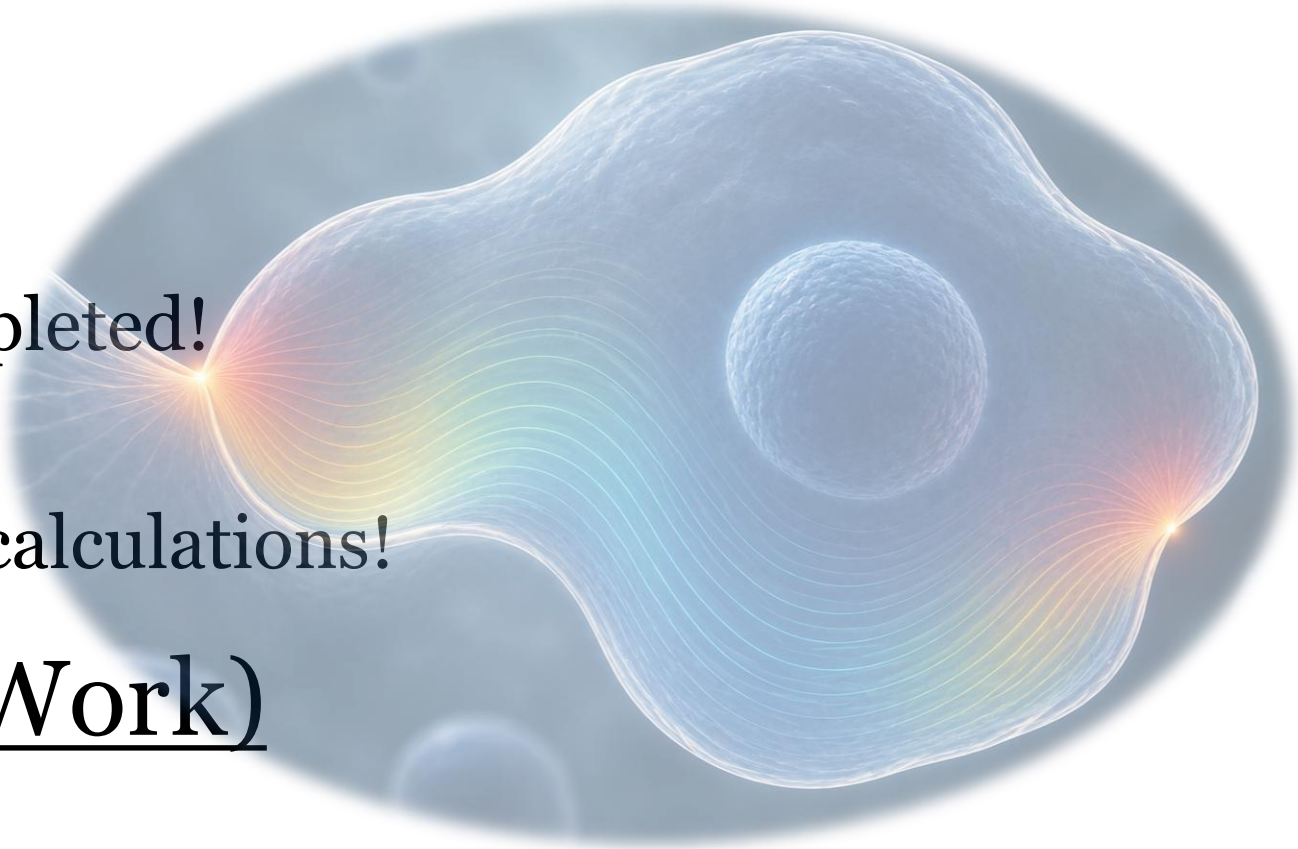
$$\tau = 1 \quad D_u = 0.2, \quad D_v = 20, \quad b = 0.4, \quad \gamma = 0.25.$$

Change Surface tension $\times \frac{1}{4}$

$$\begin{cases} \tau V = au - b - \gamma\kappa & \text{on } \Gamma(t), \\ \partial_t u = D_u \Delta u + f(u,v) & \text{in } \Omega(t), \\ \partial_t v = D_v \Delta v - f(u,v) & \text{in } \Omega(t), \\ D_u \partial_\nu u + uV = 0 & \text{on } \Gamma(t), \\ D_v \partial_\nu v + vV = 0 & \text{on } \Gamma(t). \end{cases}$$



結果 (Conclusion)



○Wave-Pinning Model in 1-D

Error analysis in has been completed!

○Wave-Pinning Model in 2-D

Be able to carry out numerical calculations!

今後の課題 (Future Work)

○Wave-Pinning Model in 1-D

- Check whether there are any errors in the proof.
- Compiling the results into a paper.

○Wave-Pinning Model in 2-D

- Conduct an error analysis.
- Perform numerical branch analysis

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ご清聴ありがとうございました！

Thank you for attention!