Reaction-Diffusion Systems

Let $c(x,t) \equiv$ Concentration of a species (cells, chemicals, heat)

$J(x,t) \equiv$ Flux $\equiv$ amount of material being transported

Fickian diffusion: $J \propto -\frac{\partial c}{\partial x}$

diffusion transports matters from high-to-low concentration

$$J = -D \frac{\partial c}{\partial x}$$

diffusion coefficient

e.g.) Blood molecules: $D = 10^{-7} \frac{cm^2}{sec}$

oxygen in blood: $D = 10^{-5} \frac{cm^2}{sec}$

Conservation Equation

$$\begin{bmatrix} \text{Rate of change} \\ \text{of some material} \\ \text{in a region} \end{bmatrix} = \begin{bmatrix} \text{rate of flow} \\ \text{across} \\ \text{boundary} \end{bmatrix} + \begin{bmatrix} \text{material created} \\ \text{inside} \end{bmatrix}$$

$$\underbrace{\frac{\partial}{\partial t}\underbrace{\int_{x_0}^{x_1} c(x,t)\,dx}_{\text{Total amount of material}}}_{\text{rate of change}} = \underbrace{J(x_0,t)-J(x_1,t)}_{\text{rate of flow across } x_0<x<x_1} = -\int_{x_0}^{x}$$

$$\Vert$$

$$\int_{x_0}^{x_1} \frac{\partial c}{\partial t}(x,t)\,dx = -\int_{x_0}^{x_1} \frac{\partial J}{\partial x}\,dx$$

$$\boxed{\int_{x_0}^{x_1}\left(\frac{\partial c}{\partial t}+\frac{\partial J}{\partial x}\right)dx = 0}$$

Integral Conservation Law

$\int (\cdot)\, dx = 0$ for arbitrary regions

$\Rightarrow (\cdot) = 0$

Diffusion Eq.

Since $J = -D \frac{\partial c}{\partial x} \Rightarrow$ $\boxed{\frac{\partial c}{\partial t} - \frac{\partial}{\partial x}\left(D \frac{\partial c}{\partial x}\right)}$

If D = constant $\Rightarrow$ $\boxed{\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}}$

Let V = 3D space

$S \equiv$ Arbitrary surface enclosing V

$$\frac{\partial}{\partial t}\int_V c(\vec{x},t)\,dV = -\int_S \vec{J}\cdot d\vec{s} + \int_V \underset{\uparrow\,(c,\vec{x},t)}{f}\,dV$$

Assume c to be continuous

Recall: $\displaystyle\int_V \nabla\cdot\vec{J}\,dV = \int_S \vec{J}\cdot d\vec{s}$

$$\int_V \boxed{\left(\frac{\partial c}{\partial t} + \nabla\cdot\vec{J} - f(c,\vec{x},t)\right)}\,dV = 0$$

$$\Rightarrow \boxed{\frac{\partial c}{\partial t} + \underbrace{\nabla\cdot\vec{J}}_{\text{scalar}} = f(c,\vec{x},t)}$$

Conservation Eq. for c

$$\frac{\partial c}{\partial t} = \underbrace{f + \nabla \cdot (D \underbrace{\nabla c}_{\text{gradient}})}_{\text{scalar}}$$

$D = \cancel{D(x, c)}$, i.e. biomedical appl.

$$D = \text{constant} \Rightarrow \boxed{\frac{\partial c}{\partial t} = \underbrace{f}_{\text{reaction}} + \underbrace{D \nabla^2 c}_{\text{diffusion}}}$$

Generalization

$$\vec{u} = \begin{pmatrix} u_1(\vec{x}, t) \\ u_2(\vec{x}, t) \\ \vdots \\ u_m(\vec{x}, t) \end{pmatrix}, \quad D = \begin{pmatrix} D_{11} & \underbrace{\dots \quad D_{1m}}_{\text{cross diffusivity}} \\ & \\ D_{m1} & \dots \quad D_{mm} \end{pmatrix}$$

Without cros[s] diffusivity:

$$D = \begin{pmatrix} D_1 & & \\ & D_2 & \\ & & \ddots \end{pmatrix}$$

$$\frac{\partial \vec{u}}{\partial t} = f + \underbrace{\nabla \cdot \left(D \underbrace{\nabla \vec{u}}_{\text{tensor}}\right)}_{\text{vector}}$$

Turing Patterns (1952)

$$\frac{\partial u}{\partial t} = f(u,v) + D_u \nabla^2 u$$

$$\frac{\partial v}{\partial t} = g(u,v) + D_v \nabla^2 v$$

stability

"diffusion driven instability"

e.g.) $\vec{x} \equiv$ field of dry gra
grass

$g \equiv$ grass hoppers

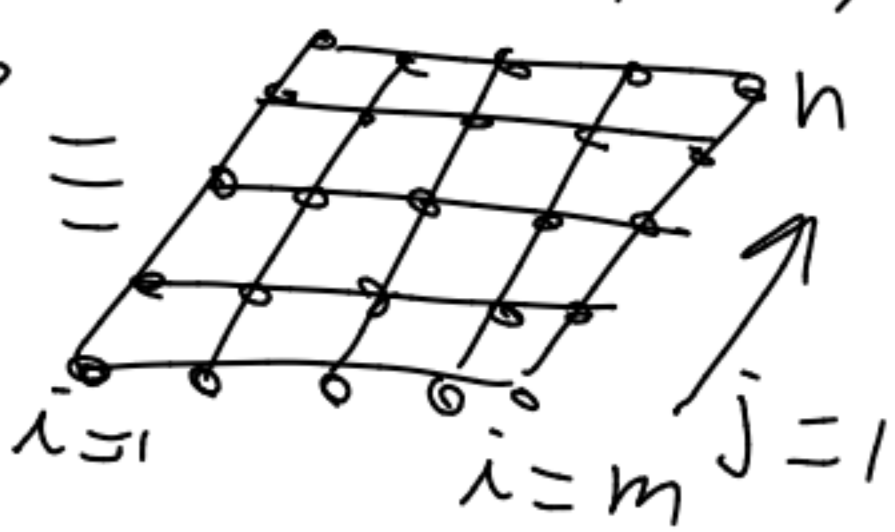
(moisture $\equiv$ inhibito

$f \equiv$ flame front/activa

Let $\vec{x} \in \mathbb{R}^2, \mathbb{R}^3$

$$u(\vec{x},t),\ v(\vec{x},t)$$

$\vec{x} \equiv$



$$\vec{x} = \begin{bmatrix} x_{11} \\ \vdots \\ x_{1m} \\ x_{21} \\ \vdots \\ x_{2m} \\ \vdots \\ x_{mn} \end{bmatrix}$$

$g = 0$: no moisture

$\Rightarrow$ fire spreads uniformly

$\Rightarrow$ steady-state $\equiv$ uniformed charred area

$g > 0$ and $D_g > D_f$

$\Rightarrow$ moisture moves quickly ahead of flame front

$\Rightarrow$ charred area is restricted to a finite domain

$\Rightarrow$ Pattern Formation

Conditions for Instability

Assume: $(u, v) = (u_0, v_0) \equiv$ Steady-State or Equilibrium
Spatially homogeneous sol.

$$\left.\frac{\partial u}{\partial t}\right|_{(u_0,v_0)} = 0 \Rightarrow f(u_0, v_0) + D_u \nabla^2 u_0 = 0$$

$$\left.\frac{\partial v}{\partial t}\right|_{(u_0,v_0)} = 0 \Rightarrow g(u_0, v_0) + D_v \nabla^2 v_0 = 0$$

$(u_0, v_0) \equiv$ Equil. $\xRightarrow{\text{Perturbation}}$

$$u = u_0 + \tilde{u}$$
$$v = v_0 + \tilde{v}$$

perturbation $\|\tilde{u}\|, \|\tilde{v}\| \ll 1$

Linearization

$$\frac{\partial u}{\partial t} = f(u,v) + D_u \nabla^2 u \equiv F(u,v)$$

$$\frac{\partial v}{\partial t} = g(u,v) + D_v \nabla^2 v \equiv G(u,v)$$

$\Downarrow$ Linearization

$$\frac{\partial \tilde{u}}{\partial t} = \underbrace{\left.\frac{\partial f}{\partial u}\right|_{(u_0,v_0)}}_{a} \tilde{u} + \underbrace{\left.\frac{\partial f}{\partial v}\right|_{(u_0,v_0)}}_{b} \tilde{v} + D_u \nabla^2 \tilde{u}$$

$$\frac{\partial \tilde{v}}{\partial t} = \underbrace{\left.\frac{\partial g}{\partial u}\right|_{(u_0,v_0)}}_{c} \tilde{u} + \underbrace{\left.\frac{\partial g}{\partial v}\right|_{(u_0,v_0)}}_{d} \tilde{v} + D_v \nabla^2 \tilde{v}$$

$$\boxed{\begin{aligned}\frac{\partial \tilde{u}}{\partial t} &= a\tilde{u} - b\tilde{v} + D_u \nabla^2 \tilde{u} \\ \frac{\partial \tilde{v}}{\partial t} &= c\tilde{u} - d\tilde{v} + D_v \nabla^2 \tilde{v}\end{aligned}}$$

Linearized System

$a, b, c, d > 0 \Rightarrow$ u – activator
v – inhibitor

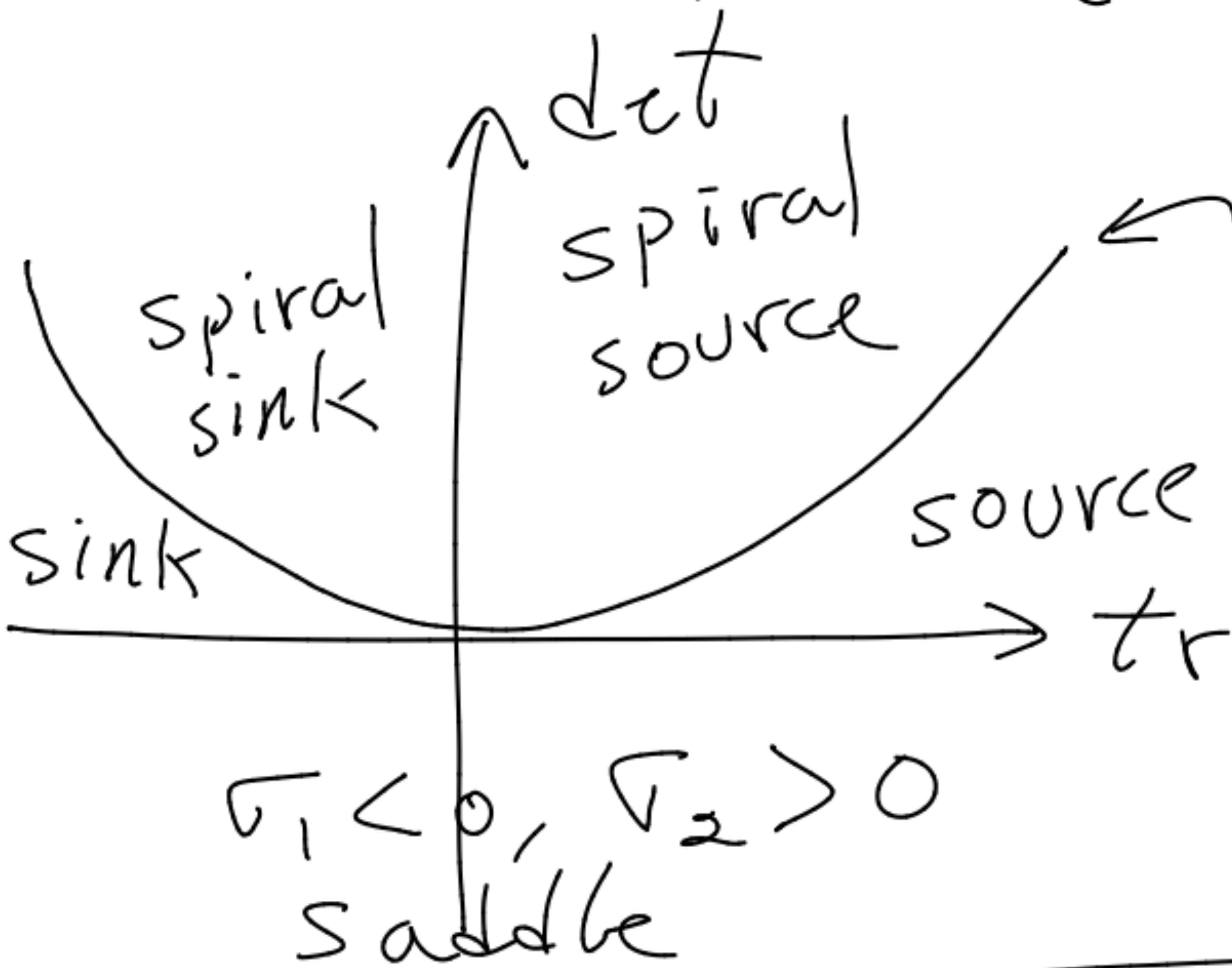
Special Case: $D_u = D_v = 0$

$$\begin{bmatrix} \frac{\partial \tilde{u}}{\partial t} \\ \frac{\partial \tilde{v}}{\partial t} \end{bmatrix} = \underbrace{\begin{bmatrix} a & -b \\ c & -d \end{bmatrix}}_{J} \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix} = J \begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix}$$

Set: $\left.\begin{aligned} \tilde{u} &= \hat{u} e^{\sigma t} \\ \tilde{v} &= \hat{v} e^{\sigma t} \end{aligned}\right\}$ $\begin{aligned} &\sigma < 0 \Rightarrow \tilde{v}, \tilde{u} \downarrow 0 \Rightarrow (u_0, v_0) \text{ stable} \\ &\sigma > 0 \Rightarrow \tilde{u}, \tilde{v} \nearrow \infty \Rightarrow (u_0, v_0) \text{ unstable} \end{aligned}$

Char. Poly: $\boxed{\sigma^2 - tr(\sigma)\sigma + \det J = 0}$

$$\sigma^2 - (a-d)\sigma + (-ad+bc) = 0$$



$$\underbrace{(\mathrm{tr}J)^2}_{x} - \underbrace{4\det J}_{y} = 0$$

$$\mathrm{Re}\{\sigma\} < 0$$

$$\Downarrow$$

$$\mathrm{tr}J < 0 \ \& \ \det J > 0$$

$$\boxed{a < d \ \& \ ad < bc}$$

$$\sigma = -\frac{1}{2}\mathrm{tr}J \pm \frac{1}{2}\underbrace{\sqrt{(\mathrm{tr}J)^2 - 4\det J}}_{(|\mathrm{tr}J| - \varepsilon)}$$

Full System

Let

Fourier Expansion

$$\tilde{u}(\vec{x},t) = \hat{u}\, e^{i\vec{k}\cdot\vec{x}+\sigma t} + c.c.$$

$$\tilde{v}(\vec{x},t) = \hat{v}\, e^{i\vec{k}\cdot\vec{x}+\sigma t} + c.c.$$

Fourier Modes

$\vec{k}$ = wave vector