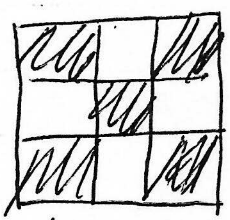
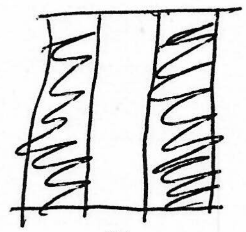
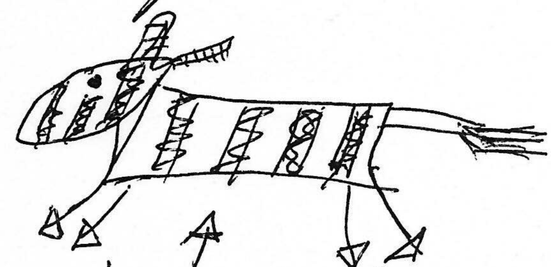
Fronts

Cf: J.D. Murray: "Mathematical Biology"

Turing-Instability (2D) — Pattern/Fronts

i.) Introduction

→ Turing Instability is simple mechanism for generating heterogeneous spatial patterns via reaction-diffusion systems

i.e.  v.s.  ⇒ 

black, white > reactants ?

?

marking pattern of zebra, etc.

→ generic structure and preview:

$$\left.\begin{aligned} \frac{\partial A}{\partial t} &= F(A,B) + D_A \nabla^2 A \\ \frac{\partial B}{\partial t} &= G(A,B) + D_B \nabla^2 B \end{aligned}\right\} \text{structure of system}$$

- pattern formation results from instability if $D_A \neq D_B$, even if $D = 0$ system supports homogeneous, linearly stable equilibria!

[Note: Remarkable as here diffusion triggers instability, unlike usually stabilizing behavior]

↓

ala' convection

→ Can understand relation of pattern formation to unequal D_A, D_B via "example" of fire and grasshoppers.

reaction

Consider: grasshoppers: sweat when $T > T_c$. Sweat quenches/prevents fire.

inhibitor

together in field of dry grass

fire: triggers inhibition response

activator

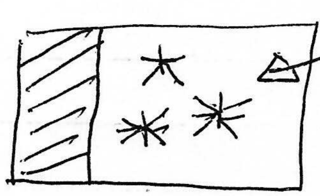
activator, inhibitor } generic biological model

also: grasshoppers: highly mobile (D_g)

fire: less mobile (D_f)

$\boxed{D_g \gg D_f}$

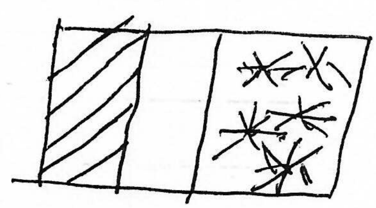
dry grass field



initially burning region

grasshoppers

→



$D_g > D_f$ (grasshoppers outrun fire)

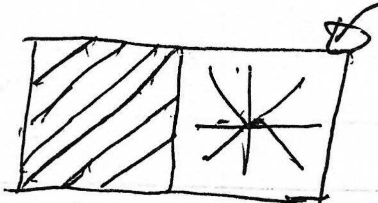
fire spreads onto here

high concentration of grasshoppers wets grass ⇒ avoids fire

Key element:

- time scale disparity
- diffusion/mobility disparity

→



hoppers (wet)

charred

Point is that spatial scale of charred region

set by $\begin{cases} \text{reaction rate} \leftrightarrow \text{sweet production, burn} \\ D_G / D_F \leftrightarrow \text{relative mobility.} \end{cases}$

i.e. rather obvious that:

* → boundary, initial conditions important

* → critical time scales : $\frac{D_G}{L^2}$, $\frac{D_F}{L^2}$, γ
  ↓
  reaction rate

(i.e. size of burnt region set by

$\frac{D_G}{L^2}$ vs $\frac{D_F}{L^2}$ → how much faster hoppers out-hop fire

γ vs. $\frac{D_F}{L^2}$ → sweet vs burn rate.)

ii.) Analysis – Basic Example

$$\rightarrow \frac{\partial A}{\partial t} = F(A,B) + D_A \nabla^2 A$$

$$\frac{\partial B}{\partial t} = G(A,B) + D_B \nabla^2 B$$

here:

Schnackenberg

$$F(A,B) = k_1 - k_2 A \underbrace{+ k_3 A^2 B}_{\text{auto-catalytic effect}}$$

self-saturation

$$G(A,B) = k_4 - k_3 A^2 B$$

or

Gierer + Mienhardt

$$F = k_1 - k_2 A + \frac{k_3 A^2}{B}$$

$$G = k_4 A^2 - k_5 B$$

A → activator
B → inhibitor

etc.

Will examine Schnackenberg system:

→ de-dimensionalizing:

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

$$\frac{\partial v}{\partial t} = \gamma (b - u^2 v) + d \nabla^2 v$$
$$= \gamma g(u,v) + d \nabla^2 v$$

where:

$\gamma = k_2 / (D_A / L^2)$; $d = D_B / D_A$

ratio reaction to diffusion time

ratio of diffusions

$L \equiv$ box size

and: $t^* = \dfrac{D_A t}{L^2}$, $x^* = \dfrac{x}{L}$

$u = A (k_3/k_2)^{1/2}$, $v = B (k_3/k_2)^{1/2}$

$a = (k_1/k_{12})(k_3/k_{12})^{1/2}$, $b = (k_4/k_2)(k_3/k_{12})^{1/2}$

note: structure of form:

$\partial/\partial t \, u = \gamma f(u, v) + \nabla^2 u$

$\dfrac{\partial v}{\partial t} = \gamma g(u, v) + d \nabla^2 v$

is generic!

boundary/initial condition

no in/out flux

$\hat{n} \cdot \nabla \begin{pmatrix} u \\ v \end{pmatrix} = 0$

on bndry

$u(\underline{r}, 0)$, $v(\underline{r}, 0)$ given

→ To analyze:

— first, ignore diffusion:

∴ u_0 , v_0 → fixed point

→ linearly stable

For stability: (linear) community/stability matrix

$$\frac{\partial}{\partial t}\begin{pmatrix}\tilde{u}\\ \tilde{v}\end{pmatrix} = \gamma \begin{pmatrix}\frac{\partial f}{\partial u}, & \frac{\partial f}{\partial v}\\ \frac{\partial g}{\partial u}, & \frac{\partial g}{\partial v}\end{pmatrix}_{\substack{u_0\\ v_0}} \begin{pmatrix}\tilde{u}\\ \tilde{v}\end{pmatrix}$$

$\sim e^{\lambda t}$

growth rate

$\therefore$ seek $\det|\gamma \underline{\underline{A}} - \lambda \underline{\underline{I}}| = 0$

$$\Rightarrow \quad \begin{vmatrix}\gamma f_u - \lambda, & \gamma f_v\\ \gamma g_u, & \gamma g_v - \lambda\end{vmatrix} = 0$$

$$\lambda^2 - \lambda\gamma(f_u + g_v) + \gamma^2(f_u g_v - f_v g_u) = 0$$

$$\lambda = \frac{1}{2}\left[\gamma(f_u + g_v) \pm \left[\gamma^2(f_u+g_v)^2 - 4\gamma^2(f_u g_v - f_v g_u)\right]^{1/2}\right]$$

$$= \frac{\gamma}{2}\left[\operatorname{tr} A \pm \left((\operatorname{tr} A)^2 - 4\det A\right)^{1/2}\right]$$

re $\lambda < 0$ (stability) $\Rightarrow \begin{cases}\operatorname{tr}\underline{\underline{A}} < 0\\ \det\underline{\underline{A}} > 0\end{cases}$ $\rightarrow$ {stability conditions note: $\mathrm{tr}\, A < 0$, $\det A > 0$ obviously impose constraints on f_u, f_v, g_u, g_v etc.

→ now, with diffusion:

if $\underline{W} = \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix}$, then for linear stability:

$$\frac{\partial}{\partial t} \underline{W} = \underline{\underline{D}} \cdot \nabla^2 \underline{W} + \gamma \underline{\underline{A}} \cdot \underline{W}$$

$$\underline{\underline{D}} = \begin{bmatrix} 1, & 0 \\ 0, & d \end{bmatrix}$$

as usual:

$$\underline{W} = \sum_k c_k e^{\lambda t} \underline{W}_k(\underline{r}) \qquad \sim e^{ik\cdot r}$$

$$\nabla^2 W_k + k^2 W_k = 0 \quad ; \quad \hat{n} \cdot W = 0 \text{ on bndry}$$

$$1D \Rightarrow W \sim \cos\left(\frac{n\pi x}{a}\right) \qquad a \equiv \text{box size}$$

$$k = k_n = \frac{n\pi}{a}$$

$\therefore$ stability $\Leftrightarrow$

$$\lambda W_k = \gamma \underline{\underline{A}} \cdot \underline{W}_k - k^2 \underline{\underline{D}} \cdot \underline{W}_k$$

$$\Rightarrow \det(\gamma \underline{\underline{A}} - k^2 \underline{\underline{D}} - \lambda \underline{\underline{I}}) = 0$$

Thus, for stability condition:

$$\begin{vmatrix} \gamma f_u - k^2 - \lambda, & \gamma f_v \\ \gamma g_u, & \gamma g_v - k^2 d - \lambda \end{vmatrix} = 0$$

$$\Rightarrow \begin{cases} \lambda^2 + \lambda\left[k^2(1+d) - \gamma(f_u + g_v)\right] + h(k^2) = 0 \\ h(k^2) = d k^4 - \gamma(d f_u + g_v)k^2 + \gamma^2 \det A \end{cases}$$

disp. rel'n

$$2\lambda = -\left(k^2(1+d) - \gamma \, \mathrm{tr} A\right) \pm \left[\left(k^2(1+d) - \gamma \, \mathrm{tr} A\right)^2 - 4h(k^2)\right]^{1/2}$$

recall stable uniform state $\Rightarrow$ $\left.\begin{matrix} \mathrm{tr} A < 0 \\ \det A > 0 \end{matrix}\right\}$

Here, expect instability for finite k. Thus, need

$$\boxed{h(k^2) < 0} \rightarrow \left.\begin{matrix}\text{condition for} \\ \underline{\text{instability}}\end{matrix}\right\} \begin{matrix} - \text{ of } \pm \\ \text{wins.}\end{matrix}$$

but $h(k^2) = dk^4 - \gamma(df_u + g_v)k^2 + \gamma^2 \det A$

$$= \underbrace{dk^4 + \gamma^2 \det A}_{>0,\ \text{as } \det A > 0} - \gamma(df_u + g_v)k^2$$

but $\underbrace{\operatorname{tr} A < 0}_{\text{uniform state stability}}$ $\Rightarrow$ $\boxed{h(k^2) < 0 \ \text{only if } d \neq 1}$

$\Rightarrow$ have demonstrated $D_A \neq D_B$ for instability

$\because \begin{cases} \operatorname{tr} A < 0 \\ df_u + g_v > 0 \end{cases} \Rightarrow \begin{cases} d \neq 1 \\ g_u, f_v \text{ have opposite signs} \end{cases}$

Now, more rigorously, $h(k^2)_{min} < 0$ for instability!

$$\frac{dh}{dk^2} = 2dk^2 - \gamma(df_u + g_v)$$

$$k^2_{min} = \frac{\gamma(df_u + g_v)}{2d} \quad \rightarrow k^2 \text{ for } h_{min}$$

$\Rightarrow$

$$h(k^2)_{min} = \gamma^2\left[\det A - \frac{(d f_u + g_v)}{4d}\right]$$

$\therefore$ condition for instability for finite, $\neq 0$ k^2 is $h_{min}(k^2) < 0 \Rightarrow$

$$\boxed{\frac{(d f_u + g_v)^2}{4d} > \det A}$$

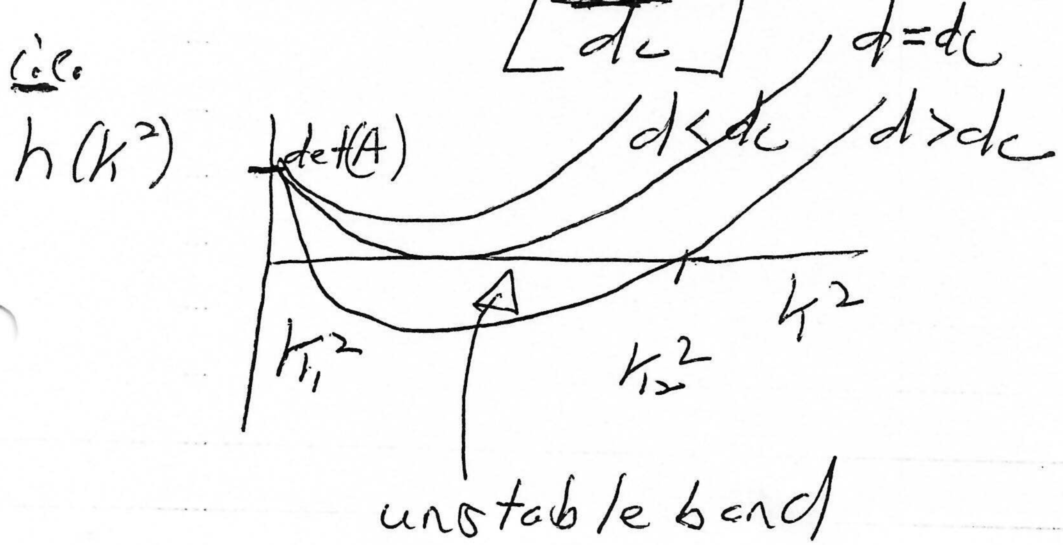
Note: - defines condition for Turing instability
- defines critical value d for Turing instability: i.e.

$$d_{crit}^2 f_u^2 + 2(2 f_v g_u - g_v f_u) d_c + g_v^2 = 0$$

- defines k_{crit}

$$k_{crit}^2 = \gamma\left[\frac{\det A}{d_c}\right]^{1/2}$$

i.e.



$\frac{\partial u}{\partial t} = \gamma f(u,v) + \nabla^2 u$
$\partial v/\partial t = \gamma g(u,v) + d\nabla^2 v$ $\Big\}$ 2 Field Reaction-Diffusion (Turing)

...) Reaction-Diffusion Systems - Example II

→ Recall conditions/characteristics of Turing instability:

① linearly stable fixed point of homogeneous system i.e. for u_0, v_0:

$$\frac{\partial \underline{w}}{\partial t} = \gamma \underline{\underline{A}} \cdot \underline{w} + \underline{\underline{D}} \cdot \underline{w}''$$

$$\mathrm{tr} A = f_u + g_v < 0$$
$$\det A = f_u g_v - f_v g_u > 0$$

② mode structure from Helmholtz equation

$$\nabla^2 \psi + k^2 \psi = 0 \quad ; \quad \hat{n} \cdot \underline{\nabla} \psi = 0 \text{ on boundary}$$

③ instability with diffusion (i.e. spatial coupling), i.e. $h(k^2) < 0$

$$h(k^2) = dk^4 - \gamma(d f_u + g_v) k^2 + \gamma^2 \det A$$

$$\Rightarrow d f_u + g_v > 0 \Rightarrow d \neq 1$$

then obtain spatio-temporal instability (pattern) with:

- threshold $\frac{(d f_u + g_v)^2}{4d} > \det A$

$\Rightarrow$ critical d (d_c):

$$d_c^2 f_u^2 + 2(2 f_v g_u - f_u g_v) d_c + g_v^2 = 0$$

② $K_{crit} = \gamma \left[\frac{\det A}{d_c}\right]^{1/2} = \gamma \left[\frac{f_u g_v - f_v g_u}{d_c}\right]^{1/2}$

i.e. unstable wave-# at threshold → sets pattern scale

③ range of unstable wave #'s:

$$k_1^2 < k^2 < k_2$$

$$k_1^2 = \left[\gamma(d f_u + g_v) - \gamma\{(d f_u + g_v)^2 - 4 d \det A\}^{1/2}\right] / 2d$$

$$k_2^2 = \left[\gamma(d f_u + g_v) + \gamma\{(d f_u + g_v)^2 - 4 d \det A\}^{1/2}\right] / 2d$$

→ Consider some generic questions in pattern formation;

① How does structure in pattern depend on size of system? (as embryo grows ⟷ structure increases)

i.e. consider 1D system

$$u'' + \gamma f(u,v) = 0 \qquad u'(0) = u'(1) = 0$$

$$d v'' + \gamma g(u,v) = 0 \qquad v'(0) = v'(1) = 0$$

(i) $\otimes u$
(ii) $\otimes v$ } and integrating, adding

$$H=\int_0^1 (u'^2+v'^2)\,dx = \frac{\gamma}{d}\int_0^1 \left[d\,u f(u,v)+v g(u,v)\right]dx \quad \underline{B.}$$

heterogeneity function } measure of spatial structure in pattern (akin energy in statics)

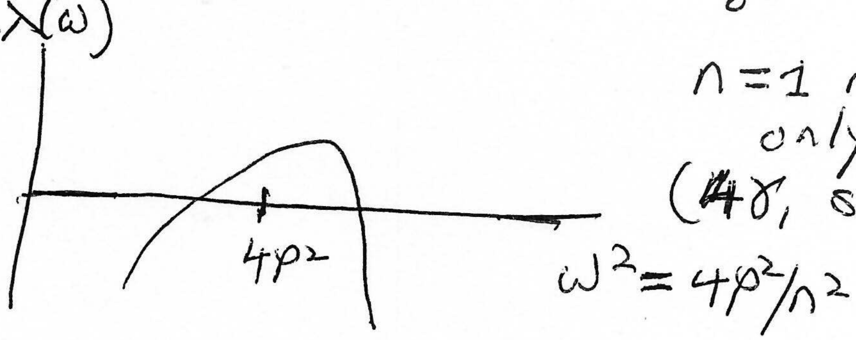
now $H \geq 0$; $H=0$ for const. solution (diffn)

$H \sim \gamma/d \sim L^2$! ⇒ heterogeneity increases as square of box size! ($\underline{1D}$)

② → What kind of spatial structure results?
→ What is role of macro-geometry? → What is impact of symmetry and what kind of patterns result?

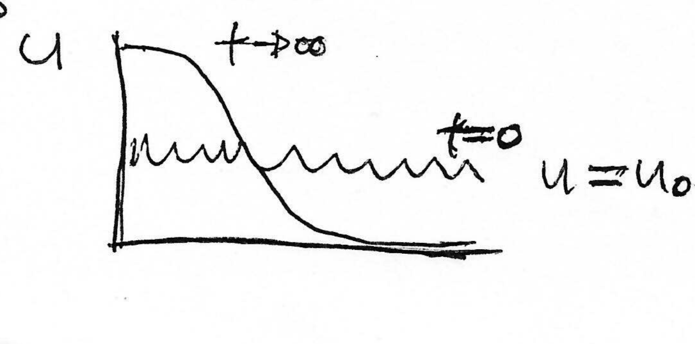
→ All $\underline{\text{spatial}}$ structure follow from $\nabla^2\psi + k^2\psi = 0$. B.C.'s quantize k!

i.e. in 1D,

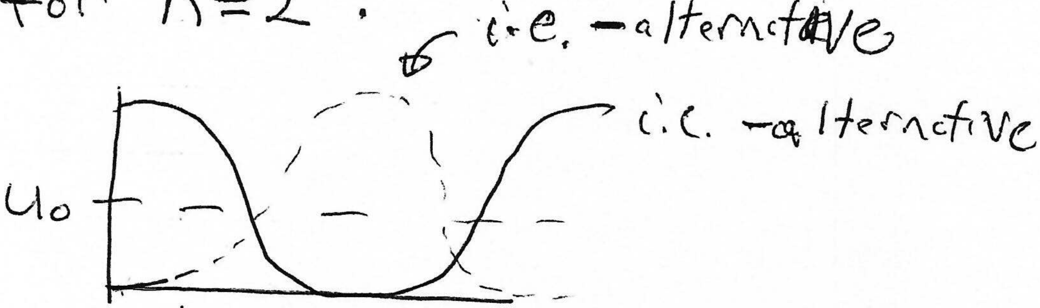


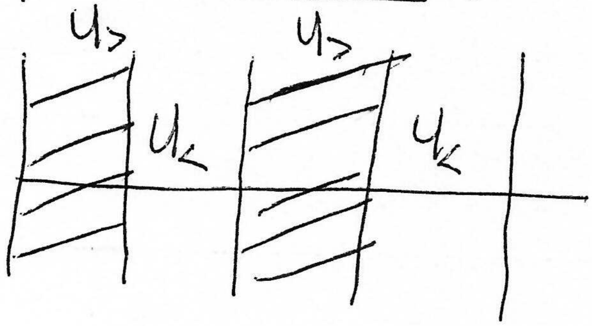
n = 1 mode only (4γ, size)

⇒



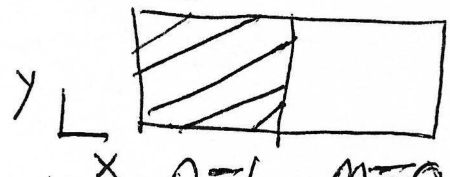
for $n=2$:





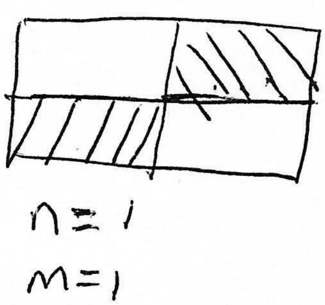
etc.

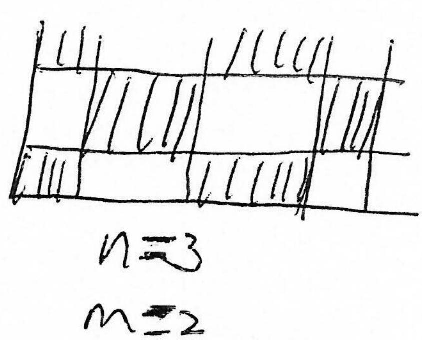
i.e. in 2D → checkerboard pattern



etc.

$n \leftrightarrow x$
$m \leftrightarrow y$





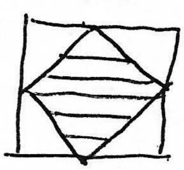
etc.

→ can also demand

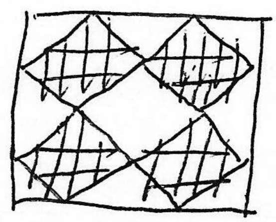
- pattern cover surface
- " " exhibit symmetry { i.e. square, hexagonal, rhombic

∴ set is tesselations of plane by Helmholtz solutions of symmetry

e.g. a) Square symmetry



$k = \pi$



$k = 2\pi$

etc.

$$\underset{\substack{\uparrow \\ \text{square symm.}}}{S}\, \psi(r, \theta) = \psi\left(r, \theta + \frac{\pi}{2}\right) = \psi(r, \theta)$$

square symm. – invariance under $\frac{\pi}{2}$ rotation.

soln: $\psi_s = \dfrac{\cos kx + \cos ky}{2}$ { standing wave in both directions

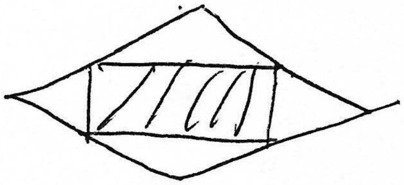
$$= \frac{\cos(kr\cos\theta) + \cos(kr\sin\theta)}{2}$$

clearly $S\psi_s = \psi_s$ ✓

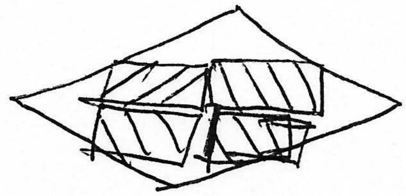
b) rhombic

$$R\,\psi(r,\theta,\phi) = \psi(r,\theta+\pi,\phi) = \psi(r,\theta,\phi)$$

rhombus ∡ (phase)



$k=\pi$



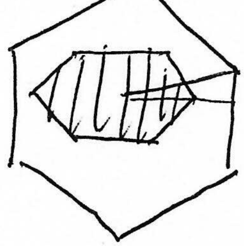
$k = 2\pi$

$$\psi(x,y) = \left[\cos kx + \cos k(x\cos\phi + y\sin\phi)\right]/2$$
$$= \left[\cos(kr\cos\theta) + \cos(kr\cos(\theta-\phi))\right]/2$$

c) hexagonal

ψ invariant under $\pi/3$ rotation

i.e.



etc.

$$H\,\psi(r,\theta) = \psi(r,\theta+\pi/3) = \psi(r,\theta)$$

$$\psi(x,y) = \left[\cos(kr(\theta+\pi/6)) + \cos(kr(\theta-\tfrac{\pi}{6})) + \cos(kr(\theta-\tfrac{\pi}{2}))\right]/3$$

3) Give detailed example !?

Consider Schnackenberg system (10):

$$\frac{\partial}{\partial t} u = \gamma f(u,v) + u_{xx}$$
$$= \gamma(a - u + u^2 v) + u_{xx}$$

$$\frac{\partial}{\partial t} v = \partial_t v = \gamma(b - u^2 v) + d\, v_{xx}$$

stationary states: $f = g = 0$

$$v_0 = \frac{u_0 - a}{u_0^2} \qquad \Rightarrow \begin{cases} u_0 = a + b \\ v_0 = b/(a+b)^2 \end{cases}$$
$$b = u_0 - a$$

$\Rightarrow$

$$f_u = \frac{b-a}{a+b}, \quad f_v = (a+b)^2$$

$$g_v = -(a+b)^2, \quad g_u = \frac{-2b}{a+b}.$$

$\therefore$ $\operatorname{tr} A < 0$ $\quad f_u + g_v < 0$

$\Rightarrow$ $0 < b - a < (a+b)^3$

$\det A > 0$

$\Rightarrow (a+b)^2 > 0$ ✓

also need: $\quad d f_u + g_v > 0 \qquad (h<0)$

$$\Rightarrow d(b-a) > (a+b)^3$$

$$(d f_u + g_v)^2 > (\det A)\, 4d \qquad \text{(threshold)}$$

$$\Rightarrow \left[d(b-a) - (a+b)^3\right]^2 > 4d(a+b)^4$$

$\Rightarrow (a, b, d)$ define <u>Turing space</u> via constraints:

$\operatorname{tr} A < 0, \quad h < 0, \quad$ threshold

- space defines regime of Turing instability
- overlap of space with geometrically allowed $k_i \Rightarrow$ eigenvalues

For range unstable modes:

$$\gamma L = k_1^2 < k^2 = \left(\frac{n\pi}{a}\right)^2 < k_2^2 = \gamma M$$

$$\begin{matrix} L \\ M \end{matrix}(a,b,d) = \left(\left[d(b-a) - (a+b)^3\right] \mp \left\{\left[d(b-a) - (a+b)^3\right]^2 - (a+b)^4 4d\right\}^{1/2}\right) \Big/ 2d(a+b)$$

etc.

v.) Coat Patterns in Mammals

→ Very important questions:

- why do cats have ringed tails? (usually)
- Origin of zebra scapular stripes?

embryo

melanoblasts (migrate during gestation)

→ Basic ideas of origin of markings:

- hair color determined by melanocytes located in basal epidermis

melanoblasts → ∘∘∘ → melanocytes → color (after activation)

- melanocytes generate melanin ⇒ skin and hair color

⊛ - release of diffusing activator chemical triggers release of melanin

⊛ - location of melanocytes determined by location of melanoblasts, which migrate over embryo during gestation

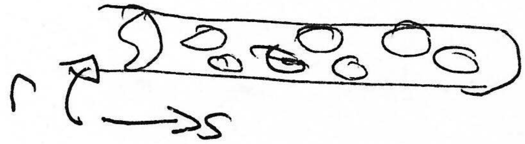
so { melanoblasts - migrates
{ melanocytes
{ activator chemical - diffuses

⇒ { classic 2-field reaction-diffusion

As results generic, can proceed using existing insight! 10%

→ cats tail

For tail 'long and thin' during embryogenesis, might expect



i.e. spots, a la' leopards body

but { reaction-diffusion system must satisfy boundary condition ⇒ quantization of eigenvalue; i.e. Helmholtz

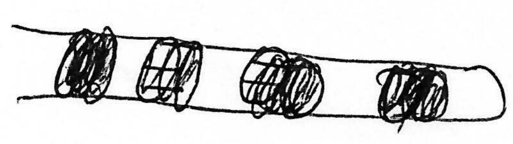
i.e. $K^2 = \frac{n^2}{r^2_{tail}} + \frac{m^2\pi^2}{S^2_{tail}}$ { cylindrical surface

$n \neq 0$ outside unstable band

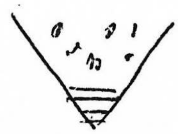
now $S^2 \gg r^2$ (long/thin) ⇒ $K^2_{n \geq 1} \gg K_c$

∴ allowed modes likely have { $n = 0$, $m =$ finite

⇒ 1D pattern of striped tail:



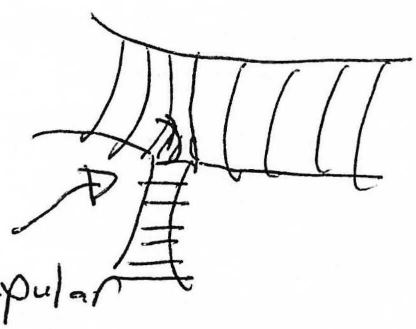
explains why - cats' tails generally ringed
- Leopard tail striped at tip

i.e. pre-natal leopard tail  → stubby

hence $r^2 \leq s^2$ ⇒ can have $r \neq 0$, except near tip ⇒ spotty tail

→ illustrates timing significance in Morphogenesis

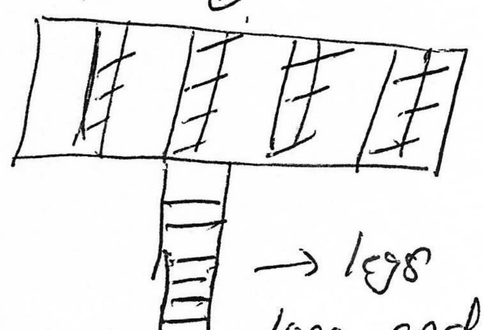
→ zebra scapular stripes



scapular stripes

from

stripes set in early embryogenesis

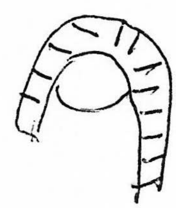


→ legs long and thin.

⇒ rings !

embryo is strongly anisotropic ⇒ stripes appear on flattened body. Legs appear later.

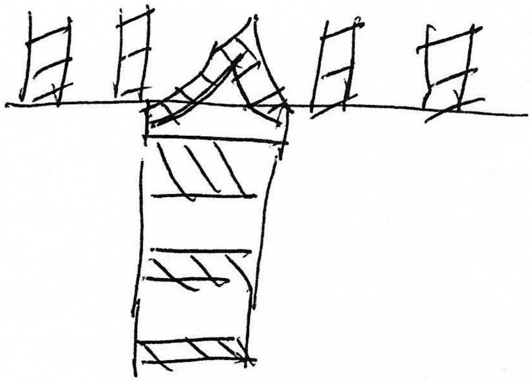
i.e.



Thus, leg - body juncture akin to "fringing field"

10%

i.e.



scapular stripes.