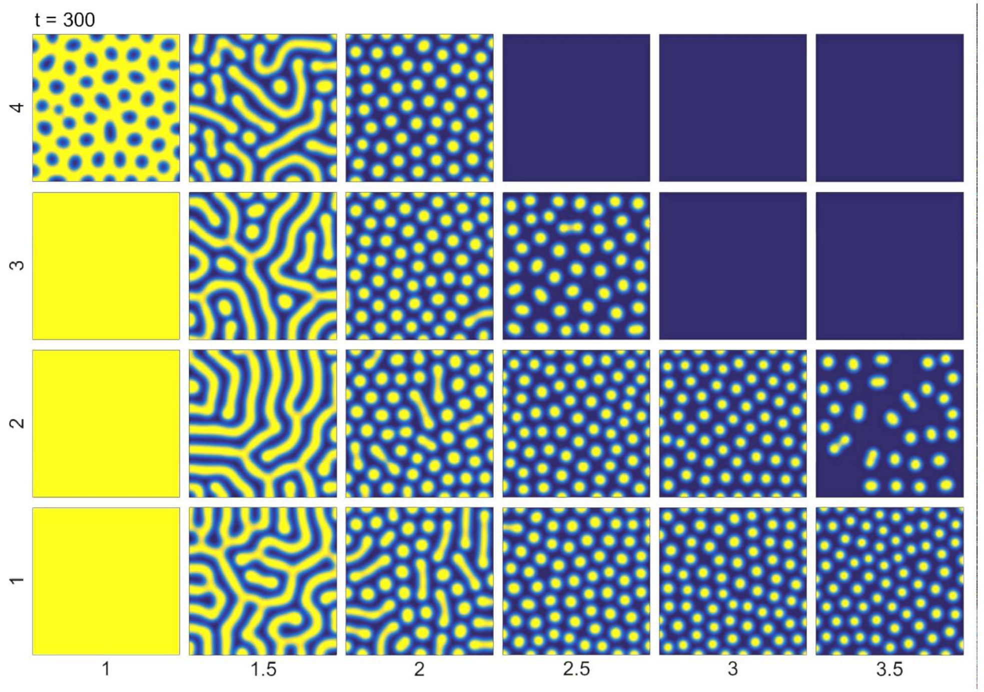
Continuous Field Models



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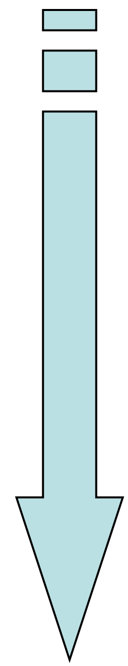
Continuous Field Models

Increasing the number of variables

- Models with small degrees of freedom
  - No spatial extension
- Models with large degrees of freedom
  - Spatial extension
- Continuous field models
  - Infinite number of variables -> Functions
  - Continuous spatial extension

Fewer variables



More variables

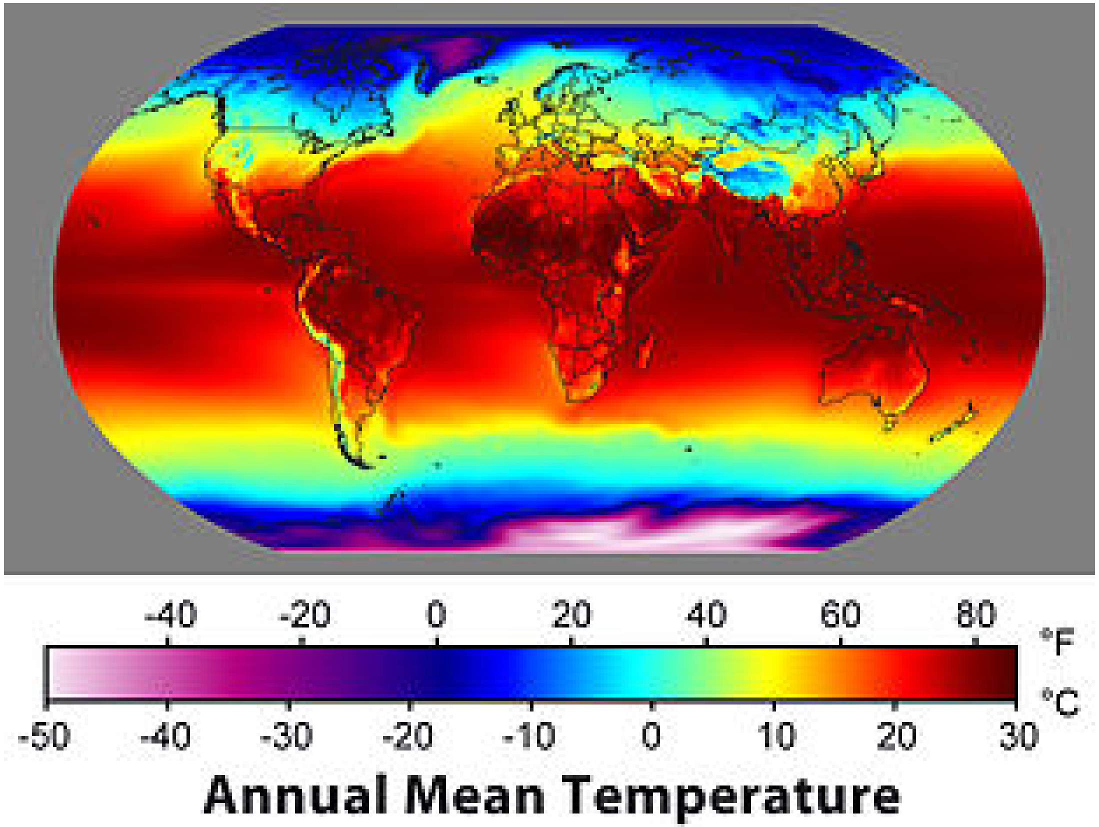
Continuous field models

- A system's state is represented by a function that maps each spatial location to a local state value/vector
- Dynamics are described typically using partial differential equations (PDEs)
- Analytical treatments may still be possible; may give us important solutions and insights

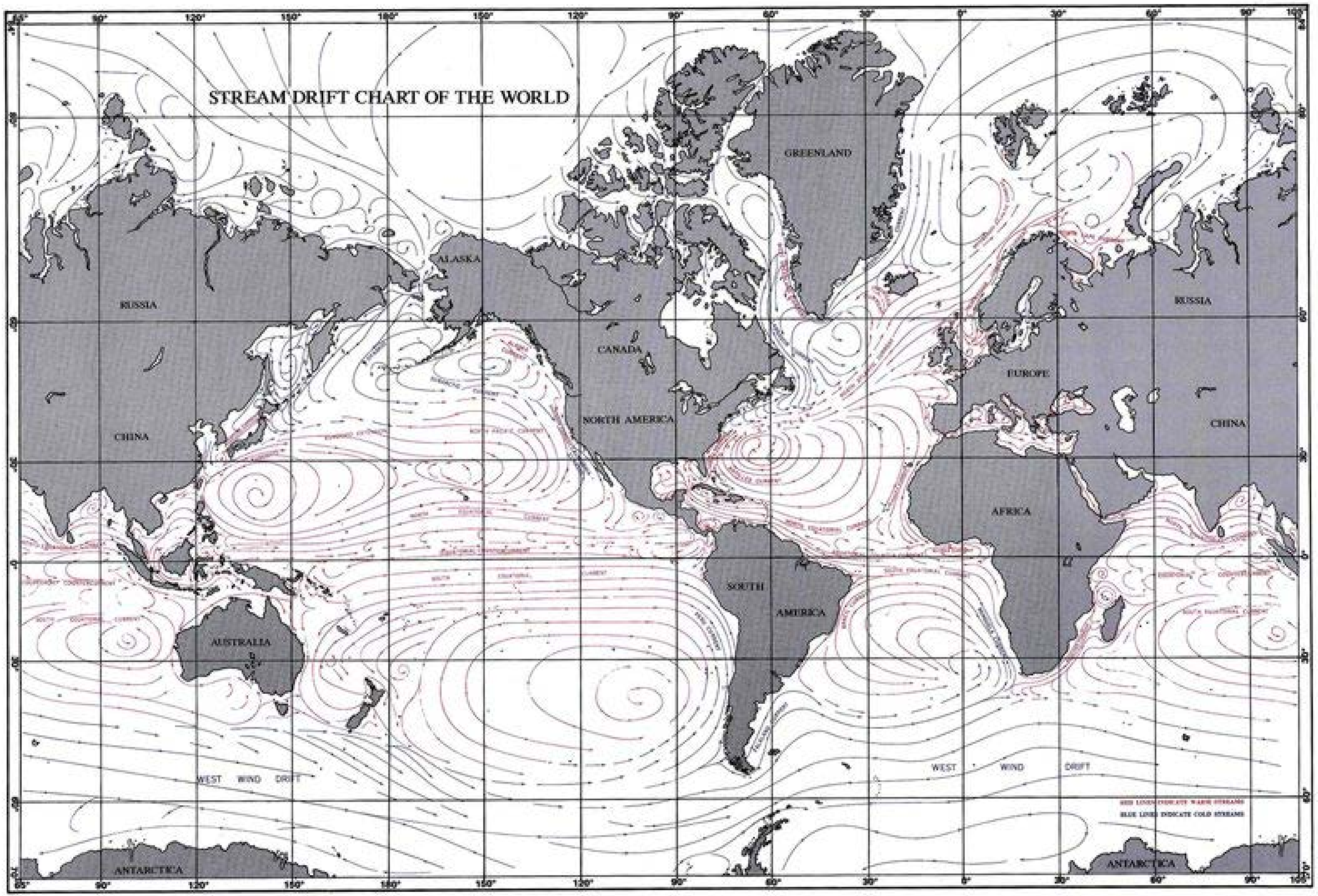
Spatial function as a "state"

- The state of a PDE-based system is defined by a function $f(x,t)$
  - A **field** made of local states defined over a continuous spatial domain
- **x:** spatial location (vector)
- **f(x,t):** local state (scalar or vector)
  - Population density (scalar)
  - Chemical concentration (scalar or vector)
  - Local flow (vector)

Example of a scalar field



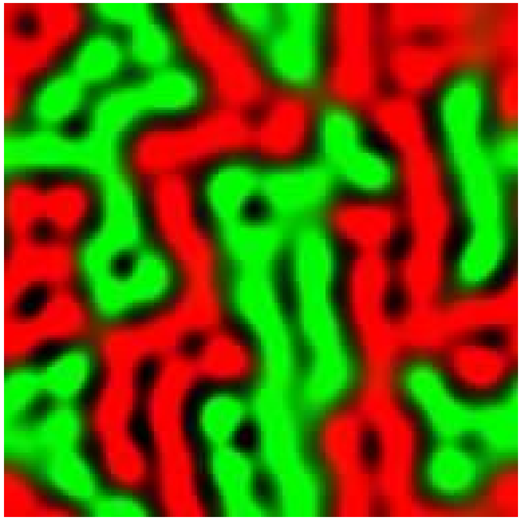
Example of a vector field



Global ocean current in 2004. Source: National Geospatial intelligence agency

Spatio-temporal patterns

- If a system has spatial extension, nonlinear interactions among local parts may spontaneously create patterns from initially uniform conditions
  - May be static or dynamic
  - Seen in many aspects of biological systems
    - Morphogenesis
    - Neural/muscular activities
    - Population distribution



A couple of fundamentals (1)

- Contour (aka. level curve/surface):
  - a set of points x that satisfy $f(x)$ = constant for a scalar field f
- Gradient:
  - a vector locally defined by $\nabla f = (\partial f/\partial x_1, \partial f/\partial x_2, \ldots)$ for a scalar field f
    - ∇ is read "del" or "nabla"
    - Shows direction of steepest ascending slope
    - Magnitude tells the steepness
    - Always perpendicular to level curve/surface (unless it is a zero vector at critical points)

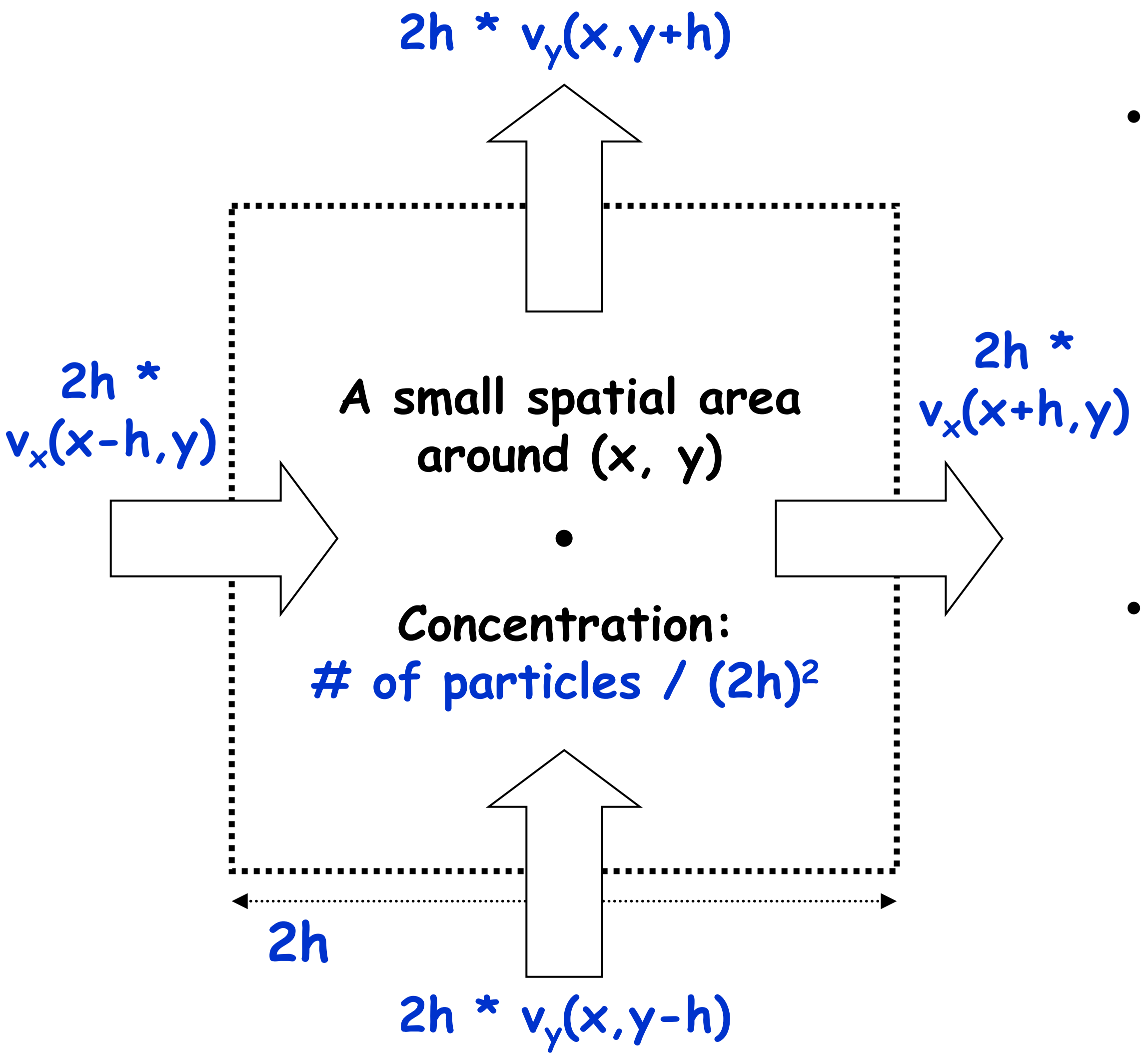
A couple of fundamentals (2)

- **Gradient field:**
  - a vector field ∇f defined over a scalar field f
- **Divergence:**
  - a scalar field

    $$\nabla \cdot \mathbf{v} = (\partial/\partial x_1, \partial/\partial x_2, \ldots) \cdot (v_1, v_2, \ldots)$$
    $$= \partial v_1/\partial x_1 + \partial v_2/\partial x_2 + \ldots ,$$

    defined over a vector field $\mathbf{v}$
    - Quantifies the tendency of the vector field to diverge from the location $(x_1, x_2, \ldots)$

What a divergence means



- Divergence > 0 means something is draining out of the point ("divergence")
- Divergence < 0 means something is coming in to the point

A couple of fundamentals (3)

- Laplacian:
  - a scalar field

    $\nabla^2 f = \nabla \cdot \nabla f$

    $= (\partial/\partial x_1,\ \partial/\partial x_2,\ \ldots) \cdot (\partial f/\partial x_1,\ \partial f/\partial x_2,\ \ldots)$

    $= \partial^2 f/\partial x_1^2 + \partial^2 f/\partial x_2^2 + \ldots\ ,$

    defined over a scalar field f
    - $\nabla \cdot \nabla$ is sometimes read "div dot grad"
    - Is positive and large around valleys of f
    - Is negative and small around peaks of f
    - Plays an important role in diffusion equations

Visualizing 2D continuous fields

- To visualize a scalar field:
  - plot_surface (needs Axes3D)
  - contour
  - imshow

- To visualize a vector field:
  - streamplot

Examples

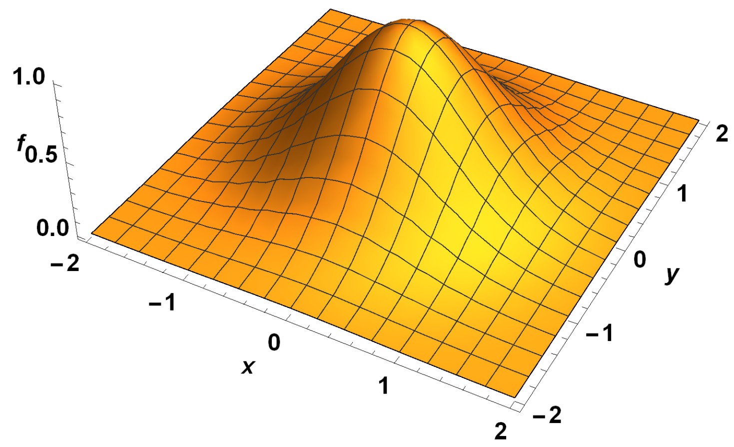


Figure 13.1: Example of a spatial function (field) defined over a two-dimensional space. The function $f(x, y) = e^{-(x^2+y^2)}$ is shown here.

Examples

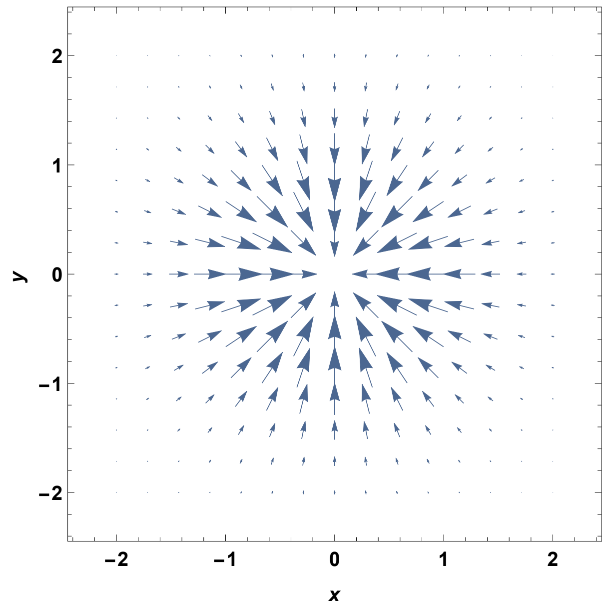


Figure 13.3: Gradient field of a spatial function $f(x, y) = e^{-(x^2+y^2)}$.

Examples

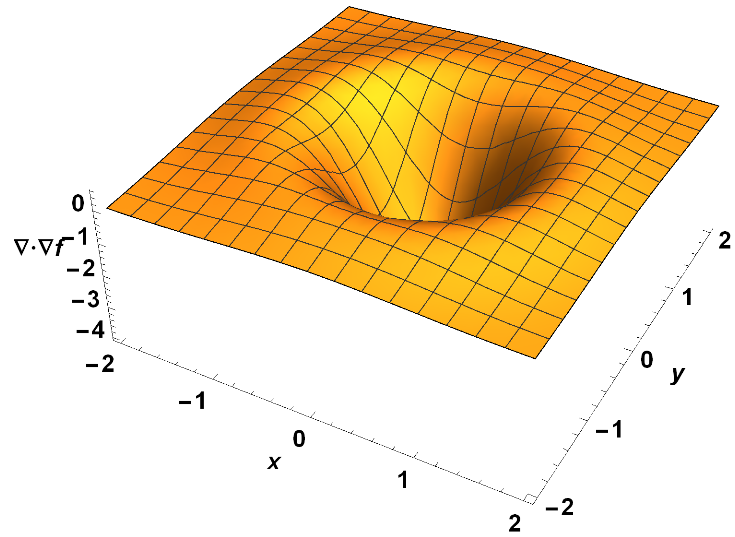


Figure 13.5: Laplacian (i.e., divergence of a gradient field) of a spatial function $f(x, y) = e^{-(x^2+y^2)}$. Compare this figure with Fig. 13.1.

Modeling Spatial Movement

Spatio-temporal dynamics in PDEs

- The dynamics of a continuous-field model may be given by:

  $$\partial f/\partial t = F(f, x, t)$$

  - If F doesn't include t, the system is autonomous
  - F may include partial derivatives of f over x_1, x_2, … etc.
  - If f is defined as a vector, separate equations should be defined for each f_i

Example: Transport equation (1)

$$\frac{\partial c}{\partial t} = -\nabla \cdot J(x,t) + s(x,t)$$

c: concentration at (x, t) (number of particles per unit of volume)

J: flux at (x, t) (a vector field that tells the number of moving particles per unit of volume & time and their direction)

s: source/sink at (x,t)

Example: Transport equation (2)

$$\frac{\partial c}{\partial t} = - \nabla \cdot (c(x,t)\, v(x,t)\ ) + s(x,t)$$

c: concentration at (x, t) (number of particles per unit of volume)

v: trend at (x, t) (a vector field that tells the velocity of moving particles)

(i.e. $v(x,t) = J(x,t) / c(x,t)$)

Deriving diffusion equation (1)

$$\frac{\partial c}{\partial t} = -\nabla \cdot J(x,t) + s(x,t)$$

- If the particles obey simple diffusion:
  - $s(x,t)$ should be zero (no source/sink)
  - $J(x,t)$ should be in the opposite direction of the gradient of $c(x,t)$, because the particles tend to move along steepest descending slopes

Deriving diffusion equation (2)

$$\frac{\partial c}{\partial t} = - \nabla \cdot J(x,t) + s(x,t)$$

$$= - \nabla \cdot (-D \nabla c(x,t))$$

(where D is the diffusion coefficient; if D is a constant that doesn't depend on x or t, this further simplifies to)

$$= D \nabla \cdot \nabla c(x,t)$$

$$= D \nabla^2 c(x,t)$$ (Fick's law)

Exercise

- Develop a two-variable PDE model that describes the spatio-temporal dynamics of the following system:
  - People are attracted toward the regions where economy is active
  - Economy is activated by having more people in the region
  - Economy would diminish without people
  - Both populations and economical activities diffuse spatially

Simulating PDE Models

Discretizing time

- Discretize time at interval Δt:

$$\partial f/\partial t = F(f,\ x,\ t)$$

$$\begin{aligned} f_{t+\Delta t}(x) &= f_t(x) + \partial f/\partial t\ \Delta t \\ &= f_t(x) + F(f_t,\ x,\ t)\ \Delta t \end{aligned}$$

  - Spatial derivatives in F should also be replaced with their discrete equivalents

Discretizing spatial derivatives

$$\partial f/\partial x = \lim_{h\to 0} \left(f(x+h,t) - f(x,t) \right) / h$$

- If we make a discrete analog of this by letting $h = \Delta x$:

$$\partial f/\partial x \sim \left(f_t(x+\Delta x) - f_t(x) \right) / \Delta x$$

- If both sides of neighbors are used:

$$\partial f/\partial x \sim \left((f_t(x+\Delta x) - f_t(x)) + (f_t(x) - f_t(x-\Delta x)) \right) / 2\Delta x$$

$$= \left(f_t(x+\Delta x) - f_t(x-\Delta x) \right) / 2\Delta x$$

Discretizing Laplacians (1)

$$\partial^2 f/\partial x^2 = \lim_{h\to 0} (f'(x+h,t) - f'(x-h,t)) / 2h$$

$$= \lim_{h\to 0} \{ \lim_{k\to 0} (f(x+h+k,t) - f(x+h-k,t)) / 2k$$

$$- \lim_{k\to 0} (f(x-h+k,t) - f(x-h-k,t)) / 2k \} / 2h$$

$$= \lim_{h\to 0} (f(x+2h,t) + f(x-2h,t) - 2f(x,t)) / (2h)^2$$

- If we make a discrete analog of this by letting $h = \Delta x/2$:

$$\partial^2 f/\partial x^2$$

$$\sim (f_t(x+\Delta x) + f_t(x-\Delta x) - 2f_t(x)) / \Delta x^2$$

Discretizing Laplacians (2)

- Similarly, for 2-D space:

$$\nabla^2 f = \partial^2 f/\partial x^2 + \partial^2 f/\partial y^2$$

$$\sim (f_t(x+\Delta x,y)+f_t(x-\Delta x,y)-2f_t(x,y)) / \Delta x^2$$

$$+(f_t(x,y+\Delta y)+f_t(x,y-\Delta y)-2f_t(x,y)) / \Delta y^2$$

$$= (f_t(x+\Delta k,y) + f_t(x-\Delta k,y) + f_t(x,y+\Delta k)$$

$$+ f_t(x,y-\Delta k) - 4f_t(x,y)) / \Delta k^2$$

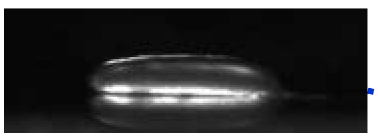
(if $\Delta x = \Delta y = \Delta k$)

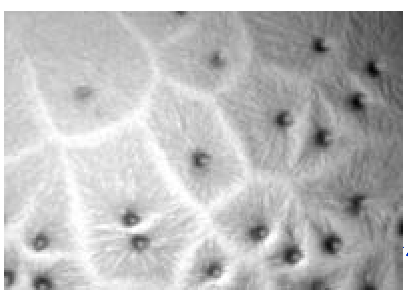
Exercise

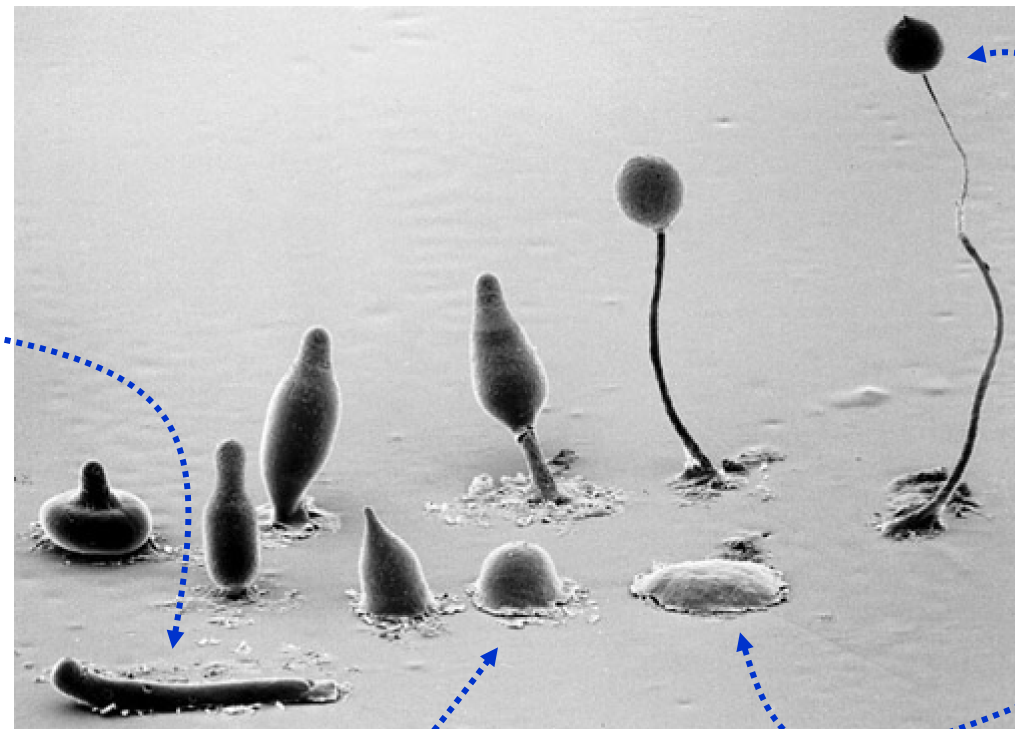
- Simulate the following continuous field models in a 2-D space:
  - Diffusion: $\partial c/\partial t = D\, \nabla^2 c(x,t)$
  - Transport: $\partial c/\partial t = -\nabla \cdot (c(x,t)\, v)$
    - v is a constant vector that represents the velocity of a homogeneous trend

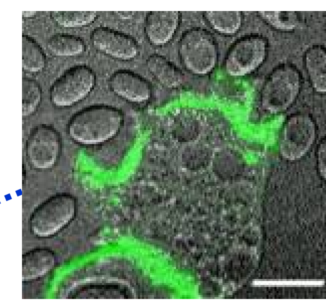
Biological example: Cellular slime mold aggregation

- Model organism: Dictyostelium discoideum









Model of slime mold aggregation

- Developed by Keller & Segel (1970)
- Assumptions:
  - Initially homogeneous distribution of cells
  - Cells undergo random motion (diffusion) and chemotaxis toward cAMP (attractant)
  - Cells neither die nor divide
  - Each cell constantly produce cAMP
  - cAMP shows diffusion and exponential decay

Keller-Segel equations

$$\partial a/\partial t = \mu\nabla^2 a - \chi a\nabla^2 c$$

$$\partial c/\partial t = D\nabla^2 c + fa - kc$$

a: density of cellular slime molds

c: concentration of cAMP

μ: motility of cells

χ: chemotactic coefficient of cells

D: diffusion coefficient of cAMP

f: rate of cAMP secretion by cells

k: rate of cAMP degradation

Reaction-Diffusion Equations

Reaction-diffusion equations

- Continuous field models whose dynamical equations are made of reaction terms and diffusion terms:

$$\partial f_1/\partial t = R_1(f_1, f_2, \ldots) + D_1 \nabla^2 f_1$$

$$\partial f_2/\partial t = R_2(f_1, f_2, \ldots) + D_2 \nabla^2 f_2 \quad \ldots$$

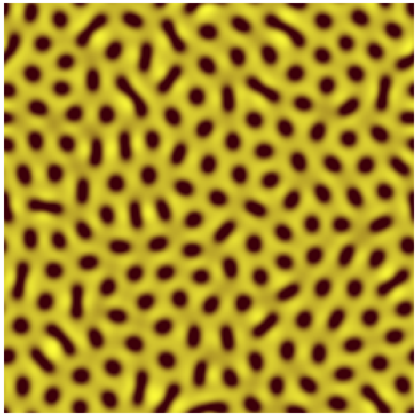
  - R_1, R_2, …: Reaction functions
  - D_1, D_2, …: Diffusion coefficients

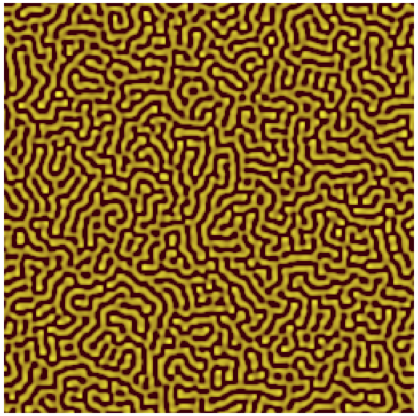
Turing pattern formation

- One of the first R-D systems developed by A. M. Turing in early 1950's

$$\frac{\partial u}{\partial t} = a(u-h) + b(v-k) + D_u \nabla^2 u$$
$$\frac{\partial v}{\partial t} = c(u-h) + d(v-k) + D_v \nabla^2 v$$

  - Explains how animal coat patterns may emerge out of chemical processes





Images generated using online applet by C.G. Jennings at SFU

Belousov-Zhabotinsky reaction (1)

- An "oscillatory" chemical reaction found by B. P. Belousov and then confirmed by A. M. Zhabotinsky in 1950's and 1960's, respectively
- A complex oxidation process of malonic acid ($CH_2(COOH)_2$) by an acidified bromate solution, involving about 30 different chemicals

Belousov-Zhabotinsky reaction (2)

- A simplified "Oregonator" model with no spatial dimension:

$$\epsilon \frac{\partial u}{\partial t} = u(1-u) - \frac{u-q}{u+q} f v + D_u \nabla^2 u$$

$$\frac{\partial v}{\partial t} = u - v + D_v \nabla^2 v$$

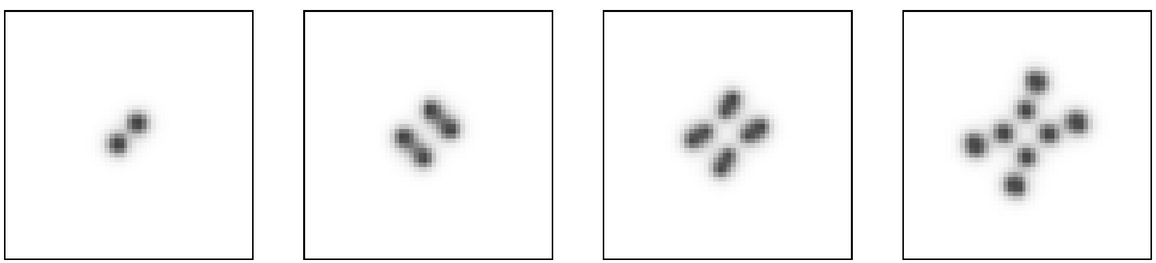
  - **u**: concentration of "activator"
  - **v**: concentration of "inhibitor"

Gray-Scott pattern formation

- Another famous R-D model developed by P. Gray and S. K. Scott in 1983; popularized by J. E. Pearson in 1993

$$\frac{\partial u}{\partial t} = F(1-u) - uv^2 + D_u \nabla^2 u$$
$$\frac{\partial v}{\partial t} = -(F+k)v + uv^2 + D_v \nabla^2 v$$

  - May show biological-looking growth, division & death of "spots"



Analytical Treatments of Continuous Field Models

Review: Stability of equilibrium points

- If a system at its equilibrium point is slightly perturbed, what happens?
- The equilibrium point is called:
  - Stable (or asymptotically stable) if the system eventually falls back to the equilibrium point
  - Lyapunov stable if the system doesn't go far away from the equilibrium point
  - Unstable otherwise

Similar analysis is possible for continuous field models

1. Find equilibrium states (i.e., functions, not just points)
   - Homogeneous equilibrium states are often used in analytical treatments
2. Add small perturbations to the equilibrium states
3. Linearize the model equations and see if the perturbations added will grow or shrink

Finding homogeneous equilibrium states

- If the system is in its homogeneous equilibrium state, i.e, $f(x,t)= f_h$:
  - No spatial variation
    - $\rightarrow$ Ignore all spatial derivatives
  - No temporal variation
    - $\rightarrow$ Equate all equations with 0
- Solving the resulting equations tells you homogeneous equilibrium states

Exercise

- Obtain the homogeneous equilibrium state(s) of the Keller-Segel model:

$$\partial a/\partial t = \mu\nabla^2 a - \chi a\nabla^2 c$$

$$\partial c/\partial t = D\nabla^2 c + fa - kc$$

Rescaling variables

- Dynamics of a system won't change qualitatively by linear rescaling of variables (e.g., $x \to \alpha x'$)
- You can set arbitrary rescaling factors for variables to simplify the model equations
- If you have k variables (including time t and space x/y/z…), you may eliminate k parameters

Exercise

- Simplify the Keller-Segel model by rescaling $a \rightarrow \alpha\, a'$, $c \rightarrow \beta\, c'$, $x \rightarrow \gamma\, x'$, (also $y \rightarrow \gamma\, y'$), and $t \rightarrow \delta\, t'$

$$\partial a/\partial t = \mu \nabla^2 a - \chi a \nabla^2 c$$
$$\partial c/\partial t = D\nabla^2 c + fa - kc$$

Linear stability analysis

- Let $\Delta f(x,t)$ be a small, spatially non-homogeneous perturbation between the system's current state $f(x,t)$ and its homogeneous equilibrium state f_h, i.e. $f(x,t) = f_h + \Delta f(x,t)$
- Plug the above form into the model and ignore quadratic terms of $\Delta f(x,t)$
- Study how $\Delta f(x,t)$ behaves over time

A trick for linearization

- Even after ignoring quadratic terms of $\Delta f(x,t)$, the model equations may still include differential operators (e.g., $\partial^2/\partial x^2$)
- But if $\Delta f(x,t)$ is in the shape of an "eigenfunction" of these operators…

$\rightarrow$ They will be replaced by scalar values (eigenvalues) and the equations will be in simple, linear form!!

Eigenfunctions

- An "eigenfunction" f of an operator L is defined by:

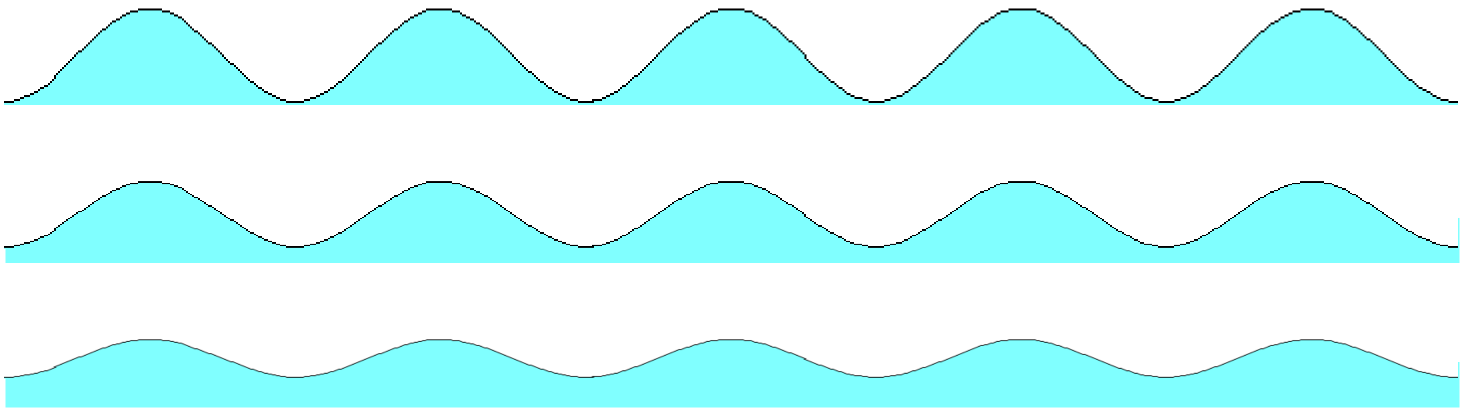
$$L\, f = \lambda\, f$$

  - Where λ is (again) called an "eigenvalue"
  - f is similar to eigenvectors of matrices
  - For $L = \partial/\partial x$: $f(x) = C\, e^{\lambda x}$
  - For $L = \partial^2/\partial x^2$: $f(x) = C_1\, e^{\lambda^{1/2} x} + C_2\, e^{-\lambda^{1/2} x}$
    - This includes sin and cos functions for $\lambda < 0$

What does this mean?

- For $L = \partial^2/\partial x^2$: $f(x) = C_1\, e^{\lambda^{1/2}x} + C_2\, e^{-\lambda^{1/2}x}$
  - This includes sin and cos functions for $\lambda < 0$

- This means that sine waves will not change their shape through diffusion



Exercise

- Sine waves will not change their shape through diffusion
- Show the above fact mathematically in a 1-D space
  - Let $f(x,0) = \sin(qx+p)$ (initial condition)
  - Let $\partial f/\partial t = D\nabla^2 f$ (dynamics)
  - Solve the above equation and show that the solution is still the original sine wave

Linearizing model equations

- For 1-D diffusion-based models, the following perturbation is often used:

$$\Delta f(x,t) = \Delta f(t) \sin(qx+p)$$

  - $\Delta f(t)$: amplitude of small perturbation
  - q: wavenumber (spatial frequency)
  - p: phase offset (you may ignore this)

Exercise

- Linearize the 1-D Keller-Segel model

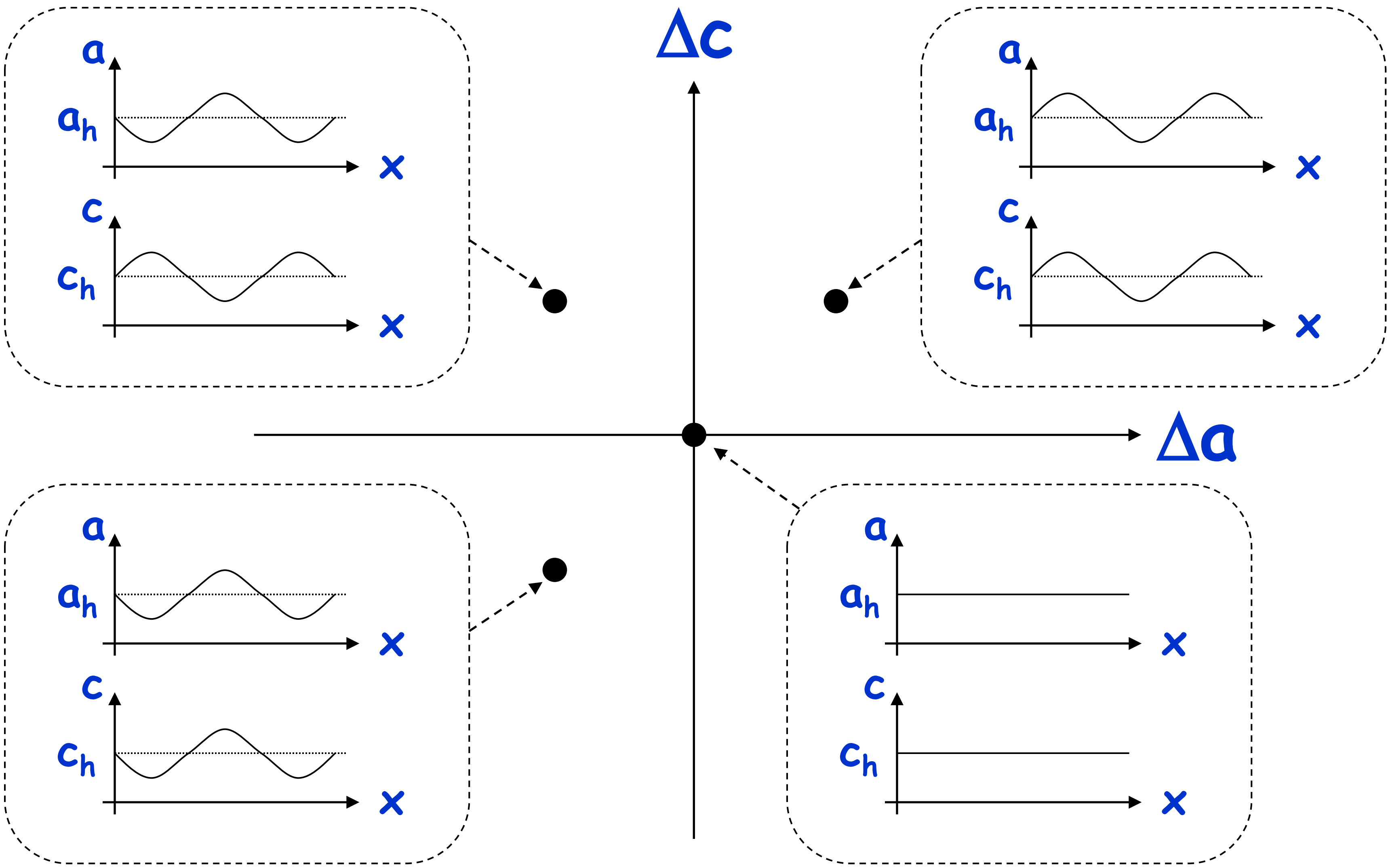
$$\partial a/\partial t = \mu\nabla^2 a - \chi a\nabla^2 c$$

$$\partial c/\partial t = D\nabla^2 c + fa - kc$$

around its homogeneous equilibrium state (a_h, c_h), by assuming

$$a(x,t) = a_h + \Delta a(t)\sin(qx+p)$$
$$c(x,t) = c_h + \Delta c(t)\sin(qx+p)$$

Exercise (continued)



Exercise (continued)

- Then cancel all the sin(qx+p) to obtain linearized dynamical equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\Delta a \\ \Delta c\end{pmatrix} = M \begin{pmatrix}\Delta a \\ \Delta c\end{pmatrix}$$

(now we get something very familiar!)

- Study the properties of matrix **M** and obtain the conditions for which the perturbation grows or shrinks

Results

- Condition for instability of homogeneous equilibrium states (i.e., aggregation of cellular slime molds):

$$\mu(Dq^2 + k) < \chi a_h f$$

  - Perturbations whose wavenumbers satisfy this inequality will grow over time; confirm this in numerical simulations
  - Eigenvectors of matrix M tells the relative speeds of growth/shrink of perturbations of a and c

Linear stability analysis of reaction-diffusion systems

- Result of linear stability analysis can be concisely written using Jacobian matrix of reaction terms

$$\frac{\partial}{\partial t}\begin{pmatrix}\Delta f_1\\ \Delta f_2\end{pmatrix} = J\begin{pmatrix}\Delta f_1\\ \Delta f_2\end{pmatrix} - q^2\begin{pmatrix}D_1\,\Delta f_1\\ D_2\,\Delta f_2\end{pmatrix}$$

(Derive the above form yourself)

Diffusion-induced instability

- Some systems have homogeneous equilibrium states which are stable if no diffusion is assumed, but which are unstable when diffusion is allowed
- Mechanism that accounts for spontaneous emergence of Turing patterns