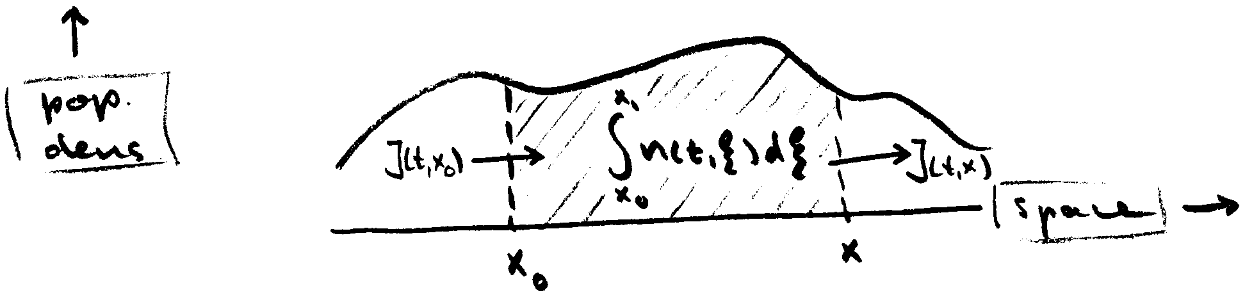
27-03-2012

Movement in space



$n(t,\xi)$ pop. dens. at time t and location ξ.

$\int_{x_0}^{x} n(t,\xi)\,d\xi$ number of individuals at time t and between locations x_0 and x

$J(t,\xi)$ net flux of individuals at time t and location ξ.

$$\Longrightarrow \quad \partial_t \int_{x_0}^{x} n(t,\xi)\,d\xi = J(t,x_0) - J(t,x)$$

Differentiation w.r.t. x gives

$$① \quad \boxed{\partial_t n(t,x) = -\partial_x J(t,x)}$$

Question is what $J(t,x)$ looks like.

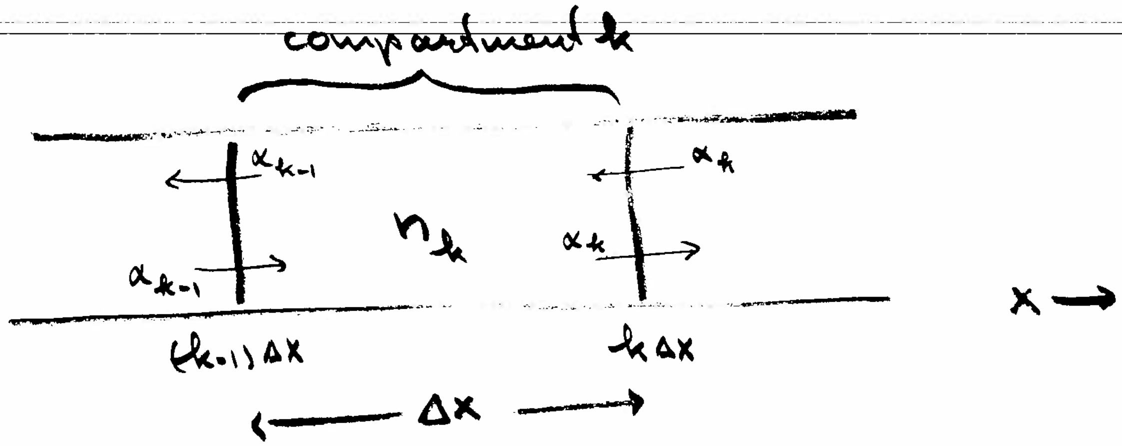
The flux $J(t,x)$ is a pop-level thing, namely, the number of individuals per unit of time moving through x from the left minus the number of individuals moving through x from the right.

How do we connect $J(t,x)$ to ind.-level phenomena.

First we make this connection for randomly moving individuals. Later we extend this to other modes of movement such as advection and taxis.

Random movement

Compartment model



$\boxed{\text{i-states}}$ N_k an individual in comp. $k \in \mathbb{Z}$.

$\boxed{\text{i-process}}$ $N_k \underset{\alpha_k}{\overset{\alpha_k}{\rightleftarrows}} N_{k+1}$ (movement between comps. k and $k+1$)

$\boxed{\text{p-state}}$ n_k number of individuals in compartment $k \in \mathbb{Z}$.

Define the net flux between compartments k and $k+1$:

(2) $$\boxed{J_k(t) := \alpha_k(t)\, n_{k+1}(t) - \alpha_k(t)\, n_k(t)}$$

The idea now is to let comp. size Δx go to zero to get a continuous description of space.

As Δx goes to zero, the α_k should go to infinity, because the prob. per unit of time of hitting the boundary of a compartment goes to infinity as the compartments become smaller.

As Δx goes to zero, we also want to describe pop size as a pop density rather than in terms of #individuals per compartment, because in the limit $\Delta x \to 0$, the notion of "compartment" becomes meaningless.

To this end we define the following continuously differentiable interpolating functions:

$$\circledast \begin{cases} n(t, k\Delta x) := \dfrac{n_k(t)}{\Delta x} & \forall k \in \mathbb{Z}. \\ \alpha(t, k\Delta x) := (\Delta x)^2 \alpha_k(t) & \forall k \in \mathbb{Z}. \end{cases}$$

and

$$J(t, k\Delta x) := J_k(t) \qquad \forall k \in \mathbb{Z}.$$

Then, from ② on page 3, we get

$$③ \quad \boxed{J(t, k\Delta x) = -\alpha(t, k\Delta x) \frac{n(t, k\Delta x + \Delta x) - n(t, k\Delta x)}{\Delta x}}$$

Letting $\Delta x \to 0$ and $k \to \infty$ such that $k\Delta x =: x$ stays constant, we get

$$④ \quad \boxed{J(t,x) = -\alpha(t,x)\, \partial_x n(t,x)}$$

- This is called "Fick's Law" for randomly moving particles.
- $\alpha(t,x)$ is called the diffusion coefficient.

Substitution of ④ (page 5) into ① (page 1) gives the diffusion equation

⑤ $$\boxed{\partial_t n(t,x) = \partial_x \big(\alpha(t,x)\, \partial_x n(t,x)\big)}$$

which is also called the heat equation (because it also describes the transport of heat in a given material).

If $\alpha(t,x) = D$ is a constant, we get the (maybe) more familiar form

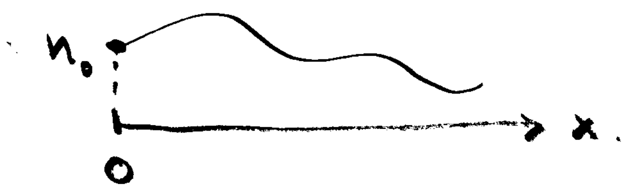
⑥ $$\boxed{\partial_t n(t,x) = D\, \partial_x^2 n(t,x)}$$

From definition ⊛ on page 5 it follows that $2\alpha(t,x)$ is the expected distance-squared travelled per unit of time per individual.

Boundary conditions

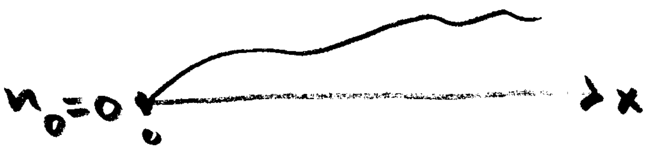
Frequently encountered boundary conditions:

- **Constant concentration boundary**



$$n(t,0) = n_0 \quad \forall t$$

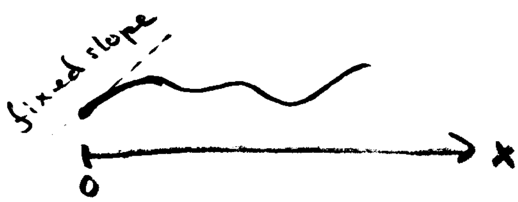
Special case: Absorbing boundary



$$n(t,0) = 0 \quad \forall t.$$

- **Constant flux boundary**

(Case of diffusion with a constant diffusion coefficient)



$$\alpha(t,0)\,\partial_x n(t,0) =$$
$$= D\,\partial_x n(t,0)$$

is constant for all t.

Special case: <u>Reflecting boundary</u>

(again for <u>constant</u> diff coeff.)

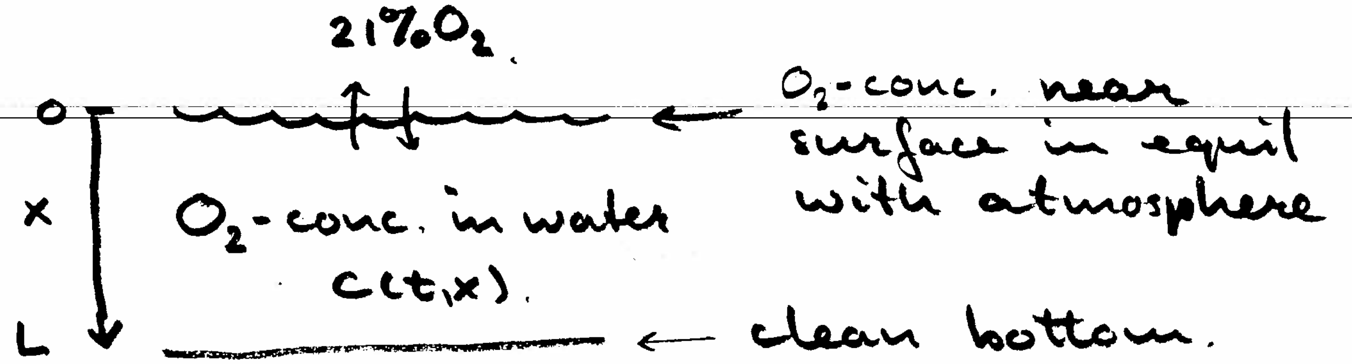
$$\alpha(t,0)\,\partial_x u(t,0) =$$

$$= D\,\partial_x u(t,0) = 0 \quad \forall t.$$

Formulation of the boundary conditions is as much a part of the model formulation as formulation of the flux:

(The bnd. cond. do not follow from the mathematics; they follow from the biology.)

Example I



$$\boxed{\partial_t c = D\,\partial_x^2 c} \quad \text{(diffusion)}$$

$$\boxed{c(t,0) = c_0} \quad \text{(const. conc. bnd. at } x=0\text{)}$$

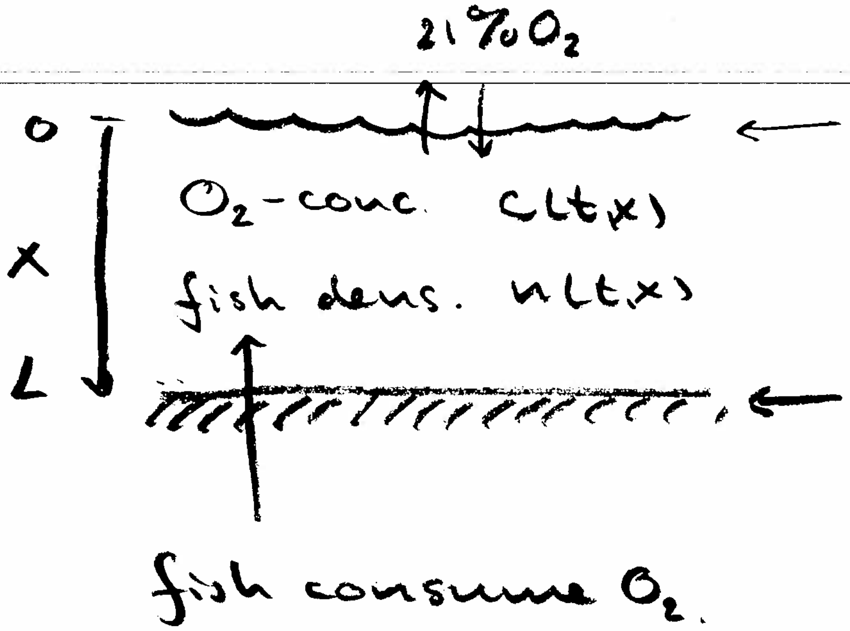
$$\boxed{\partial_x c(t,L) = 0} \quad \text{(refl. bnd. at } x=L\text{)}$$

Reaction-diffusion equations

$$\partial_t n = \partial_x(\alpha\,\partial_x n) + \underbrace{\text{Local reactions}}$$

This part is just the kind of mass-action modeling we did in the first half of the course.

Example II



O_2-conc. near surface in equil with atmosphere

Bacteria in detritus layer absorb all oxygen near bottom

$$\boxed{\begin{aligned} \partial_t c &= D_1 \partial_x^2 c - \beta c n \\ \partial_t n &= D_2 \partial_x^2 n \end{aligned}}$$

O_2 consumption by fish.

$N + O_2 \xrightarrow{\beta} N$ reaction.

$\boxed{c(t,0) = c_0 > 0}$ (constant concentration boundary at $x=0$)

$\boxed{c(t,L) = 0}$ (absorbing boundary at $x=L$)

$\boxed{\partial_x n(t,0) = 0}$ (reflecting boundary at $x=0$)

$\boxed{\partial_x n(t,L) = 0}$ (reflecting boundary at $x=L$)

Equilibrium solution.

We calculate the equilibrium solutions for example II (p. 10).

Setting $\partial_t c = 0$ and $\partial_t n = 0$ we get:

$$\circledast \quad \boxed{\begin{aligned} 0 &= D_1 \partial_x^2 c - \beta c n \\ 0 &= D_2 \partial_x^2 n \end{aligned}} \quad \begin{aligned} &(\text{oxygen}) \\ &(\text{fish}). \end{aligned}$$

From the second equation we get

$$\boxed{n(x) = a + bx}$$

The boundary conditions imply that $b = 0$. and so

$\boxed{n(x) = a}$ (constant).

Let $N_{tot} := \int_0^L n(\xi)\,d\xi$ be the total number of fish, then

$$\boxed{n(x) = \frac{N_{tot}}{L}}$$ (i.e., we write $a = \frac{N_{tot}}{L}$, the average density).

From the first equation in ⊛ we then get

$$\boxed{0 = D_1 \partial_x^2 c - \beta \frac{N_{tot}}{L} c}$$

Note that this is a linear 2^{nd}-order ODE for c.

We can re-write this as a system of 1^{st}-order ODEs:

$$\boxed{\begin{aligned} \partial_x c &= v \\ \partial_x v &= \theta^2 c \end{aligned}} \quad \text{where} \quad \boxed{\theta := \frac{\beta}{D_1} \frac{N_{tot}}{L}}$$

In matrix notation:

$$\partial_x \begin{pmatrix} c \\ v \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ \theta^2 & 0 \end{pmatrix}}_{\text{matrix } A.} \begin{pmatrix} c \\ v \end{pmatrix}$$

Eigen value problem:

$$\boxed{AB = B\Lambda}$$

where Λ is a diagonal matrix with the eigenvalues of A as entries, and where the columns of B are the corresponding eigen vectors (See Appendix A).

$$\boxed{A = B\Lambda B^{-1}}$$

$$\Rightarrow \boxed{\begin{pmatrix} c(x) \\ v(x) \end{pmatrix} = B e^{\Lambda x} B^{-1} \begin{pmatrix} c(0) \\ v(0) \end{pmatrix}}$$

$$B = \begin{pmatrix} 1 & 1 \\ -\theta & \theta \end{pmatrix}, \quad B^{-1} = \frac{1}{2}\begin{pmatrix} 1 & \frac{-1}{\theta} \\ 1 & \frac{1}{\theta} \end{pmatrix}$$

$$\Lambda = \begin{pmatrix} -\theta & 0 \\ 0 & \theta \end{pmatrix}$$

$$\Rightarrow \boxed{c(x) = \frac{v(0)}{\theta} \sinh(\theta x) + c(0) \cosh(\theta x)}$$

Applying the boundary conditions $c(0)=c_0$ and $c(L)=0$ given explicit expressions for $c(0)$ and $v(0)$:

$$\boxed{\begin{aligned} c(0) &= c_0 \\ v(0) &= -c_0\,\Theta\,\mathrm{Coth}(L\Theta) \end{aligned}}$$

and so:

$$\boxed{c(x) = c_0\,\frac{\sinh((L-x)\Theta)}{\sinh(L\Theta)}}$$

which is the equil. solution for the O_2-concentration.