Computer Science in Ocean and Climate Research

Lecture 4: Space-dependent Models

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Recall: General form of a climate model

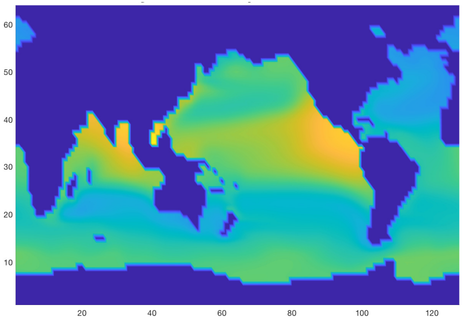
- Model in continuous form:

$$\begin{aligned} \dot{y}(t) &= f(y(t), t), \quad t \in (t_0, T) \\ y(t_0) &= y_0. \end{aligned}$$

- ... in discrete form, with Euler time-stepping:

$$\left.\begin{array}{rcl} y_{k+1} & = & y_k + \Delta t f(y_k, t_k) \\ t_{k+1} & = & t_k + \Delta t \end{array}\right\} k = 0, \ldots, n-1$$

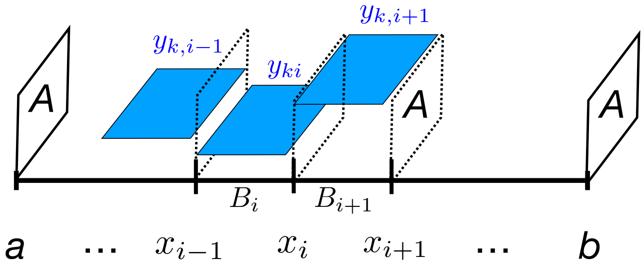
- But: Realistic climate models are space- **and** time-dependent.



simulated distribution of nutrients in one ocean layer

Example: Space discretization in 1-D

- Background/assumption: 3-D model, but all processes constant in two space dimensions.
- ⇝ Build a 1-D simplification: Consider interval $[a, b]$ in the relevant dimension.
- Separated in boxes $B_i := [x_{i-1}, x_i], i = 1, \ldots, N$, with lateral area A.

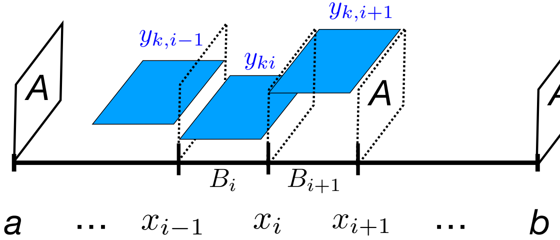


- $y_{ki} \approx y(t_k, B_i)$: mean concentration in (or at midpoint of) box B_i at time t_k.
- Now already the value at the k-th time-step is a vector

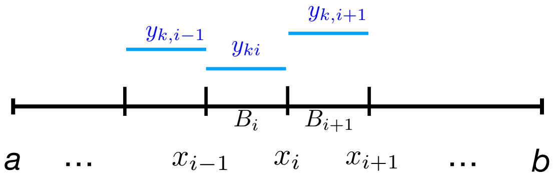
$$y_k = (y_{ki})_{i=1}^N \in \mathbb{R}^N, k = 0, \ldots, n.$$

Example: Simplification from 3-D to 1-D

- 3-D model, but all processes/values constant in two space dimensions.

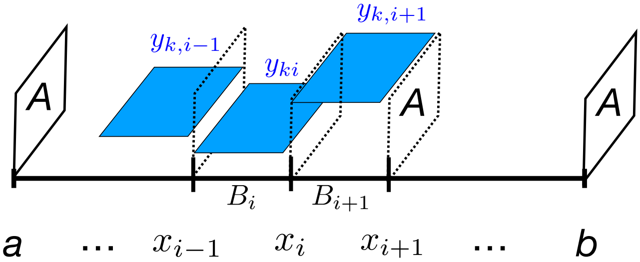


- 1-D simplification: $[a, b]$, separated in boxes $B_i := [x_{i-1}, x_i], i = 1, \ldots, N$.



Example: Space discretization in 1-D

- 1-D simplification:



- Euler time-stepping:

$$\left.\begin{array}{rcl} y_{k+1,i} & = & y_{ki} + \Delta t f_i(y_k, t_k) \\ t_{k+1} & = & t_k + \Delta t \end{array}\right\} \quad k = 0, \ldots, n-1, i = 1, \ldots, N.$$

- Model function/rhd side is now a vector-valued function $f = (f_i)_{i=1}^N$,
- ... one component for every box.

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Predator-prey model in a spatial domain

- Original model (ODE system with two equations):

$$\dot{x} = x(\alpha - \beta y - \lambda x) =: f_1(x, y),$$
$$\dot{y} = y(\delta x - \gamma - \mu y) =: f_2(x, y).$$

No explicit dependency on t in model function $f = (f_1, f_2)$ (**autonomous system**).

- Spatial model: $x_{ki} \approx x(t_k, B_i), y_{ki} \approx y(t_k, B_i)$, ...
- ... mean concentrations in the box or concentrations at midpoint.
- Here, x is the symbol for value of prey species (not for the spatial coordinate).

$$x_k = \begin{pmatrix} x_{k1} \\ \vdots \\ x_{kN} \end{pmatrix}, y_k = \begin{pmatrix} y_{k1} \\ \vdots \\ y_{kN} \end{pmatrix} \in \mathbb{R}^N.$$

- Reactions (growth, death, eating) are point-wise.

$\rightsquigarrow$ Original model is applied in every box independently.

Predator-prey model in a spatial domain

- Original model:

$$\begin{aligned} \dot{x} &= x(\alpha - \beta y - \lambda x) =: f_1(x,y), \\ \dot{y} &= y(\delta x - \gamma - \mu y) \ =: f_2(x,y). \end{aligned}$$

- With explicit Euler:

$$\left.\begin{aligned} x_{k+1} &= x_k + \Delta t\, f_1(x_k, y_k) \\ y_{k+1} &= y_k + \Delta t\, f_2(x_k, y_k) \end{aligned}\right\} \quad k = 0, \dots, n-1.$$

- Spatial model: $x_{ki} \approx x(t_k, B_i), y_{ki} \approx y(t_k, B_i)$, applied in every box independently.
- Model functions f_1, f_2 are now both vector-valued.

$$\left.\begin{aligned} f_{1i}(x_{ki}, y_{ki}) &= x_{ki}(\alpha - \beta y_{ki} - \lambda x_{ki}) \\ f_{2i}(x_{ki}, y_{ki}) &= y_{ki}(\delta x_{ki} - \gamma + \mu y_{ki}) \end{aligned}\right\} \quad i = 1, \dots, N, k = 0, \dots, n-1.$$

Predator-prey model in a spatial domain

- Spatial model: $x_{ki} \approx x(t_k, B_i), y_{ki} \approx y(t_k, B_i)$, applied in every box independently.
- Model functions f_1, f_2 are now both vector-valued.

$$\left.\begin{array}{rcl} f_{1i}(x_{ki}, y_{ki}) & = & x_{ki}(\alpha - \beta y_{ki} - \lambda x_{ki}) \\ f_{2i}(x_{ki}, y_{ki}) & = & y_{ki}(\delta x_{ki} - \gamma + \mu y_{ki}) \end{array}\right\} \quad i = 1, \dots, N, k = 0, \dots, n-1.$$

- Vector notation: $x_k = (x_{ki})_{i=1}^N \in \mathbb{R}^N$, same for y_k.

$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_2(x_k, y_k) & = & y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \dots, n-1,$$

- ... where $x_k * y_k$ means element-wise vector multiplication.
- All boxes independent, interaction between boxes? Movement of individuals?

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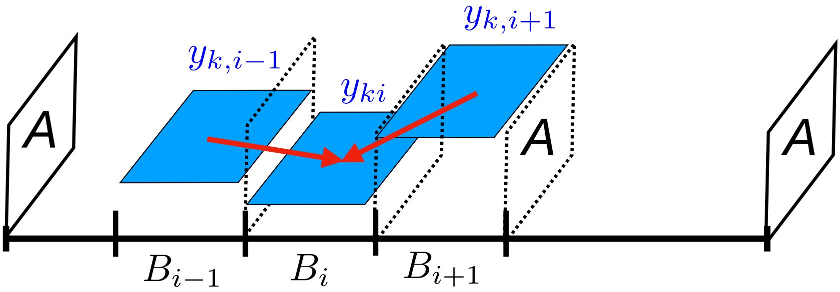
Modeling one important spatial process: Diffusion

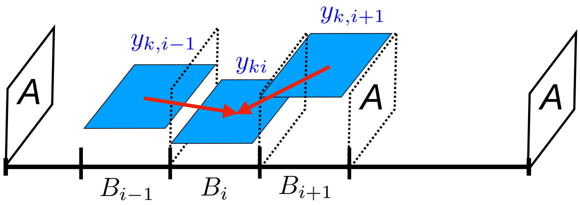
- Diffusion: molecular exchange at box boundaries.
- Evens different concentrations out in spatial neighborhood (i.e., here: boxes).
- Exchange from boxes with high concentrations into boxes with smaller ones.



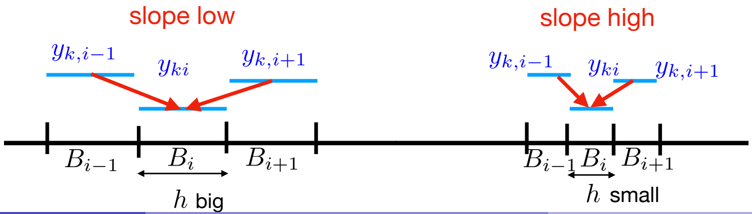
- Exchange depends on the slope of the concentration at the box boundaries.

Modeling one important spatial process: Diffusion

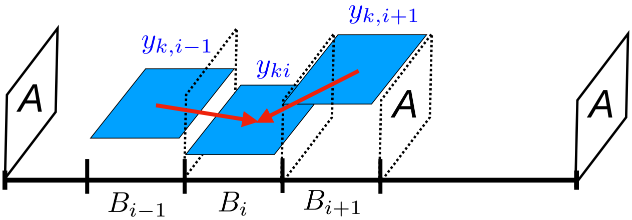
- Exchange from boxes with high concentrations into boxes with smaller ones.



- Exchange depends on the slope of the concentration at the boundaries and thus, on *h*:



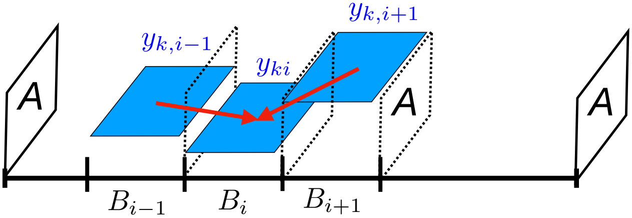
Modeling one important spatial process: Diffusion



- Exchange depends on the slope of the concentration at the boundaries and thus, on h:

$$\underbrace{A\frac{y_{k,i-1} - y_{ki}}{h}}_{\text{exchange } B_{i-1}\to B_i} + \underbrace{A\frac{y_{k,i+1} - y_{ki}}{h}}_{\text{exchange } B_{i+1}\to B_i} = \underbrace{A\frac{y_{k,i-1} - 2y_{ki} + y_{k,i+1}}{h}}_{\text{total exchange } \to B_i} \qquad h : \text{box length (in 1-D).}$$

Modeling one important spatial process: Diffusion



- Total exchange for box B_i:

$$A\frac{y_{k,i-1} - 2y_{ki} + y_{k,i+1}}{h}.$$

- Division by box volume Ah gives change of concentration in box B_i:

$$\frac{y_{k,i-1} - 2y_{ki} + y_{k,i+1}}{h^2}.$$

Modeling one important spatial process: Diffusion

- Change in concentration in box B_i:
$$\frac{y_{k,i-1} - 2y_{ki} + y_{k,i+1}}{h^2}$$
- Change from time-step $k \to k+1$ in box B_i with diffusion constant κ:
$$y_{k+1,i} = y_{ki} + \Delta t \frac{\kappa}{h^2}(y_{k,i+1} - 2y_{ki} + y_{k,i-1}), \quad \text{same for } x_{ki}.$$
- This operation can be described by a matrix:
$$y_{k+1} = y_k + \Delta t\, D y_k \quad \text{with } D = \frac{\kappa}{h^2}\begin{pmatrix} -1 & 1 & & & 0 \\ 1 & -2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & -2 & 1 \\ 0 & & & 1 & -1 \end{pmatrix}$$
- Special behavior at boundaries (no exchange).

Predator-prey model with diffusion

- Recall: Predator-prey model without diffusion,
  Model functions using vector notation: $x_k = (x_{ki})_{i=1}^N \in \mathbb{R}^N$, same for y_k.

$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_1(x_k, y_k) & = & y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \ldots, n-1,$$

- ... where $x_k * y_k$ means element-wise vector multiplication.
- Now: Predator-prey model with diffusion:

$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & Dx_k + x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_2(x_k, y_k) & = & Dy_k + y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \ldots, n-1.$$

- Matrix $D \in \mathbb{R}^{NxN}$: Tridiagonal matrix, N^2 entries, ...
- ... but only $\approx 3N$ nonzeros $\rightsquigarrow$ **sparse** matrix.

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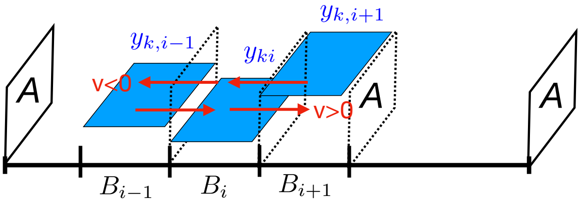
Another spatial process: Transport or advection

- Movement with a given velocity v (e.g., ocean circulation or individual motion).



- Transport into and out of box B_i:

$$v > 0: \quad \underbrace{Avy_{k,i-1}}_{\text{transport into } B_i} - \underbrace{Avy_{ki}}_{\text{transport from } B_i} = Av(y_{k,i-1} - y_{ki})$$

$$v < 0: \quad \underbrace{Avy_{k,i+1}}_{\text{transport into } B_i} - \underbrace{Avy_{ki}}_{\text{transport from } B_i} = Av(y_{k,i+1} - y_{ki}).$$

Another spatial process: Transport or advection

- Transport into and out of box B_i:

$$v > 0 : Av(y_{k,i-1} - y_{ki}), \quad v < 0 : Av(y_{k,i+1} - y_{ki}).$$

- Division by box volume Ah $\rightsquigarrow$ change in concentration due to transport/advection:

$$v > 0 : v\frac{y_{k,i-1} - y_{ki}}{h}, \quad v < 0 : v\frac{y_{k,i+1} - y_{ki}}{h}.$$

$\rightsquigarrow$ Transport/advection matrix:

$$v > 0 : T = \frac{v}{h}\begin{pmatrix} -1 & & & 0 \\ 1 & \ddots & & \\ & \ddots & -1 & \\ 0 & & 1 & \color{red}{0} \end{pmatrix}, \quad v < 0 : T = \frac{v}{h}\begin{pmatrix} \color{red}{0} & 1 & & 0 \\ & -1 & \ddots & \\ & & \ddots & 1 \\ 0 & & & -1 \end{pmatrix}$$

- No transport through boundary (only last element changed).

Predator-prey model with transport and diffusion

- Recall: Predator-prey model without diffusion:

$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_1(x_k, y_k) & = & y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \ldots, n-1,$$

- ... where $x_k * y_k$ means element-wise vector multiplication.
- Predator-prey model with diffusion:

$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & Dx_k + x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_2(x_k, y_k) & = & Dy_k + y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \ldots, n-1.$$

- Predator-prey model with transport and diffusion:

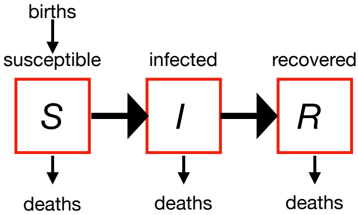
$$\left.\begin{array}{rcl} f_1(x_k, y_k) & = & Tx_k + Dx_k + x_k * (\alpha - \beta y_k - \lambda x_k) \\ f_2(x_k, y_k) & = & Ty_k + Dy_k + y_k * (\delta x_k - \gamma - \mu y_k) \end{array}\right\} \quad k = 0, \ldots, n-1.$$

Contents

Classic endemic model (SIR-model)

- ODE system with three equations:

$$\dot{S} = \alpha N - \delta S - \beta S \frac{I}{N},$$
$$\dot{I} = \beta S \frac{I}{N} - \gamma I - \mu I,$$
$$\dot{R} = \gamma I - \delta R.$$



with

$N = S + I + R$: total population
α: birth rate
δ: dying rate of not infected
μ: dying rate of infected
β: contact rate
γ: recovery rate.

- Diffusion and transport also makes sense.

What is important

- Realistic climate models have a spatial distribution and are space- and time-dependent.
- Modeling of space-dependency can be done in the discretized form.
- A 1-D modeling is a rough simplification, but we can get some basic ideas.
- Diffusion and transport are two main processes in spatial models.
- They lead to linear terms in the discretized models.
- Both are described by sparse matrices.
- The predator-prey model can be extended to a spatially distributed version.
- Also other models from other disciplines have a similar structure.