Random Walk

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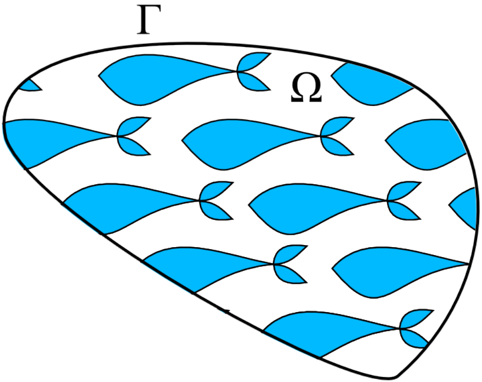
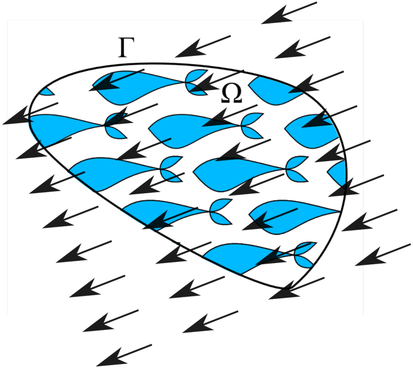
Euler's description



Euler's description



Continuity equation

for concentration

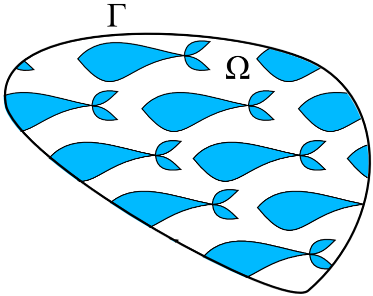
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} c\,\mathrm{d}\Omega = \int_{\Gamma} c\boldsymbol{v}\mathbf{n}\,\mathrm{d}\Gamma$$

Gauss's theorem

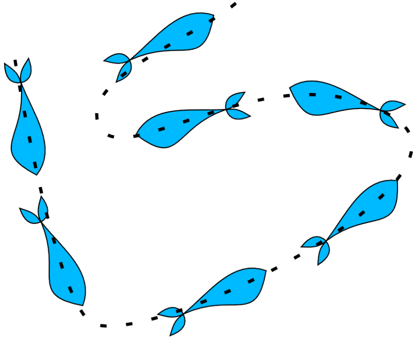
$$\frac{\mathrm{d}c}{\mathrm{d}t} = \mathrm{div}\, c\boldsymbol{v}$$

in local form

Euler's description



Lagrange's description



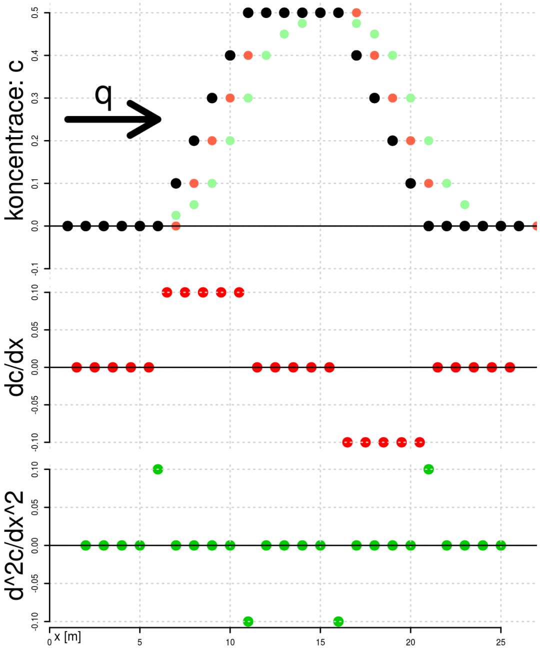
Advekčně disperzní rovnice

$$\frac{\partial \theta c}{\partial t} = \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) - \frac{\partial qc}{\partial x} + R$$

Disperzní koeficient (hydromechanická disperze) D $[L^2.t^{-1}]$:

$$\theta D = D_L|q| + \theta D_w \tau_w$$

c - koncentrace $[mmol, mg/l, ...]$; D_L - mechanická disperze (podélná) $[L]$; D_w - molekulární difuze $[L^2.t^{-1}]$;q - objemoví tok $[L.t^{-1}]$; τ_w - tortuozita $[-]$



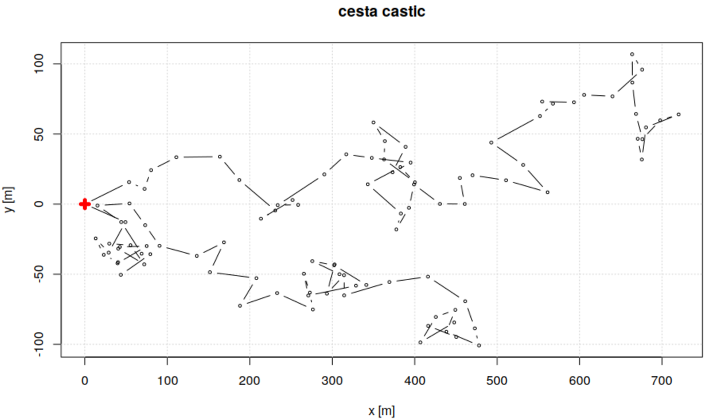
$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - q\frac{\partial c}{\partial x}$$

$$-q\frac{\partial c}{\partial x}$$

$$D\frac{\partial^2 c}{\partial x^2}$$

Random walk

- use when numerical diffusion occurs
- for tracking of particles trajectory
- changing coordinates (steps) of discrete count of particles



Random walk

How does it work?

- particles travel through a space
- each step has a constant part of length A
- and a random part of length B

Step length probability

$$
\begin{array}{ll}
p(x) = 0 & \text{pro } x < (A - B) \\
p(x) = 1/2B & \text{pro } (A - B) < x < (A + B) \\
p(x) = 0 & \text{pro } x > (A + B)
\end{array}
$$

This leads to s step with mean size m of
$m = A$
and variation σ^2
$\sigma^2 = B^2/3$

Probability of particle occurrence in a given distance has a statistical distribution

$$P(x) = \frac{1}{\sqrt{2\pi S^2}} \exp\left(-\frac{(x-M)^2}{2S^2}\right)$$

$$M = Nm = NA$$

$$S^2 = N\sigma^2 = NB^2/3$$

where N is a particle steps count.

Probability of particle occurrence in a given distance has a statistical distribution

$$P(x) = \frac{1}{\sqrt{2\pi S^2}} \exp\left(-\frac{(x-M)^2}{2S^2}\right) \tag{1}$$

$$M = Nm = NA$$

$$S^2 = N\sigma^2 = NB^2/3$$

where N is a particle steps count.

Analytical solution of advection-dispersion equation

$$c/c_0 = \frac{1}{\sqrt{2\pi Dt}} \exp\left(-\frac{(x-Vt)^2}{4Dt}\right) \tag{2}$$

$$M = Vt$$

$$S^2 = 2Dt$$

where V is the velocity and D is the dispersion coefficient.

Random walk

Constant and random part of each step can be expressed from equations 1 and 2

$$NA = Vt -> \ A = Vt/N[L]$$

$$NB^2/3 = 2Dt -> \ B = \sqrt{(}6DA/V) \ [L]$$

Each step in the Random walk procedure has a deterministic step of length A (which represents advection) and random step of maximum size B (which represents diffusion).

Random walk - the procedure

Each next step of particle can be in **1D** calculated as

$$x_{i+1} = x_i + A + 2[rand() - 0.5]B$$

Each next step of particle can be in **2D** calculated as

$$x_{i+1} = x_i + A + 2[rand() - 0.5]B_l$$

$$y_{i+1} = y_i + 2[rand() - 0.5]B_t$$

where $B_l = \sqrt{(}6D_l A/V)$ a $B_t = \sqrt{(}6D_t A/V)$

Formulas for assignment:
particle position:

$$x_{i+1} = x_i + A + 2[rand() - 0.5]B_l$$

$$y_{i+1} = y_i + 2[rand() - 0.5]B_t$$

Constant and random step size:

$$A = Vdt$$

$$B_l = \sqrt{(}6D_l A/V), \ where \ D_l = a_l V$$

$$B_t = \sqrt{(}6D_t A/V), \ where \ D_t = 0.2D_l$$

Water flow in the aquifer: Darcy's law: $q = K\nabla H$
Mean porous flow velocity: $V = q/n$, where n stands for porosity

Úkol

Using MS Excel, build a random walk model and simulate the 2D propagation of **1000** particles through a fully saturated porous medium for **3500** days, set the time step length to **50 days**. The medium is isotropic with saturated hydraulic conductivity **10 m/d**, porosity **48%** and longitudinal dispersivity **20 m**. Consider transverse dispersivity **5 times** less than longitudinal dispersivity. Determine the flow velocity using data from two piezometers **2000 m** apart, with the water table at **350 mnm** in piezometer 1 and **310 mnm** in piezometer 2. Use Darcy's law to calculate the mean pore velocity. The geographic position of the contaminant source is: $x0 = 0\,m$, $y0 = 0\,m$.

According to the relation from the "theory", calculate the value of the mean step length due to advection (A) and the value of the maximum longitudinal and transversal deviation (B_l, B_t)). Calculate the x and y positions of each particle at each time. Use the random number function (RAND()) to randomize the particle progression.

Plot the position of each particle in day 750 and 3500.

Plot the histogram of particle number and concentration at 750 days and 3500 days along x and y axis. Use an interval width of 20 metres. Use the following to plot the histogram function `FREQUENCY` and `Array formula`.

Formula for calculating concentration. One particle represents 0.5 mmol. Show the resulting concentration in mmol/l.

$$C = (number\ of\ particles\ in\ mmol)/(histogram\ interval) * porosity$$

Use of FREQUENCY and Array formula

1. Select all cells in which the frequency output is required.

2. Then type the FREQUENCY formula in Excel. The FREQUENCY. Formula has the following mandatory arguments:

- Data_array: is an array or reference to a set of certain values whose frequencies we need to count.
- Bins_array: It is an array or reference to intervals into which you want to group the values in data_array.

3. Press "CTRL + Shift + enter" to apply Array formula