Universität Potsdam

Earth Surface Process Modelling course

Diffusion equation

Jean Braun 2020

Diffusion

Application to hillslope processes

Soil creep

Landsliding

Rock fall

Diffusion

Diffusive flux

A *flux* is a quantity measuring the rate of flow of a substance or property across a unit surface area per unit time. It is a *vector*. Examples include the flux of water in a fluid, the flux of heat in a solid or the flux of soil at the surface of the Earth.

A *transport model* often corresponds to a given expression for a flux. A *diffusive flux* is one that is directly proportional to the gradient of the quantity it transports (this is also called Fick's first law):

$$\vec{q} = -K\,\overrightarrow{grad}\,h = -K\,\vec{\nabla}\,h$$

The *gradient* is a *differential operator*; it combines the three spatial derivatives of a scalar field (h) to form a vector field:

$$\vec{\nabla}\,h = [\partial_x h, \partial_y h, \partial_z h]$$

The proportionality constant, K, is called the *diffusivity* and has units of $[L]^2[T]^{-1}$ regardless of the units of h.

The negative sign implies that the flux points in the direction of decreasing values of h.

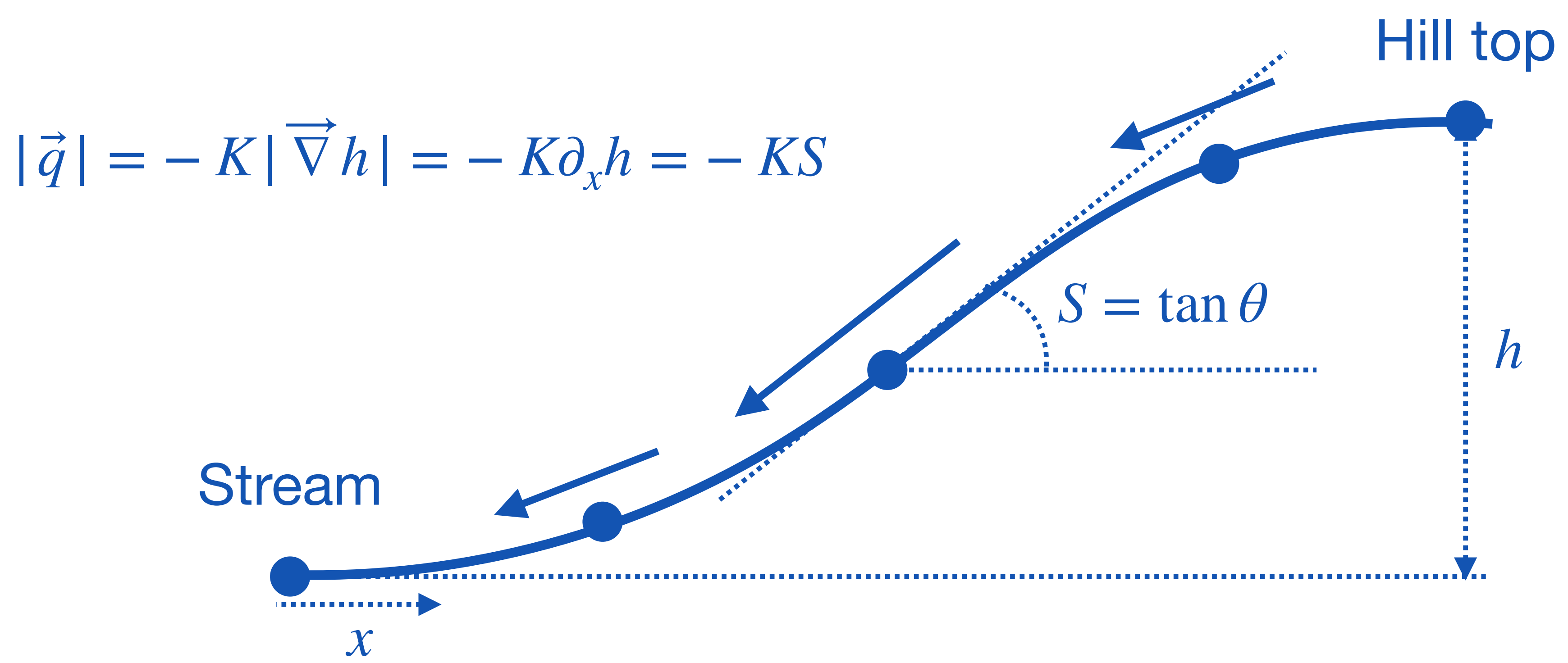
Diffusion

Application to hillslope processes

A variety of processes are responsible for the transport of mass along hill slopes. They include soil creep, rain splash, overland flow, etc. Most of these processes are controlled by gravity and therefore by the local slope. They are often represented by a simple (linear) diffusion transport law:

$$\vec{q} = -K\overrightarrow{\nabla} h$$

where h is the thickness of soil (or any transportable layer). In a *transport-limited system*, it is assumed that the availability of material is unlimited and that the efficiency of transport determines its rate alone. In such a situation, h can also be regarded as the topographic height or *elevation*.



Diffusion

Conservation law

A *conservation law* states that in a close system a given quantity does not change as the system evolves through time. Examples include the conservation of mass, conservation of energy, etc.

The most general way to express a conservation law is through a *continuity equation* that states that the rate of change of a quantity is equal to (-) the divergence of the flux of the quantity:

$$\partial_t h = -\, div\vec{q} = -\, \vec{\nabla} \cdot \vec{q}$$

The *divergence* is another differential operator that transforms a vector field into a scalar field by adding the spatial derivatives of its components:

$$\vec{\nabla} \cdot \vec{q} = \partial_x q_x + \partial_y q_y + \partial_z q_z$$

The divergence of a flux is a measure of the spatial rate of change of the flux at a given point. It can be regarded as “how much comes out minus how much comes in” of the quantity transported (by the flux).

Diffusion

Application to hillslope processes

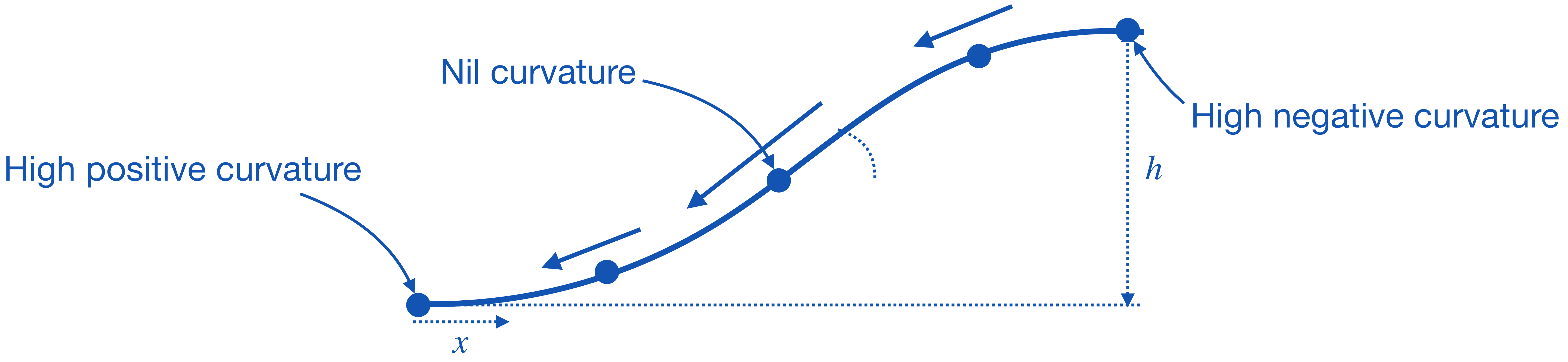
Combining the transport law, $\vec{q} = -K\vec{\nabla}h$, with the conservation law, $\partial_t h = -\vec{\nabla}\cdot\vec{q}$, leads to the *diffusion equation*:

$$\partial_t h = \vec{\nabla}\cdot K\vec{\nabla}h$$

Assuming that K is a constant, we obtain the following equation describing the evolution of topography along a hillslope:

$$\partial_t h = K\nabla^2 h = K(\partial_{xx}h + \partial_{yy}h)$$

where $\nabla^2 h$ is the *Laplacian operator* which transform a scalar field into another scalar field by summing it second spatial derivatives. The Laplacian is a good measure of the "mean" curvature of the topography.



Diffusion

Initial and boundary conditions

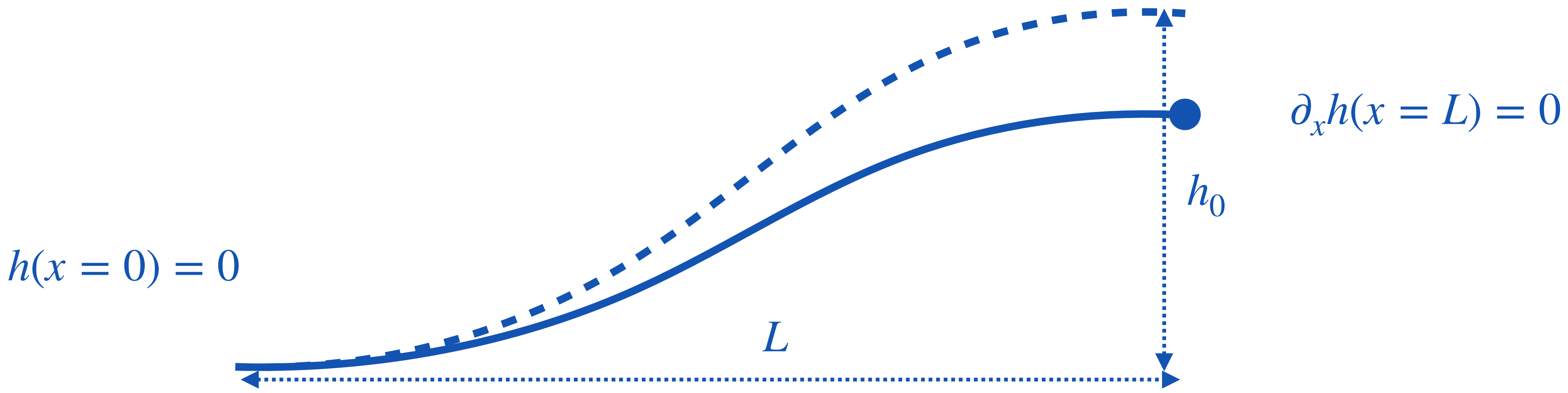
The diffusion equation:

$$\partial_t h = K \partial_{xx} h$$

was introduced by Fick in 1855 to describe the diffusion of matter in a binary medium and by Fourier in 1822 to describe the transport of heat by conduction. It is an *initial value problem equation* that describes the temporal evolution of a quantity as a function of its spatial distribution. It requires an *initial condition*:

$$h(x, t=0) = h_0(x)$$

as well as boundary conditions that are commonly of two types: *Dirichlet* conditions where h is specified and *Neumann* conditions where the gradient of h in the direction normal to the boundary is specified.



Diffusion

Numerical solution: discretisation

We wish to solve the diffusion equation using a computer. For this we must first *discretize* the problem, that is decide at which points in space, x_i, and time, t_i, we wish to compute the solution. Usually these points are chosen to be regularly spaced:

$x_i = i\Delta x$ for $i = 0,\cdots,n_x - 1$ and $t_k = k\Delta t$ for $k = 1,\cdots,n_t - 1$

but this does not need to be the case. We will call h_i^k the numerical solution of the equation at position x_i and time t_k. Such a solution can be represented by a table (or grid) with elements of a given row, k, representing the spatial variation of the solution at a given time t_k, and a given column, i, representing the solution through time at a given point x_i:

$$
\begin{array}{ccccc}
h_1^1 & h_2^1 & h_3^1 & \cdots & h_{n_x}^1 \\
h_1^2 & h_2^2 & h_3^2 & \cdots & h_{n_x}^2 \\
h_1^3 & h_2^3 & h_3^3 & \cdots & h_{n_x}^3 \\
\vdots & \vdots & \vdots & \cdots & \vdots \\
h_1^{n_t} & h_2^{n_t} & h_3^{n_t} & \cdots & h_{n_x}^{n_t}
\end{array}
$$

Diffusion

Numerical solution: finite difference method

To solve the equation, we need to find ways of computing derivatives. Let's focus first on the spatial derivative(s). The definition of a derivative is:

$$\partial_x h = \lim_{\epsilon \to 0} \frac{h(x+\epsilon) - h(x)}{\epsilon}$$

The *finite difference approximation* replaces this limit by a finite value for epsilon, taken to be the spacing between two adjacent points of our discretisation:

$$\partial_x h(x_i, t_k) \approx \Delta_x h_i^k = \frac{h_{i+1}^k - h_i^k}{\Delta x}$$

We see that this approximation must depends on the size of Δx. We also see that different strategies are possible, i.e., by using the point before i to estimate the derivative at x_i^k or, by symmetry, the two points before and after i. This leads to three different estimates, called *forward*, *backward* and *centred finite difference* approximations, namely:

$$\Delta_x^+ h_i^k = \frac{h_{i+1}^k - h_i^k}{\Delta x}, \ \Delta_x^- h_i^k = \frac{h_i^k - h_{i-1}^k}{\Delta x} \text{ and } \Delta_x^c h_i^k = \frac{h_{i+1}^k - h_{i-1}^k}{2\Delta x}, \text{ respectively.}$$

Diffusion

Numerical solution: finite difference method

To obtain a finite difference approximation to the second derivative, we apply the first derivative twice, using a backward then a forward finite difference approximation, to preserve symmetry. This leads to:

$$\Delta_{xx} h_i^k = \Delta_x^+ \Delta_x^- h_i^k = \Delta_x^+ \frac{h_i^k - h_{i-1}^k}{\Delta x} = \frac{\frac{h_{i+1}^k - h_i^k}{\Delta x} - \frac{h_i^k - h_{i-1}^k}{\Delta x}}{\Delta x} = \frac{h_{i+1}^k - 2h_i^k + h_{i-1}^k}{\Delta x^2}$$

All finite difference approximations tend to the "real" value of the first or second derivative when $\Delta x \to 0$.

Using Taylor's development of a function in the vicinity of a point in terms of its derivatives, one can demonstrate that the forward and backward first derivative finite difference approximations are 1st order accurate, which means that the error they introduce decreases linearly with Δx, while the centred first derivative and second derivative finite difference approximations are 2nd order accurate, which means that the error decreases as Δx^2.

Diffusion

Numerical solution: application to the diffusion equation

We can now write the following finite difference approximation of the diffusion equation:

$$\partial_t h_i^k = K \partial_{xx} h_i^k \approx K \frac{h_{i+1}^k - 2h_i^k + h_{i-1}^k}{\Delta x^2}$$

We can also express the time derivative using a forward finite difference approximation to obtain:

$$\frac{h_i^{k+1} - h_i^k}{\Delta t} = K \frac{h_{i+1}^k - 2h_i^k + h_{i-1}^k}{\Delta x^2}$$

or, after a simple re-organisation, the following *evolution equation*, giving the solution at time t_{k+1} and position x_i as a function of the solution at time t_k and position x_{i-1}, x_i and x_{i+1}:

$$h_i^{k+1} = h_i^k + \frac{K\Delta t}{\Delta x^2}(h_{i+1}^k - 2h_i^k + h_{i-1}^k)$$

Diffusion

Numerical solution: condition for stability

From the form of this evolution equation:

$$h_i^{k+1} = h_i^k + \frac{K\Delta t}{\Delta x^2}(h_{i+1}^k - 2h_i^k + h_{i-1}^k)$$

one can derive the following stability criterion:

$$\frac{K\Delta t}{\Delta x^2} < 0.5 \text{ or } \Delta t < \frac{\Delta x^2}{2K}$$

that is necessary for the solution to evolve in a stable manner. This condition implies that the time step Δt must be smaller than a certain limit that depends on the square of the spatial step Δx.

Diffusion

Exercise 1: Sinusoidal topography

Develop a simple code to solve the 1D diffusion equation:

$$\partial_t h = K \partial_{xx} h$$

assuming a sinusoidal initial condition:

$$h(t=0,x) = h_0 \sin(2n\pi x/L)$$

and homogeneous Dirichlet boundary conditions at both ends of the domain of length L:

$h(t, x=0) = 0$ and $h(t, x=L) = 0$

Use $h_0 = 1$, $K = 1$ and $L = 1$ and vary the value of n between 1 and 10. Solve the equation for different spatial resolution (Δx) but adjusting the temporal resolution (Δt) to satisfy the stability condition. Carry the computation from time $t = 0$ to time $t = 0.005$.

Diffusion

Exercise 2: Comparison to analytical solution

The problem of the diffusion of a sinusoidal topography possesses an analytical solution:

$h(x,t) = h_0 e^{-t/\tau_n} \sin(2n\pi x/L)$ with $\tau_n = \dfrac{L^2}{4\pi^2 n^2 K}$ for $x \in [0,L]$ and $t \in [0,\infty[$

that corresponds to a sinusoidal function of same period as the original one but of amplitude decreasing exponentially at a rate given by the time scale τ_n. This time scale is proportional to the square of the wavelength of the sinusoidal function, L/n, and inversely proportional to the diffusivity, K.

Compare your solution to the analytical solution and determine how the error varies as a function of Δx and Δt.

Diffusion

Numerical solution: Implicit vs explicit methods

The method we have used to derive the finite difference evolution equation approximating the diffusion equation is called *explicit* because the second spatial derivative, $\partial_{xx}h_i^k$, is estimated at time t_k. A more stable approximation can be obtained if we estimate this derivative at time t_{k+1} as follows:

$$h_i^{k+1} = h_i^k + \frac{K\Delta t}{\Delta x^2}(h_{i+1}^{k+1} - 2h_i^{k+1} + h_{i-1}^{k+1})$$

This method is called an *implicit* method. Unlike the explicit method, it is *unconditionally stable* (there is no stability condition on Δt). It requires, however, the solution of a system of coupled equations as every equation contains now three unknown values: h_i^{k+1}, h_{i-1}^{k+1} and h_{i+1}^{k+1}. This system can be represented in matrix form as follows:

$$Ah^{k+1} = h^k$$

where A is a *tridiagonal* matrix, $h^{k+1}$is the vector of unknown heights at $t_{k+1}$and h^k is the vector of known heights at t_k. The diagonal elements of A are given by: $A_{j,j} = 1 + \frac{2K\Delta t}{\Delta x^2}$ and the upper and lower diagonal elements are given by: $A_{j-1,j} = A_{j,j+1} = -\frac{K\Delta t}{\Delta x^2}$. The matrix first and last rows must also be adapted for the solution to satisfy the boundary conditions such that $A_{0,0} = 1$, $A_{0,1} = 0$ and $A_{n_x-1,n_x-1} = 1$ and $A_{n_x-1,n_x-2} = 1$. Note that solving a tridiagonal system of n_x equations is of complexity $O(n_x)$ such that the computational time is only marginally higher (compared to an explicit scheme).

Diffusion

Numerical solution: Implicit vs explicit methods

$$h_{i-1}^{k+1} = h_{i-1}^{k} + \frac{K\Delta t}{\Delta x^2}(h_{i}^{k+1} - 2h_{i-1}^{k+1} + h_{i-2}^{k+1}) \quad \rightarrow \quad -Fh_{i-2}^{k+1} + (1+2F)h_{i-1}^{k+1} - Fh_{i}^{k+1} = h_{i-1}^{k}$$

$$h_{i}^{k+1} = h_{i}^{k} + \frac{K\Delta t}{\Delta x^2}(h_{i+1}^{k+1} - 2h_{i}^{k+1} + h_{i-1}^{k+1}) \quad \rightarrow \quad -Fh_{i-1}^{k+1} + (1+2F)h_{i}^{k+1} - Fh_{i+1}^{k+1} = h_{i}^{k}$$

$$h_{i+1}^{k+1} = h_{i+1}^{k} + \frac{K\Delta t}{\Delta x^2}(h_{i+2}^{k+1} - 2h_{i+1}^{k+1} + h_{i}^{k+1}) \quad \rightarrow \quad -Fh_{i}^{k+1} + (1+2F)h_{i+1}^{k+1} - Fh_{i+2}^{k+1} = h_{i+1}^{k}$$

$$\begin{bmatrix} -F & 1+2F & -F & 0 & 0 \\ 0 & -F & 1+2F & -F & 0 \\ 0 & 0 & -F & 1+2F & -F \end{bmatrix} \begin{bmatrix} h_{i-2}^{k+1} \\ h_{i-1}^{k+1} \\ h_{i}^{k+1} \\ h_{i+1}^{k+1} \\ h_{i+2}^{k+1} \end{bmatrix} = \begin{bmatrix} h_{i-2}^{k} \\ h_{i-1}^{k} \\ h_{i}^{k} \\ h_{i+1}^{k} \\ h_{i+2}^{k} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 \\ \cdots & \end{bmatrix} \begin{bmatrix} h_{1}^{k+1} \\ h_{2}^{k+1} \end{bmatrix} = \begin{bmatrix} h_{1}^{k} \\ h_{2}^{k} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \cdots & \\ 0 & 1 \end{bmatrix} \begin{bmatrix} h_{n-1}^{k+1} \\ h_{n}^{k+1} \end{bmatrix} = \begin{bmatrix} h_{n-1}^{k} \\ h_{n}^{k} \end{bmatrix}$$

Diffusion

Exercise 3: Implicit solution to the diffusion equation

Solve the same problem as in exercise 2 but using an implicit method. Check the accuracy and stability of the solution by comparing it to the analytical solution for various values of the time step.

Diffusion

Exercise 4: Application to hillslope geometry

Using your explicit or implicit code, find the steady-state shape of a hill of width L pinned at a nil elevation at both ends and subjected to a constant and uniform uplift at a rate U assuming diffusive transport. For this you must modify your code to include the uplift term:

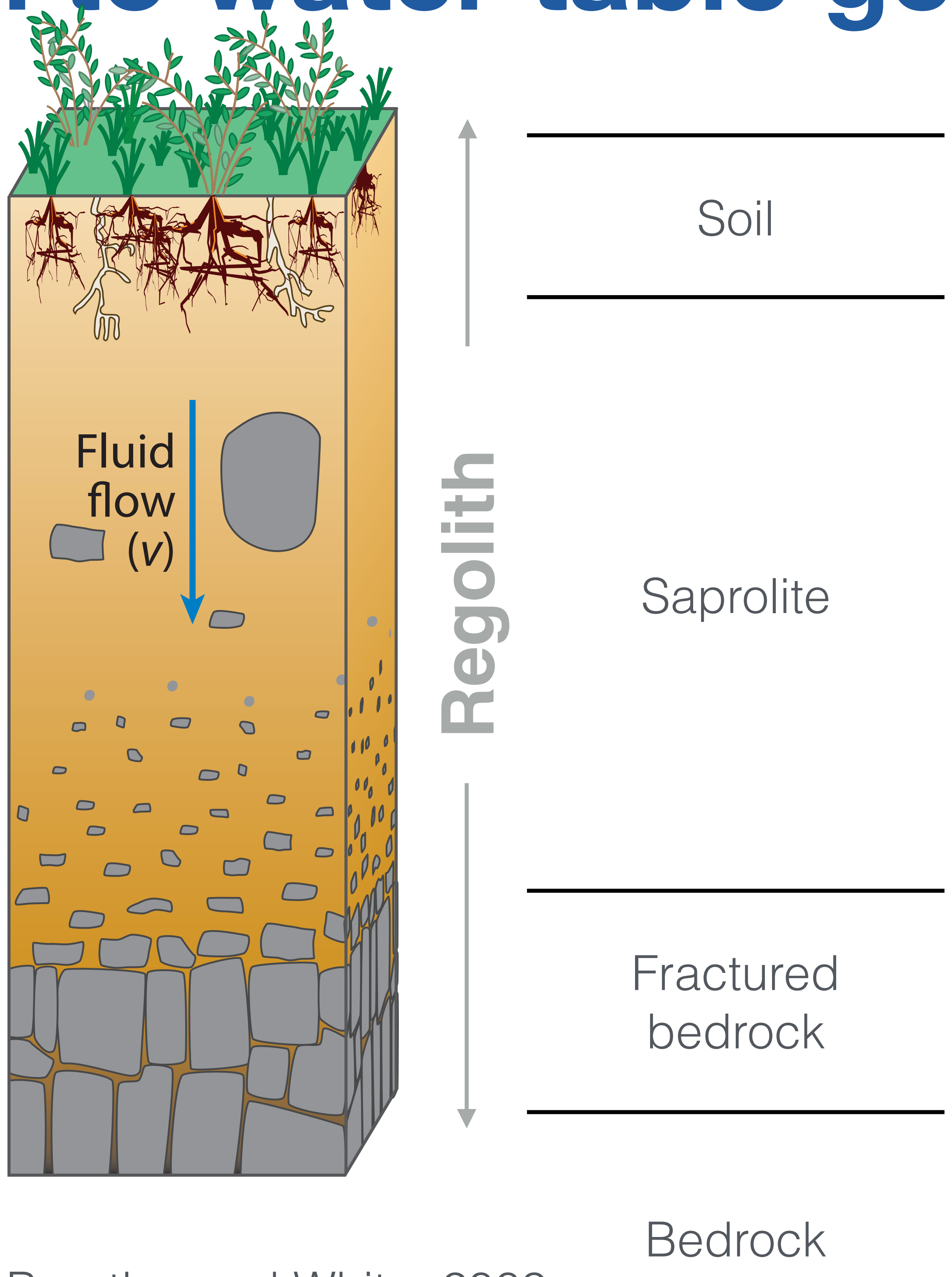
$$\partial_t h = U + K\partial_{xx} h$$

Compare your solution to an analytical solution for the steady-state elevation:

$$h = -\frac{U}{2K} x(x - L) \text{ for } x \in [0,L]$$

Diffusion

Application to water table geometry



From Brantley and White, 2009

Diffusion

Application to water table geometry

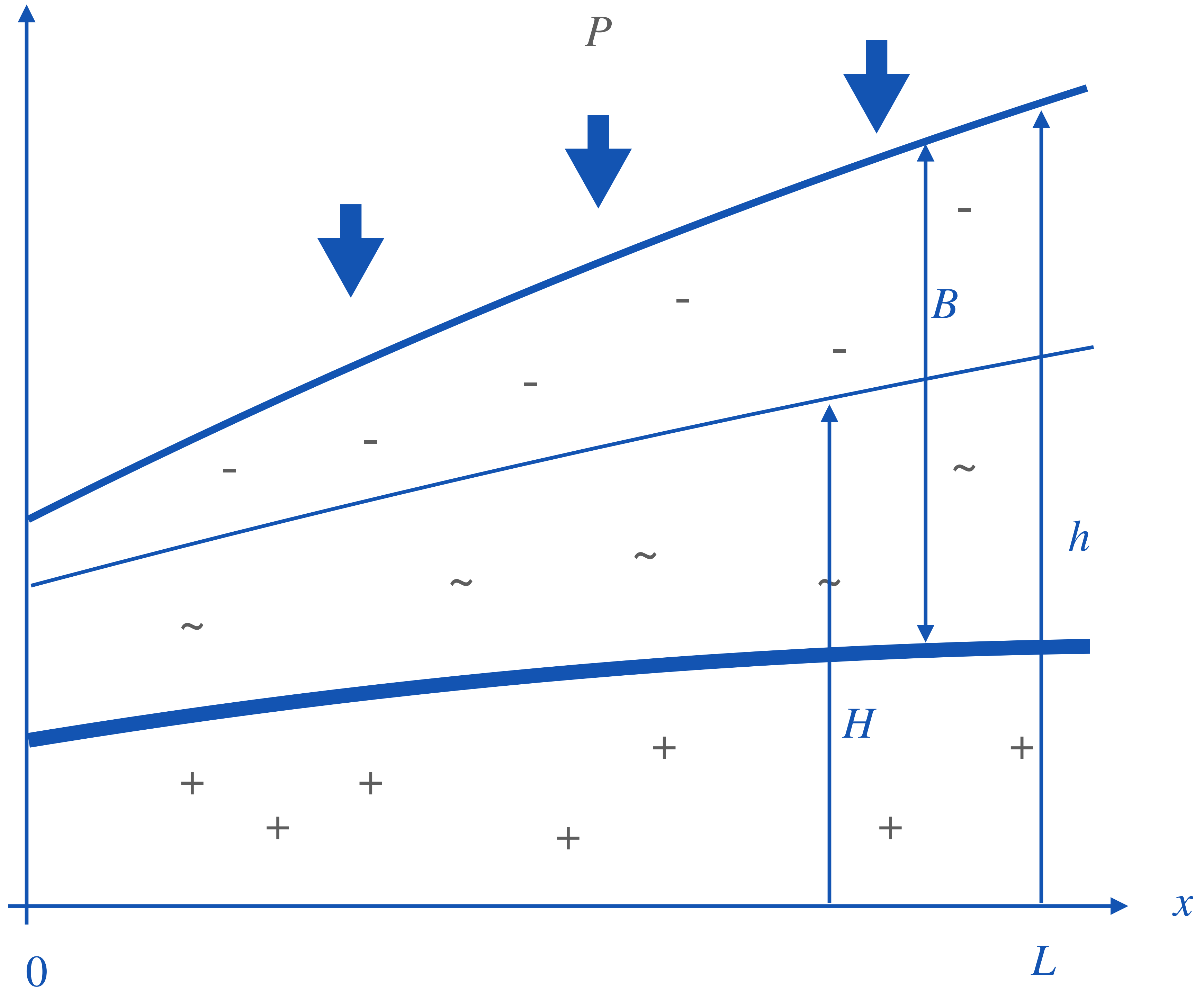
The flow of water within an unconfined aquifer in a homogeneous permeable layer of thickness $B(x)$ (the regolith) beneath a topographic surface $h(x)$ of length L obeys the following steady-state non-linear diffusion equation:

$$\partial_x K(H-h+B)\partial_x H + P = 0$$

following the Dupuit-Forchheimer assumptions that flow is dominantly lateral and that discharge is proportional to the saturated aquifer thickness, $H-h+B$. $H(x)$ is the height of the surface of the water table, K is hydraulic conductivity and P is infiltration rate (precipitation minus evapotranspiration and surface runoff).

We will assume that K and P are uniform and that the surface geometry $h(x)$ and the regolith thickness $B(x)$ are known. The boundary conditions are:

$H(x=0) = h(x=0) - B(x=0)/2$ and $\partial_x H(x=L) = 0$



Diffusion

Application to water table geometry

This equation can be simplified by integrating it in the x direction:

$$\int_x^L \partial_x K(H - h + B)\partial_x H \; dx + \int_x^L P \; dx = -K(H - h + B)\partial_x H + P(L - x) = 0$$

The following finite difference approximation is used:

$$K \; \frac{H_i - h_i + B_i + H_{i-1} - h_{i-1} + B_{i-1}}{2} \; \frac{H_i - H_{i-1}}{\Delta x} - P(L - \frac{x_i + x_{i-1}}{2}) = 0$$

to propagate the solution from base level ($x_0 = 0$) to the top of the hill ($x_{n_x - 1} = L$). Note that, in this case, this expression is a second order polynomial equation in the only unknown,H_i.

Diffusion

Exercise 5: Water table under a linear hill

Find the shape of the water table beneath a fully permeable hill of constant slope S and extend L. For this solves the water table equation seen in the previous slides assuming that the hill surface geometry is given by:

$$h(x) = Sx$$

And the regolith thickness is given by:

$$B(x) = h(x)$$

Such that the entire hill is made of regolith (i.e., the base of the regolith is the base of the hill). Compare your solution against the analytical solution:

$$H(x) = \sqrt{\frac{P}{K}x(2L - x)}$$

Diffusion

Exercise 6: Water table under a linear hill with variable regolith

Use your code to solve a similar problem but assuming that the regolith thickness is variable and given by:

$$B(x) = Sx/2 + \Delta B_0 \sin(6\pi x/L)$$

Interpret your result.

Diffusion

Application to glacier/ice sheet growth

Diffusion

Application to glacier/ice sheet growth

Diffusion

Application to glacier/ice sheet growth

The thickness, $h(x)$, of a glacier sliding on a topography of given elevation $b(x)$ is given by the following non-linear diffusion equation:

$$\partial_t h = \partial_x K(h) \partial_x (h + b) + A$$

where $K(h)$ is a non-linear diffusivity given by:

$$K(h) = f_d (\rho g)^3 h^5 (\partial_x s)^2$$

$s = h + b$ is the geometry of the surface of the glacier, f_d and n are constant and A is the snow/ice accumulation rate which is assumed to vary with surface ice elevation according to:

$$A = \max(\beta(s - ELA), A_c)$$

where ELA is the equilibrium line altitude and β and A_c are the lapse rate and maximum accumulation rate, respectively and assumed constant.

Diffusion

Exercise 7: Glacier growth

Compute the evolution through time of a glacier assuming that it has zero thickness at $x = 0$ and $x = L$ using an explicit finite difference scheme.

Follow the following steps:

1. From $s_i^k = b_i^k + h_i^k$, compute A_i^k

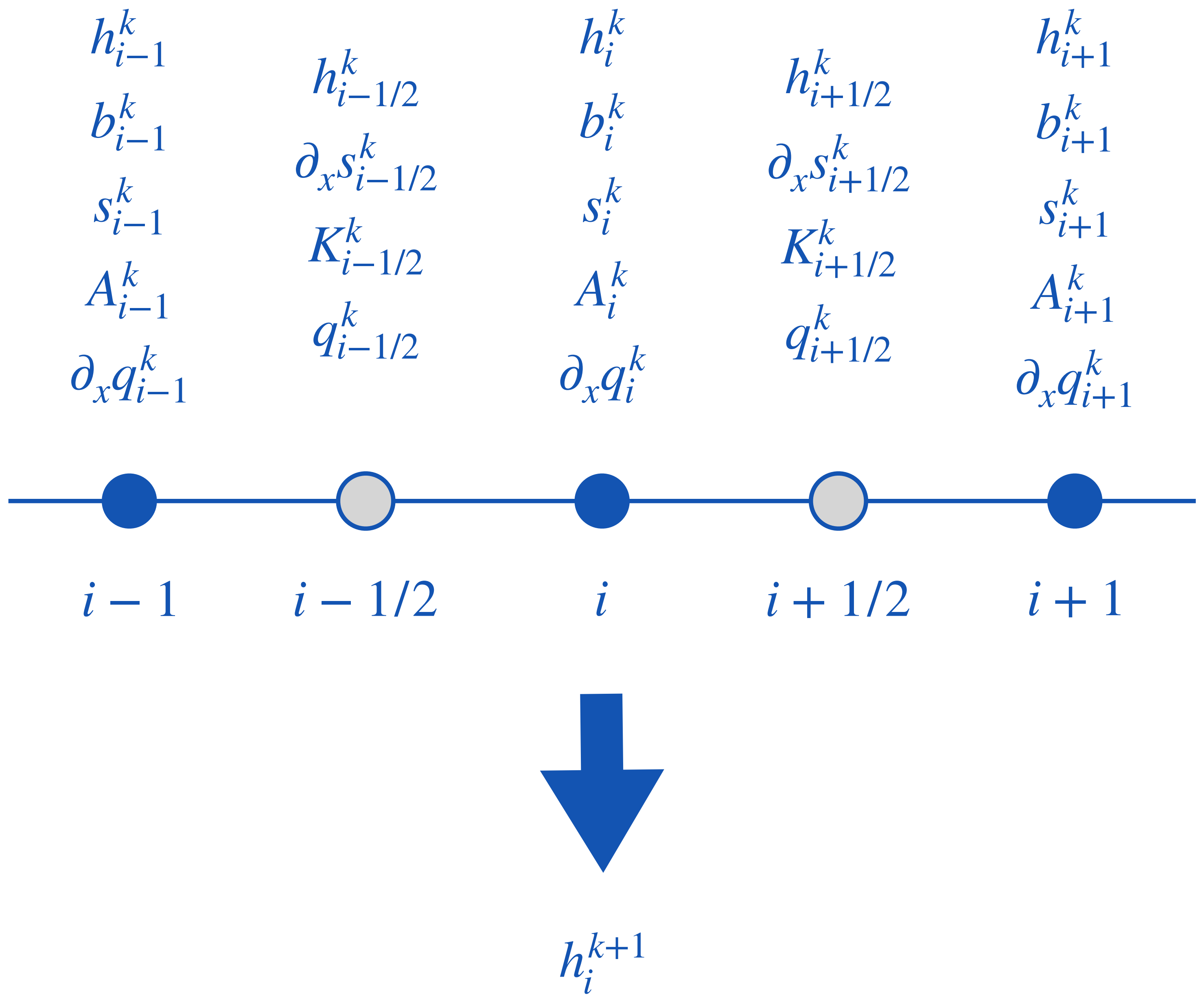
2. Compute $K_{i+1/2}^k$ using $h_{i+1/2}^k = \dfrac{h_i^k + h_{i+1}^k}{2}$ and $\partial_x s_{i+1/2}^k = \dfrac{s_{i+1}^k - s_i^k}{\Delta x}$

3. Compute the flux $q_{i+1/2}^k = K_{i+1/2}^k \partial_x s_{i+1/2}^k$

4. Compute the divergence of the flux $\partial_x q_i^k = \dfrac{q_{i+1/2}^k - q_{i-1/2}^k}{\Delta x}$

5. Find the optimal time step $\Delta t = 0.125 \dfrac{\Delta x^2}{\max K_{i+1/2}^k}$

6. Compute the new thickness $h_i^{k+1} = h_i^k + \Delta t(\partial_x q_i^k + A_i^k)$



Diffusion

Diffusion in 2D: Explicit finite difference

The 2D linear diffusion equation can be written as:

$$\partial_t h = K(\partial_{xx} h + \partial_{yy} h)$$

Using an explicit finite difference scheme it can be solved numerically using the following relation:

$$h_{i,j}^{k+1} = h_{i,j}^{k} + \frac{K\Delta t}{\Delta x^2}(h_{i+1,j}^{k} - 2h_{i,j}^{k} + h_{i-1,j}^{k}) + \frac{K\Delta t}{\Delta y^2}(h_{i,j+1}^{k} - 2h_{i,j}^{k} + h_{i,j-1}^{k})$$

The solution is stored in a 3D matrix, the elements of which, $h_{i,j}^{k}$, contain the height at location $x_i = i\Delta x$, $y_j = j\Delta y$ and time $t_k = k\Delta t$.

Diffusion

Exercise 8: Explicit finite difference scheme in 2D

Implement a 2D explicit finite difference scheme to solve the 2D diffusion equation. Compute the evolution through time of the elevation of a hill of dimension $L \times L$ and of initial elevation given by:

$$h(x, y, t = 0) = h_0 \sin(2n\pi x/L) \ \sin(2m\pi y/L)$$

Compare your solution to the following analytical solution:

$h(x, y, t) = h_0 \ e^{-t/\tau_n} \sin(2n\pi x/L) \ e^{-t/\tau_m} \sin(2m\pi y/L)$ with $\tau_n = \dfrac{L^2}{4\pi^2 n^2 K}$ and $\tau_m = \dfrac{L^2}{4\pi^2 m^2 K}$ for $x \in [0,L]$, $y \in [0,L]$ and $t \in [0,\infty[$

Diffusion

Diffusion in 2D: the ADI method

The ADI (Alternating Direction Implicit) algorithm is a simple generalisation of the 1D implicit algorithm to solve the linear diffusion equation to 2D and 3D. Assuming that the problem has been discretised on a mesh of dimension $n_x \times n_y$, it consists in solving n_y 1D problems of size n_x for half a time step followed by solving n_x 1D problems of size n_y for another half time step.

First solve:

$$h_{i,j}^{k+1/2} = h_{i,j}^{k} + \frac{K\Delta t}{2\Delta x^2}(h_{i+1,j}^{k+1/2} - 2h_{i,j}^{k+1/2} + h_{i-1,j}^{k+1/2}) + \frac{K\Delta t}{2\Delta y^2}(h_{i,j+1}^{k} - 2h_{i,j}^{k} + h_{i,j-1}^{k})$$

then solve:

$$h_{i,j}^{k+1} = h_{i,j}^{k+1/2} + \frac{K\Delta t}{2\Delta x^2}(h_{i+1,j}^{k+1/2} - 2h_{i,j}^{k+1/2} + h_{i-1,j}^{k+1/2}) + \frac{K\Delta t}{2\Delta y^2}(h_{i,j+1}^{k+1} - 2h_{i,j}^{k+1} + h_{i,j-1}^{k+1})$$

For ease of implementation, one first writes a routine/function solving implicitly a 1D problem by solving a tridiagonal matrix (as done earlier in the course). One then writes a series of loops calling the function n_x then n_y times. The algorithm remains of complexity $O(n_x \times n_y)$.

Diffusion

Exercise 9: 2D diffusion problem using the ADI method

Solve the 2D problem described in exercise 8 but using the ADI finite difference scheme. Compare the stability of the method (and its accuracy) to the explicit scheme.