Diffusion equation

Basics

The Diffusion equation is one of the most frequently used partial differential equations in exact sciences. In the simple case of one spatial variable one considers the evolution of a quantity $u(x,t)$ which depends on space x and time t. The diffusion equation has the form

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

where D is called the diffusion constant. In different applications the variable u has different meanings: it can be a temperature if one describes heat conduction; it can be a level of underground water in hydrogeology; or it can be the concentration of a solute in an unmoving medium. A "derivation" of the diffusion equation is as follows. Convervation of the quantity u requires that the total amount of u within an interval changes with a velocity given by the difference between an influx and an outflux

$$\frac{d}{dt}M = \frac{d}{dt}\int_{x_A}^{x_E} u(x,t)dx = J(x_A,t) - J(x_E,t).$$

Integral calculus tells us, that $-\partial u/\partial t$ must be the derivative of J resulting in the conservation equation

$$\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}.$$

The diffusive flux is proportional to the difference in u at different positions and in the direction from larger to lower values, i.e. it equilibrates concentrations. In continuous media J is in the opposite direction of the derivative of u

$$J = -D\frac{\partial u}{\partial x}.$$

This is known as Darcy's law for the water level in a porous medium, as Fourier's law for the heat flux, and as Fick's law for the diffusion of a solute. Substituting J into the conservation equation yields the diffusion equation.

Self-similar solution in an infinite domain

Let us interprete $u(x,t)$ as the ground water level. The integral of the water level is the volume

$$M = \int_{-\infty}^{\infty} u(x,t)dx$$

which is conserved for incompressible fluids and proportional to the total mass. There is a simple solution given by a time-dependent Gaussian function

$$u(x,t) = \frac{M}{(4\pi Dt)^{1/2}} \exp\left(-\frac{x^2}{4Dt}\right)$$

which can be checked by a direct substitution into the diffusion equation. The area M under this curve is conserved, but the variance of the Gaussian is growing linearly in time

$$\frac{1}{M}\int_{-\infty}^{\infty} x^2 u(x,t)dx = 2Dt.$$

The standard deviation (width) grows as a square root of time, i.e. the spread is slowing down over time.

Task 1: Check that the Gaussian function $u(x,t)$ above is a solution of the diffusion equation. Draw the solution as a function of the coordinate x for several different times.

Solutions in a finite domain

In a finite spatial domain $0 \leq x \leq L$, one has to supply boundary conditions. Typically, two types of boundary conditions are considered:

(1) No-flux boundary conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=0,L} = 0$$

(2) and absorbing boundary conditions (this means that water "leaks away" from the system at the boundaries):

$$u(0,t) = u(L,t) = 0$$

For no-flux boundary conditions the total amount $M = \int_0^L u(x,t)dx$ remains constant in time. The field $u(x,t)$ tends to a constant as $t \to \infty$. For absorbing boundary conditions the total amount M decreases and tends exponentially to zero as $t \to \infty$.

Numerical solution of the diffusion equation in a finite domain

For a numerical solution of the diffusion equation one introduces a grid with spatial step Δx and temporal step Δt. The field at position $k\Delta x$ and at time $n\Delta t$ is denoted as u_k^n with $k = 0 \ldots K$ and $n = 0 \ldots N$. Derivatives in the diffusion equation are replaced by finite differences

$$\frac{\partial u(x,t)}{\partial t} \to \frac{u_k^{n+1} - u_k^n}{\Delta t}, \qquad \frac{\partial^2 u}{\partial x^2} \to \frac{u_{k-1}^n - 2u_k^n + u_{k+1}^n}{(\Delta x)^2}.$$

This yields a numerical scheme for solving the evolution in time :

$$u_k^{n+1} = u_k^n + \frac{\Delta t D}{(\Delta x)^2}(u_{k-1}^n - 2u_k^n + u_{k+1}^n)$$

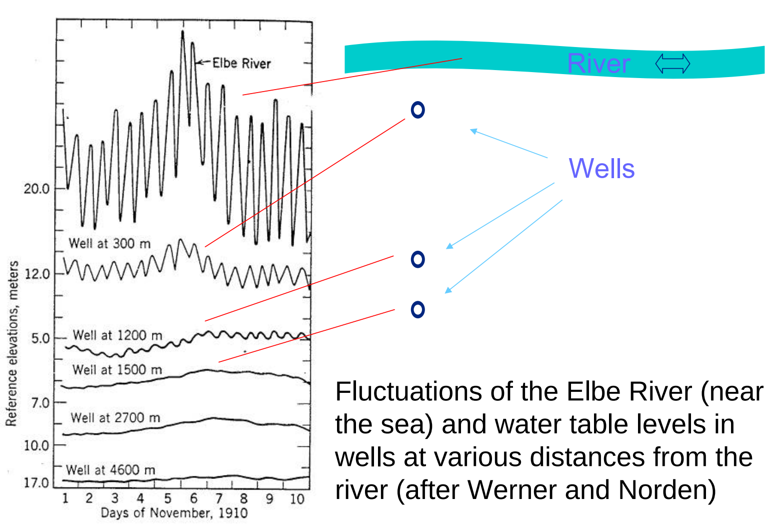
Because of the references to values u_{k-1}^n and u_{k+1}^n in the spatial derivative you can apply the numerical scheme only to the inner points of the array. The update at the end points needs to be calculated seperately in accordance with imposed boundary conditions, i.e. $u_{-1}^n = u_1^n$, $u_{K+1}^n = u_{K-1}^n$ for non-flux boundaries, and $u_{-1}^n = u_{K+1}^n = 0$ for absorbing boundary conditions. One starts with an initial field u_k^0, and through iterations of the numerical scheme obtains fields u_k^n for future times $n > 0$. The total size of the system is $L = K\Delta x$. **Important:** *The time step should be chosen according to the stability criterion* $\Delta t < \frac{(\Delta x)^2}{2D}$. *For better accuracy one takes* Δt *to be much smaller than* $\frac{(\Delta x)^2}{2D}$, *e.g. by a factor* 100.

Task 2: Implement a numerical solution of the diffusion equation with no-flux boundary conditions. Take $D = 1$, $L = 5$, $K = 500$ and initial condition $u(x, 0) = (4x(L - x)/L^2)^{10}$. Present solutions graphically at $t = 0, 0.25, 0.5, 0.75, 1.0$. Check, with which accuracy the total ammount of u is conserved.

Task 3: Implement a numerical solution of the diffusion equation with absorbing boundary conditions. Take $D = 1$, $L = 5$, $K = 500$ and initial condition $u(x, 0) = (4x(L - x)/L^2)^{10}$. Present solutions graphically at $t = 0, 0.25, 0.5, 0.75, 1.0$. Show in a separate graph the evolution of the total amount during the time interval $0 \leq t \leq 20$. Use a logarithmic scale for the amount to visualize the exponential law of its decay at large times. Determine the exponent of the decay.

Bonus : Non-stationary diffusion equation

Quite often one has a non-stationary problem for the diffusion equation. The following example considers oscillations of the underground water level close to a river, where the level of the river changes periodically in time. Prof. J. Barker (University of Southampton) illustrates this with the following observations close to Elbe river:



Fluctuations of the Elbe River (near the sea) and water table levels in wells at various distances from the river (after Werner and Norden)

One can model this effect of "spreading of oscillations" by solving the diffusion equation with a time-dependent boundary condition at $x = 0$ and an absorbing boundary condition at $x = L$

$$u^n_{-1} = A \sin\left(2\pi \frac{n\Delta t}{T}\right), \qquad u^n_{K+1} = 0.$$

Here A is the amplitue of the "river level oscillations" and T is the period.

Bonus Task : Solve the diffusion equation with periodic forcing at one boundary. Take $D = 1$, $L = 10$, $K = 1000$, $A = 1$, $T = 5$ and initial condition $u(x, 0) = 0$. Plot levels $u(x, t)$ as functions of time for $x = 1, 2, 3, 4, 5, 6, 7, 8, 9$, for a time interval of 25 periods and describe the results.