Dear student,

Next Tuesday Ferbruar 23 we have a matlab exercise in PC room Pallas, 10:45-12:30.

We will solve three problems, a chemical reaction, the 1-D time-dependent heating of a metal bar and the 1D stationary heating of a metal bar. We do this using matlab. I will give you so-called skeleton matlab programs which you have to adapt.

The start of all numerical programming should be preparation on paper. If you have time, can you please prepare the following on paper BEFORE we have the exercise on Thursday and take your work with you next Thursday. If there are difficulties/questions, then ask me/email me. If questions are be relevant to all students I will put the question and the answer on the website/tell everybody.

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The cases which I would like you to prepare are:

- discretisation of $\frac{dC}{dt} = KC$ with two time-stepping schemes.
- discretisation of a 1-D in-stationary heat conduction problem with a source term using the finite volume method.
- discretisation of a 1-D stationary heat conduction problem with a source term using the finite volume method.

Note, that useful material is on the lecture sheets. The finite volume method for the diffusion equation is given below. However, you also need to discretise the boundary conditions and the source term. For the boundary conditions we offer some help below, the source term you have to include by repeating the steps shown below with a source term added.

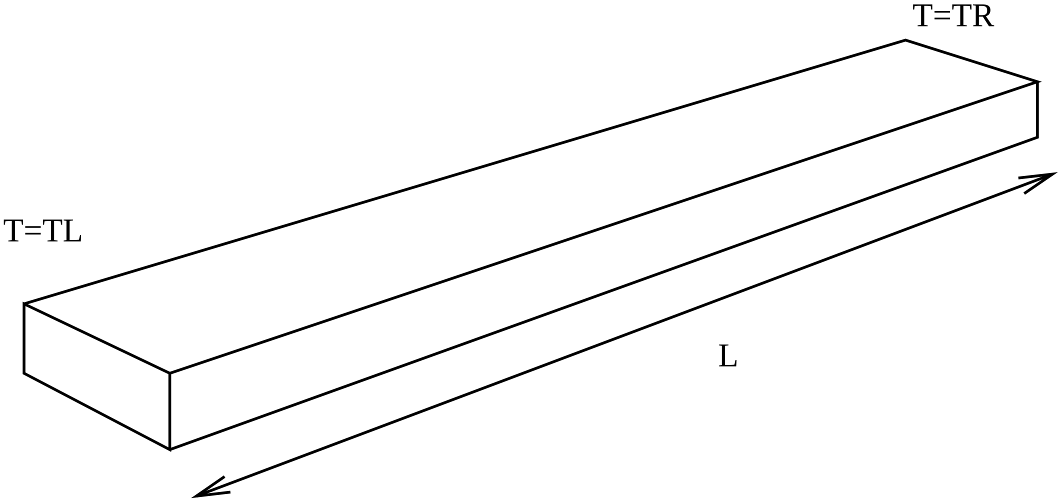
The chemical reaction

In this exercise, the equation $\frac{dC}{dt} = KC$ is solved using finite differeces. Replace $\frac{dC}{dt}$ by finite differences. First take the right hand side (RHS) KC at the old time-level. Bring all known stuff to the right, all unknown stuff to the left. You get an expression like $Cn = RHS$ with only known quantities at the RHS. Implement this in the matlab skeleton program exercise1.m. Try out time-step dt=0.1 and also dt=5. What do you observe?

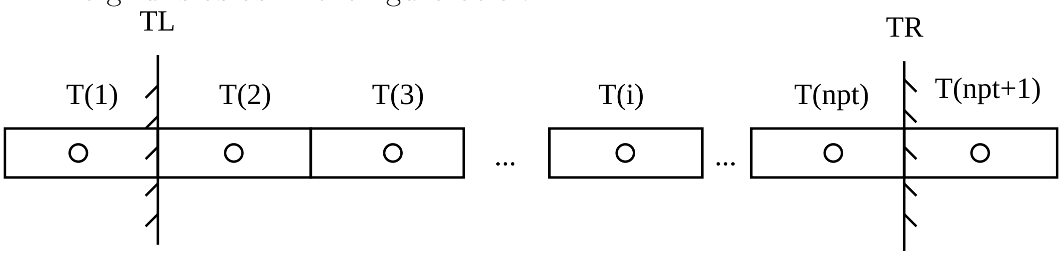
Repeat the exercise with KC at the NEW time level. Follow the same procedure as for the case above, move all the known stuff to the right, all the unknown stuff to the right. Again, you get an expression like $Cn = RHS$ with only known stuff to the right. Implement in exercise1.m. Try dt=0.1 and dt=5. What do you observe? Compare with the case above.

The geometry and the grid for the finite volume method for the diffusion equation

The geometry is a bar of length L with the temperature prescribed at left (T=TL) and right (T=TR).



The grid is as as in the figure below:



The temperature T is at the positions indicated by the circle in the middle of the grid cells. The is also a source term giving off a heat S(x) per unit volume.

The boundary conditions for the finite volume method for the diffusion equation

Note that we have a grid with the variables in the middle of the grid cell. The left boundary is between points 1 and 2, the right boundary between points npt and npt+1 Note that point 1 and point npt+1 are OUTSIDE the calculation domain. After every time-step we update them so that the boundary condition is fulfilled exactly.

Points 1 and npt+1 are called VIRTUAL POINTS or GHOST POINTS. In the figure we see that if we use linear interpolation then (T(1) + T(2))/2 = TL Use this to express T(1) in TL and T(2). Do similarly for the right boundary. This is to be used in the matlab program.

The finite volume method for the diffusion equation

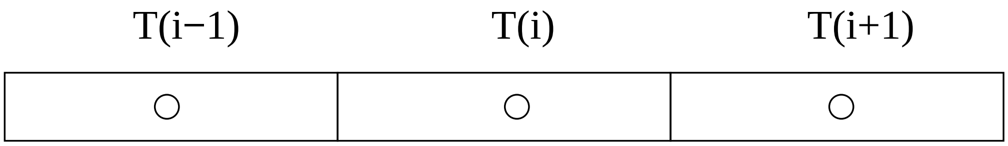
- set up an integral balance
- discretise the volume integrals and the surface fluxes
- we will assume k, ρ, c constant

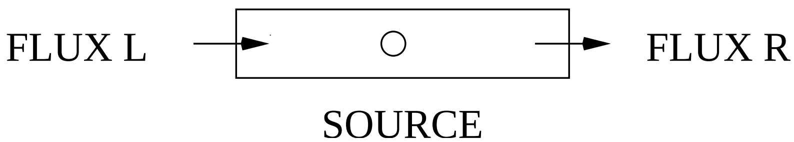
Heat balance over volume i, see figure here and on the next page.

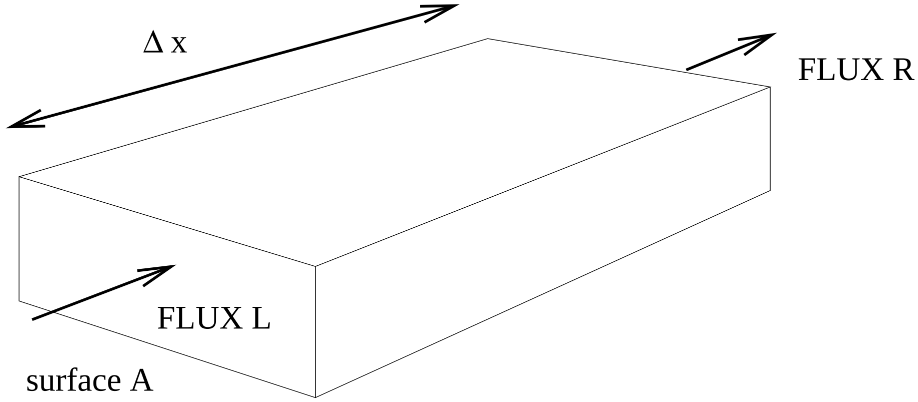
$$\int \rho c \frac{\partial T}{\partial t} = q_L A - q_R A$$

Approximate the volume integral (which represents the heat content in volume i) using the midpoint rule

$$\rho c \frac{\partial T(i)}{\partial t} \Delta x A = q_L A - q_R A$$
$$\rho c \frac{\partial T(i)}{\partial t} = \frac{q_L - q_R}{\Delta x}$$







$$\rho c \frac{\partial T(i)}{\partial t} = \frac{q_L - q_R}{\Delta x}$$

Determine the fluxes at the left and right with Fourier's law
approximate the derivatives using point $T(i)$ and its neighbors

$$q_L = -k \frac{\partial T}{\partial x}$$
$$q_L \approx -k \frac{T(i) - T(i-1)}{\Delta x}$$
$$q_R \approx -k \frac{T(i+1) - T(i)}{\Delta x}$$

Discretisation in space, constant k

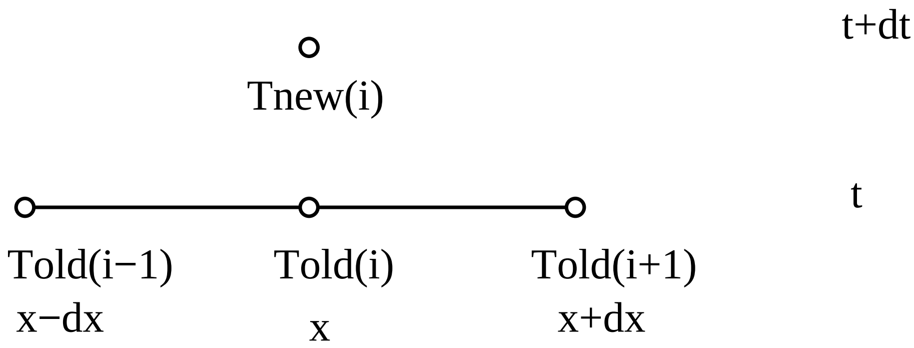
$$\frac{q_L - q_R}{\Delta x} \approx k \frac{T(i+1) - 2T(i) + T(i-1)}{\Delta x^2}$$

Then, the whole balance reads:

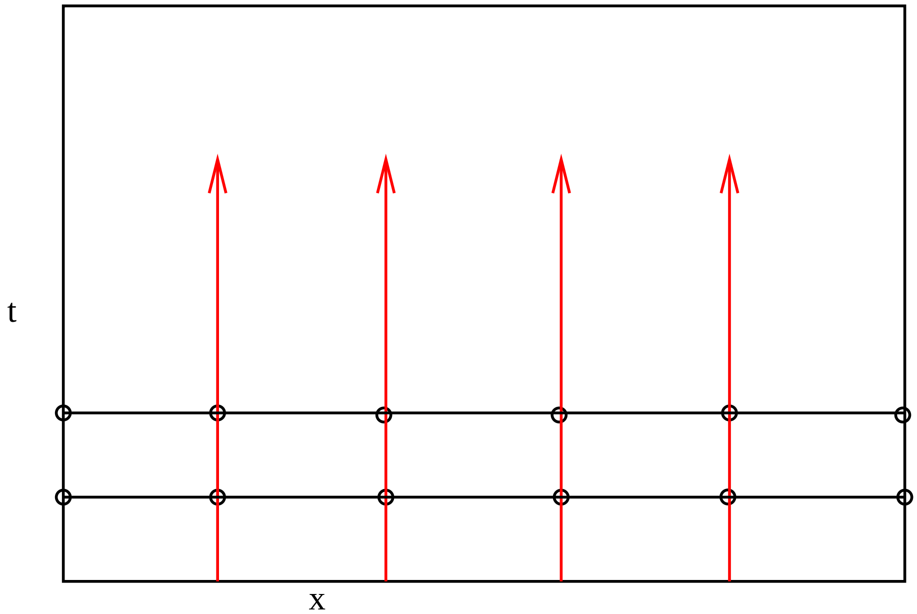
$$\rho c \frac{\partial T(i)}{\partial t} = k \frac{T(i+1) - 2T(i) + T(i-1)}{\Delta x^2}$$
$$\frac{\partial T(i)}{\partial t} = \alpha \frac{T(i+1) - 2T(i) + T(i-1)}{\Delta x^2}$$

Euler forward in time:

$$Tnew(i) = Told(i) + \Delta t \alpha \frac{Told(i+1) - 2Told(i) + Told(i-1)}{\Delta x^2}$$



- solving PDE this way (discretization in space → system ODE) is called 'the method of lines'



The stationary diffusion equation

Next we look at the stationary case including a source. The dimensions of the problem are the same as for the in-stationary problem. The left boundary condition is T=1, the boundary condition at the right is 0. From the instionary case, you can determine how the stationary discretisation looks like. You can write it in the following form:

$$aT(i+1) + bT(i) + cT(i-1) = RHS(i)$$

This is solved using Jacobi iteration. That means: rewrite the equation so that ONLY the term $bT(i)$ is at the left and divide both sides by b so that we have an equation like $T(i) = RHS(i)$ with RHS containing $T(i-1)$ and $T(i+1)$. Then we choose the left hand side at the old iteration level and the right hand side at the new itaration level. Implement this in program exercise3.m Also implement the boundary conditions. Calculate the temperature distribution for a zero source term, this gives a straight line. Next calculate the temperature distribution for another type of source, for instance with source term 1 in one discrete point and 0 in the others.