

Numerische Methoden 1 – B.J.P. Kaus

4 Fun with boundary conditions

4.1 Flux boundary conditions and fictious boundary points

Sofar we have always assumed that the boundary condition for the temperature equation was a fixed temperature. This condition is also called a Dirichlet boundary condition. We can however, also assume a case where the boundary has a constant flux of temperature. An example would be a given flux of heat from the mantle at the base of the lithosphere. This condition is called a Neuman boundary condition, and can be expressed as

$$\frac{\partial T(x=0,t)}{\partial x} = c_1 \tag{1}$$

$$\frac{\partial T(x=L,t)}{\partial x} = c_2 \tag{2}$$

There are two ways in which you can program this boundary conditions, which will be discussed in the following two sections.

4.1.1 Directly implementing the boundary condition

In here, you simply use a forward or backward finite difference approximation. Setting a flux at x = 0 than becomes:

$$\frac{T_2 - T_1}{\Delta x} = c_1 \tag{3}$$

If you use an implicit finite difference method, this will change your matrix \mathbf{A} and right-hand-side vector **rhs** into

$$\mathbf{A} = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ -\mathbf{s} & (1+2\mathbf{s}) & -\mathbf{s} & 0 & 0 & 0 \\ \dots & & & & & & \end{pmatrix}$$
(4)

$$\mathbf{rhs} = \begin{pmatrix} c_1 \Delta x \\ T_2^n \\ \dots \end{pmatrix}$$
(5)

Defining a flux boundary condition around node x = L is done similarly.

4.1.2 Using fictious boundary points

Programming the boundary conditions as indicated in the previous section works, but does not give very accurate results (for the interested ones: the resulting equation will only be first-order accurate and not second order as you have with constant temperature boundary conditions). Moreover the location where the flux condition is defined is not at T_1 but at $T_{3/2}$ or at $T_{n_x-1/2}$ instead of T_{nx} . A better way to incorporate a flux boundary conditions is therefore to use a central finite difference approximation, which is given (at i = 1) by

$$\frac{T_2^{n+1} - T_0^{n+1}}{2\Delta x} = c_1 \tag{6}$$

at $i = n_x$, the boundary condition is given by

$$\frac{T_{n_x+1}^{n+1} - T_{n_x-1}^{n+1}}{2\Delta x} = c_2 \tag{7}$$



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Figure 1: Discretization of the numerical domain with fictious boundary points, that are employed to set flux boundary conditions.

The problem is that the expressions above involve points that are not part of the numerical grid (T_0^{n+1}) and $T_{n_x+1}^{n+1}$. These points are called fictious boundary points (see Fig. 1). A way around this can be found by noting that the equation for the center nodes is given by

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \kappa \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2} \tag{8}$$

Writing this expression for the first node gives

$$\frac{T_1^{n+1} - T_1^n}{\Delta t} = \kappa \frac{T_2^{n+1} - 2T_1^{n+1} + T_0^{n+1}}{\Delta x^2} \tag{9}$$

An explicit expression for T_0^{n+1} is obtained from equation 6

$$T_0^{n+1} = T_2^{n+1} - 2\Delta x c_1 \tag{10}$$

Substituting eq. 6 into eq. 9 gives

$$\frac{T_1^{n+1} - T_1^n}{\Delta t} = \kappa \frac{2T_2^{n+1} - 2T_1^{n+1} - 2\Delta x c_1}{\Delta x^2} \tag{11}$$

Again we can rearrange this equation to bring known terms on the right-hand-side:

$$-2sT_2^{n+1} + (1+2s)T_1^{n+1} = T_1^n - 2s\Delta xc_1 \tag{12}$$

This equation only involves grid points that are part of the computational grid, and equation 11 can be incorporated into the matrix \mathbf{A} and right-hand-side **rhs**.

4.2 Exercises

- 1. Modify the implicit finite difference code from last class, to take into account a flux boundary condition. Program two cases: 1) the case in which you implement the BC directly, and 2) a case in which you use the fictious boundary point method. Computes the steady-state geotherm in a lithosphere of 100 km thickness, that has a constant temperature at the top $(T = 0^{\circ}C)$ and a constant gradient of 25 K/km at the bottom.
- 2. Modify the program to include a heat-source (generation of heat due to radioactive elements). The modified equation is than

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} + Q \tag{13}$$

Typical values for Q are 3×10^{-13} Ks⁻¹ Compute the steady state geotherm of a crust of 100 km thickness, that has a temperature of 1300 C at the bottom and 0 C at the top. Assume that the upper 30 km are composed of crust that has radioactive elements, but that the lithosphere below is free of radioactive elements.



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3. For special cases, an analytical solution exists that takes radioactive heat production into account. One case is when we set the temperature at the top of the domain to T_0 and also fix the geothermal gradient at this location (set it to $\frac{\partial T}{\partial z} = c_1$). An application for this would be the geotherm within a continent, where $T_0 = 0^{\circ}C$ and the geothermal gradient can be measured (for example in a borehole) $c_1 = 25$ K/km. The analytical solution (explained in Turcotte and Schubert, Geodynamics, 2nd edition, p. 138-144) is

$$T = T_0 + c_1 x - \frac{Q}{2\kappa} x^2 \tag{14}$$

Program this case, thereby making sure that you set the correct boundary conditions and compare the result with the analytical solution. Program your code such that x = 0 is at the Earth's surface and x = 100 km is at a depth of 100 km (in other words: positive x values mean that you go deeper into the Earth).