

## 2 Finite difference basics

The basics of the finite difference method are best understood with an example. Consider the one-dimensional transient heat conduction equation

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \quad (1)$$

where  $\rho$  is density,  $c_p$  heat capacity,  $k$  thermal conductivity,  $T$  temperature,  $x$  distance and  $t$  time. If the thermal conductivity, density and heat capacity are constant over the model domain, the equation can be simplified to

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} \quad (2)$$

where  $\kappa = \frac{k}{\rho c_p}$  is the thermal diffusivity (a common value for rocks is  $\kappa = 10^{-6} \text{ m}^2\text{s}^{-1}$ ). We are interested in the temperature evolution versus time  $T(x, t)$  which satisfies equation 2, given an initial temperature distribution (Fig. 1A). An example would be the intrusion of a basaltic dike in cooler country rocks. How long does it take to cool the dike to a certain temperature? What is the maximum temperature that the country rock experiences?

The first step in the finite differences method is to construct a grid with points on which we are interested in solving the equation (this is called discretization, see Fig. 1B).

The next step is to replace the continuous derivatives of equation 2 with their finite difference approximations. The derivative of temperature versus time  $\frac{\partial T}{\partial t}$  can be approximated with a forward finite difference approximation as

$$\frac{\partial T}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{t^{n+1} - t^n} = \frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{T_i^{\text{new}} - T_i^{\text{current}}}{\Delta t} \quad (3)$$

here  $n$  represents the temperature at the current timestep whereas  $n + 1$  represents the new (future) temperature. The subscript  $i$  refers to the location (Fig. 1B). Both  $n$  and  $i$  are integers;  $n$  varies from 1 to  $n_t$  (total number of time steps) and  $i$  varies from 1 to  $n_x$  (total number of grid points in  $x$ -direction). The spatial derivative of equation 2 is replaced by a central finite difference approximation, i.e.,

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial T}{\partial x} \right) \approx \frac{\frac{T_{i+1}^n - T_i^n}{\Delta x} - \frac{T_i^n - T_{i-1}^n}{\Delta x}}{\Delta x} = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \quad (4)$$

Substituting equation 4 and 3 into equation 2 gives

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \kappa \left( \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \right) \quad (5)$$

The third and last step is a rearrangement of the discretized equation, so that all known quantities (i.e. temperature at time  $n$ ) are on the right hand side and the unknown quantities on the left-hand side (properties at  $n + 1$ ). This results in:

$$T_i^{n+1} = T_i^n + \kappa \Delta t \left( \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} \right) \quad (6)$$

Because the temperature at the current timestep ( $n$ ) is known, we can use equation 6 to compute the new temperature. The last step is to specify the initial and the boundary conditions. If for example the country rock has a temperature of  $300^\circ\text{C}$  and the dike a width of 2 meters, with a magma temperature of  $1200^\circ\text{C}$ , we can write as initial conditions:

$$T(x < -1, x > 1, t = 0) = 300 \quad (7)$$

$$T(-1 \leq x \leq 1, t = 0) = 1200 \quad (8)$$

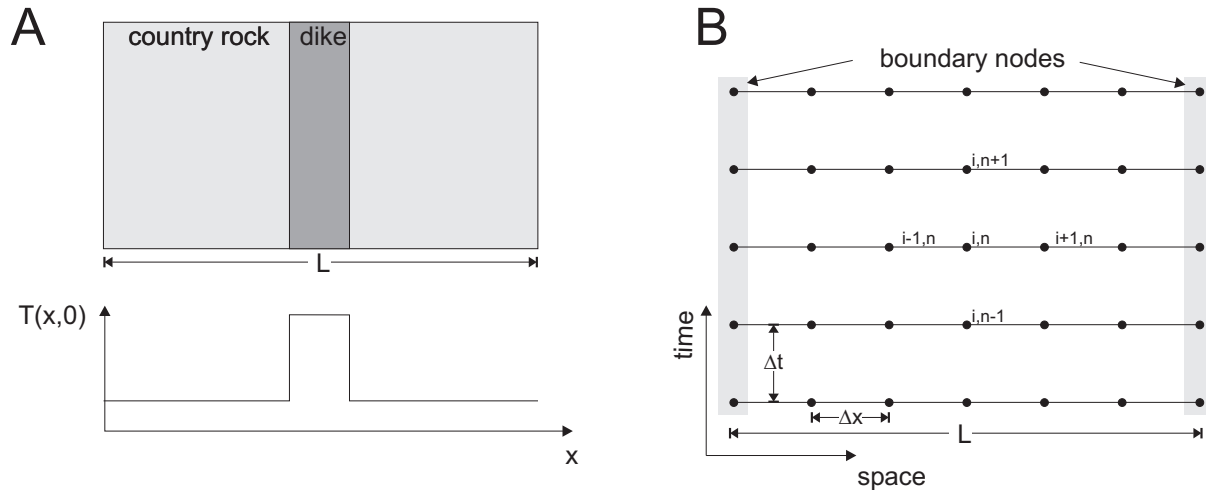


Figure 1: A) Setup of the model considered here. A hot basaltic dike intrudes cooler country rocks. Only variations in  $x$ -direction are considered; properties in the other directions are assumed to be constant. The initial temperature distribution  $T(x,0)$  has a step-like perturbation. B) Finite difference discretization of the 1D heat equation. The finite difference method approximates the temperature at given grid points, with spacing  $\Delta x$ . The time-evolution is also computed at given times with timestep  $\Delta t$ .

In addition we assume that the temperature far away from the dike center (at  $|L/2|$ ) remains at a constant temperature. The boundary conditions are thus

$$T(x = -L/2, t) = 300 \quad (9)$$

$$T(x = L/2, t) = 300 \quad (10)$$

So now you have a feeling about finite differences. The attached MATLAB code shows an example in which the grid is initialized, and a time loop is performed. In the exercise, you will fill in the questionmarks and obtain a working code that solves equation 2.

### 3 Exercises

1. Open the MATLAB editor and create an empty file with the name "heat1Dexplicit.m". Fill in the question marks and run the file by typing heat1Dexplicit in the MATLAB command window (make sure you're in the correct directory).
2. Vary the parameters (e.g. use more gridpoints, a larger timestep). Note that if the timestep is increased beyond a certain value (what does this value depend on?), the numerical method becomes unstable. This is a major drawback of explicit finite difference codes such as the one presented here. In the next lesson we will learn methods that do not have these limitations.
3. Go through the rest of the handout and see how one derives finite difference approximations.
4. Record and plot the temperature evolution versus time at a distance of 5 meter from the dike/country rock contact. What is the maximum temperature the country rock experiences at this location and when is it reached? Assume that the country rock was composed of shales, and that those shales were transformed to hornfels above a temperature of  $600^\circ\text{C}$ . What is the width of the metamorphic aureole?
5. Bonus question: Derive a finite-difference approximation for variable  $k$  and variable  $\Delta x$ .

```
%heat1Dexplicit.m
%
% Solves the 1D heat equation with an explicit finite difference scheme

clear

%Physical parameters
L      = 100;      % Length of modeled domain      [m]
Tmagma = 1200;    % Temperature of magma          [C]
Trock  = 300;     % Temperature of country rock [C]
kappa  = 1e-6;    % Thermal diffusivity of rock [m2/s]
W      = 5;      % Width of dike                    [m]
day    = 3600*24; % # seconds per day
dt     = 1*day;   % Timestep                        [s]

% Numerical parameters
nx     = 201;     % Number of gridpoints in x-direction
nt     = 500;    % Number of timesteps to compute
dx     = L/(nx-1); % Spacing of grid
x      = -L/2:dx:L/2;% Grid

% Setup initial temperature profile
T      = ones(size(x))*Trock;
T(find(abs(x)<=W/2)) = Tmagma;

time   = 0;
for n=1:nt % Timestep loop

    % Compute new temperature
    Tnew = zeros(1,nx);
    for i=2:nx-1
        Tnew(i) = T(i) + ?????;
    end

    % Set boundary conditions
    Tnew(1) = T(1);
    Tnew(nx) = T(nx);

    % Update temperature and time
    T = Tnew;
    time = time+dt;

    % Plot solution
    figure(1), clf
    plot(x,Tnew);
    xlabel('x [m]')
    ylabel('Temperature [°C]')
    title(['Temperature evolution after ',num2str(time/day),' days'])

    drawnow
end
```

Figure 2: MATLAB script to solve equation 2 (once the question marks are filled...).

## Taylor-series expansions and finite differences

Finite difference approximations can be derived through the use of Taylor series expansions. Suppose we have a function  $f(x)$ , which is continuous and differentiable over the range of interest. Let's also assume we know the value  $f(x_0)$  and all the derivatives at  $x = x_0$ . The forward Taylor-series expansion for  $f(x_0 + \Delta x)$  about  $x_0$  gives

$$f(x_0 + \Delta x) = f(x_0) + \frac{\partial f(x_0)}{\partial x} \Delta x + \frac{\partial^2 f(x_0)}{\partial x^2} \frac{(\Delta x)^2}{2!} + \frac{\partial^3 f(x_0)}{\partial x^3} \frac{(\Delta x)^3}{3!} + \frac{\partial^n f(x_0)}{\partial x^n} \frac{(\Delta x)^n}{n!} + O(\Delta x)^{n+1} \quad (11)$$

We can compute the first derivative by rearranging equation 11

$$\frac{\partial f(x_0)}{\partial x} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - \frac{\partial^2 f(x_0)}{\partial x^2} \frac{(\Delta x)}{2!} - \frac{\partial^3 f(x_0)}{\partial x^3} \frac{(\Delta x)^2}{3!} \dots \quad (12)$$

This can also be written in discretized notation as:

$$\frac{\partial f(x_i)}{\partial x} = \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x) \quad (13)$$

here  $O(\Delta x)$  is called the *truncation error*, which means that if the distance  $\Delta x$  is made smaller and smaller, the (numerical approximation) error decreases as  $\Delta x$ . This derivative is also called first order accurate.

We can also expand the Taylor series backward

$$f(x_0 - \Delta x) = f(x_0) - \frac{\partial f(x_0)}{\partial x} \Delta x + \frac{\partial^2 f(x_0)}{\partial x^2} \frac{(\Delta x)^2}{2!} - \frac{\partial^3 f(x_0)}{\partial x^3} \frac{(\Delta x)^3}{3!} + \dots \quad (14)$$

In this case, the first (backward) derivative can be written as

$$\frac{\partial f(x_0)}{\partial x} = \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x} + \frac{\partial^2 f(x_0)}{\partial x^2} \frac{(\Delta x)}{2!} - \frac{\partial^3 f(x_0)}{\partial x^3} \frac{(\Delta x)^2}{3!} \dots \quad (15)$$

$$\frac{\partial f(x_i)}{\partial x} = \frac{f_i - f_{i-1}}{\Delta x} + O(\Delta x) \quad (16)$$

By adding equations 12 and 15 and dividing by two a second order accurate first order derivative is obtained

$$\frac{\partial f(x_i)}{\partial x} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x)^2 \quad (17)$$

By adding equations 11 and 14 an approximation of the second derivative is obtained

$$\frac{\partial^2 f(x_i)}{\partial x^2} = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} + O(\Delta x)^2 \quad (18)$$

With this approach we can basically derive all possible finite difference approximations. A different way to derive the second derivative is by computing the first derivative at  $i+1/2$  and at  $i-1/2$  and computing the second derivative at  $i$  by using those two first derivatives:

$$\frac{\partial f(x_{i+1/2})}{\partial x} = \frac{f_{i+1} - f_i}{x_{i+1} - x_i} \quad (19)$$

$$\frac{\partial f(x_{i-1/2})}{\partial x} = \frac{f_i - f_{i-1}}{x_i - x_{i-1}} \quad (20)$$

$$\frac{\partial^2 f(x_i)}{\partial x^2} = \frac{\frac{\partial f(x_{i+1/2})}{\partial x} - \frac{\partial f(x_{i-1/2})}{\partial x}}{x_{i+1/2} - x_{i-1/2}} = \frac{\frac{f_{i+1} - f_i}{x_{i+1} - x_i} - \frac{f_i - f_{i-1}}{x_i - x_{i-1}}}{0.5(x_{i+1} - x_{i-1})} \quad (21)$$

Similarly we can derive higher order derivatives. Note that the highest order derivative that usually occurs in geodynamics is the 4<sup>th</sup>-order derivative.

## Finite difference approximations

The following equations are common finite difference approximations of derivatives. If you in the future need to write a finite difference approximation, come back here.

Left-sided first derivative, first order

$$\left. \frac{\partial u}{\partial x} \right|_{i-1/2} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x) \quad (22)$$

Right-sided first derivative, first order

$$\left. \frac{\partial u}{\partial x} \right|_{i+1/2} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x) \quad (23)$$

Central first derivative, second order

$$\left. \frac{\partial u}{\partial x} \right|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x)^2 \quad (24)$$

Central first derivative, fourth order

$$\left. \frac{\partial u}{\partial x} \right|_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + O(\Delta x)^4 \quad (25)$$

Central second derivative, second order

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x)^2 \quad (26)$$

Central second derivative, fourth order

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\Delta x^2} + O(\Delta x)^4 \quad (27)$$

Central third derivative, second order

$$\left. \frac{\partial^3 u}{\partial x^3} \right|_i = \frac{u_{i+2} - 2u_{i+1} + 2u_{i-1} - u_{i-2}}{2\Delta x^3} + O(\Delta x)^2 \quad (28)$$

Central third derivative, fourth order

$$\left. \frac{\partial^3 u}{\partial x^3} \right|_i = \frac{-u_{i+3} + 8u_{i+2} - 13u_{i+1} + 13u_{i-1} - 8u_{i-2} + u_{i-3}}{8\Delta x^3} + O(\Delta x)^4 \quad (29)$$

Central fourth derivative

$$\left. \frac{\partial^4 u}{\partial x^4} \right|_i = \frac{u_{i+2} - 4u_{i+1} + 6u_i - 4u_{i-1} + u_{i-2}}{\Delta x^4} + O(\Delta x)^2 \quad (30)$$

Note that the higher the order of the finite difference scheme, the more adjacent points are required. It is also important to note that derivatives of the following form

$$\frac{\partial}{\partial x} \left( k \frac{\partial u}{\partial x} \right) \quad (31)$$

should be formed as follows

$$\left. \frac{\partial}{\partial x} \left( k \frac{\partial u}{\partial x} \right) \right|_i = \frac{k_{i+1/2} \frac{u_{i+1} - u_i}{\Delta x} - k_{i-1/2} \frac{u_i - u_{i-1}}{\Delta x}}{\Delta x} + O(\Delta x)^2 \quad (32)$$

If  $k$  is spatially varying, the following approximations are wrong (but are commonly made mistakes...!!!!

$$\left| \frac{\partial}{\partial x} \left( k \frac{\partial u}{\partial x} \right) \right|_i = \frac{k_{i+1} \frac{u_{i+1} - u_i}{\Delta x} - k_i \frac{u_i - u_{i-1}}{\Delta x}}{\Delta x} \quad (33)$$

$$\left| \frac{\partial}{\partial x} \left( k \frac{\partial u}{\partial x} \right) \right|_i = k_i \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \quad (34)$$