1 Finite difference example: 1D explicit heat equation

Finite difference methods are perhaps best understood with an example. Consider the one-dimensional, transient (*i.e.* time-dependent) heat conduction equation without heat generating sources

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

where ρ 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

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

where

$$\kappa = \frac{k}{\rho c_p} \tag{3}$$

is the thermal diffusivity (a common value for rocks is $\kappa = 10^{-6}$ m^{2}s^{-1}; also see discussion in sec. **??**).

We are interested in the temperature evolution versus time, $T(x,t)$, which satisfies eq. (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 eq. (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

$$\frac{\partial T}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{t^{n+1} - t^n} = \frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{T_i^{new} - T_i^{current}}{\Delta t}. \tag{4}$$

Here, n represents the temperature at the current time step 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 eq. (2) is replaced by a central finite difference approximation (*cf.* sec. **??**), *i.e.*

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right) \approx \frac{\frac{T_{i+1}^n - T_i^n}{\Delta x} - \frac{T_i^n - T_{i-1}^n}{\Delta x}}{\Delta x} = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}. \tag{5}$$

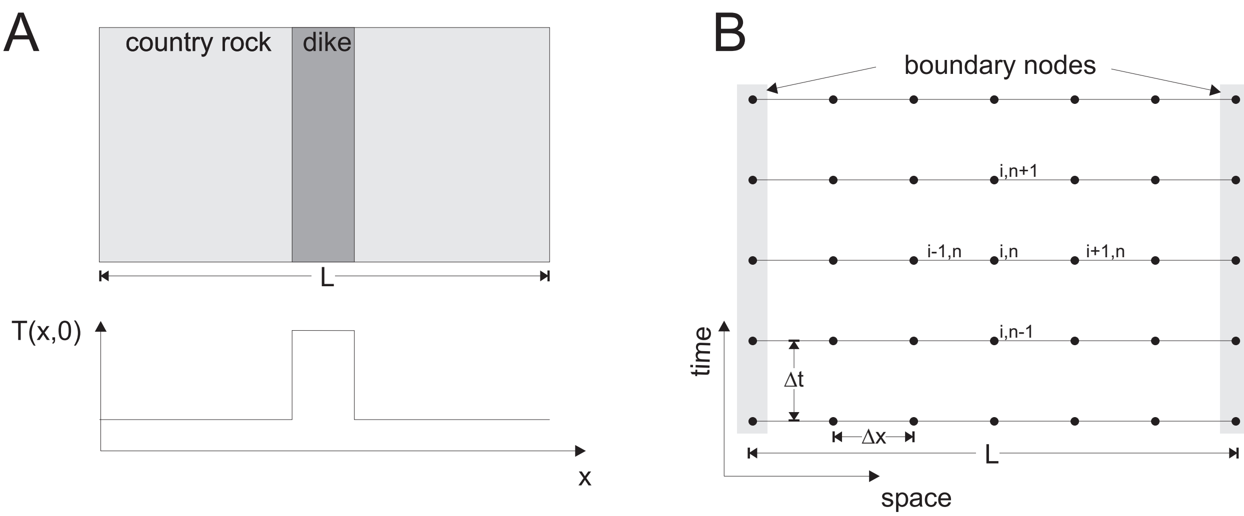

Figure 1: A) Setup of the thermal cooling model considered here. A hot basaltic dike intrudes cooler country rocks. Only variations in x-direction are considered; properties in the other directions are assumed to be constant. The initial temperature distribution $T(x, 0)$ has a step-like perturbation, centered around the origin with $[-W/2; W/2]$ B) Finite difference discretization of the 1D heat equation. The finite difference method approximates the temperature at given grid points, with spacing Δx. The time-evolution is also computed at given times with time step Δt.

Substituting eqs. (5) and (4) into eq. (2) gives

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

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:

$$T_i^{n+1} = T_i^n + \kappa \Delta t \left(\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2} \right) \tag{7}$$

Because the temperature at the current time step (n) is known, we can use eq. (7) to compute the new temperature without solving any additional equations. Such a scheme is and *explicit* finite difference method and was made possible by the choice to evaluate the temporal derivative with forward differences. We know that this numerical scheme will converge to the exact solution for small Δx and Δt because it has been shown to be consistent – that its discretization process can be reversed, through a Taylor series expansion, to recover the governing partial differential equation – and because it is stable for *certain values* of Δt and Δx: any spontaneous perturbations in the solution (such as round-off error) will either be bounded or will decay.

The last step is to specify the initial and the boundary conditions. If for example the country rock has a temperature of 300°C and the dike a total width $W = 5$ m, with a magma temperature of 1200°C, we can write as initial conditions:

$$T(x < -W/2, x > W/2, t = 0) = 300 \tag{8}$$
$$T(-W/2 \leq x \leq W/2, t = 0) = 1200 \tag{9}$$

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

$$T(x = -L/2, t) = 300 \tag{10}$$
$$T(x = L/2, t) = 300 \tag{11}$$

The MATLAB code in Figure 2, `heat1Dexplicit.m`, shows an example in which the grid is initialized, and a time loop is performed. In the exercise, you will fill in the question marks and obtain a working code that solves eq. (7).

1.1 Exercises

1. Open MATLAB and an editor and type the Matlab script in an empty file; alternatively use the template provided on the web if you need inspiration. Save the file under the name `heat1Dexplicit.m`. If starting from the template, fill in the question marks and then run the file by typing `heat1Dexplicit` in the MATLAB command window (make sure you're in the correct directory). (Alternatively, type F5 to run from within the editor.)

2. Study the time evolution of the spatial solution using a variable y-axis that adjusts to the peak temperature, and a fixed axis with range `axis([-L/2 L/2 0 Tmagma])`. Comment on the nature of the solution. What parameter determines the relationship between two spatial solutions at different times?

   Does the temperature of the country rock matter for the nature of the solution? What about if there is a background gradient in temperature such that the country rock temperature increases from 300° at $x = -L/2$ to 600° at $x = L/2$?

3. Vary the parameters (*e.g.* use more grid points, a larger or smaller time step). Compare the results for small Δx and Δt with those for larger Δx and Δt. How are these solutions different? Why? Notice also that if the time step is increased beyond a certain value, the numerical method becomes unstable and does not converge – it grows without bounds and exhibits non-physical features.

   Investigate which parameters affect stability, and find out what ratio of these parameters delimits this scheme's stability region. This is called the CFL condition, see von Neumann stability analysis in (*cf.* chap 5 of *Spiegelman*, 2004).

```
%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 [^oC]')
    title(['Temperature evolution after ',num2str(time/day),' days'])

    drawnow
end
```

Figure 2: MATLAB script `heat1Dexplicit.m` to solve eq. (2) (once the blanks indicated by the questions marks are filled in . . .).

4. Record and plot the temperature evolution versus time at a distance of 5 m from the dikecountry 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°C. What is the width of the metamorphic aureole?

5. Think about how one would write a non-dimensionalized version of the temperature solver.

6. Add a test with an analytical solution for diffusion and plot error *vrs.* resolution. A good reference for analytical solutions for heat conduction problems is *Carslaw and Jaeger* (1959), or see sec. **??**.

   The spatial discretization should be second order for a second order scheme.

7. Derive a finite-difference approximation for variable k (and variable Δx allowing for

uneven spacing between grid points should you so desire). Test the solution for the case of $k = 10$ inside the dike, and $k = 3$ in the country rock.

Bibliography

Carslaw, H. S., and J. C. Jaeger (1959), *Conduction of Heat in Solids*, 2nd ed., Oxford University Press, London, p. 243.

Spiegelman, M. (2004), *Myths and Methods in Modeling*, Columbia University Course Lecture Notes, available online at http://www.ldeo.columbia.edu/~mspieg/mmm/course.pdf, accessed 06/2006.