Appendix B

Crank-Nicolson scheme

To determine the evolution of subsurface temperature with time, the Crank-Nicolson method, obtained by computing the average of the explicit and implicit forward time centered space (FTCS) schemes, is used to solve the heat equation:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) + \rho H, \quad k\frac{\partial T}{\partial z} = F \tag{B.1}$$

where ρ is density, c is specific heat capacity, T is temperature, z is vertical coordinate, t is time, k is thermal conductivity, H is radiogenic heat production and F is heat flow. The first term of the second member of the Equation B.1 can be differentiated on an irregular grid as:

$$\frac{\partial}{\partial z} F_j = \frac{F_{j+1/2} - F_{j-1/2}}{(z_{j+1} - z_{j-1})/2} = 2\frac{k_{j+1/2}\frac{T_{j+1}-T_j}{z_{j+1}-z_j} - k_{j-1/2}\frac{T_j - T_{j-1}}{z_j - z_{j-1}}}{z_{j+1} - z_{j-1}} \tag{B.2}$$

We then obtain:

$$\begin{aligned}(\rho c)_j \frac{\partial T_j}{\partial t} =& \frac{2k_{j+1/2}}{(z_{j+1} - z_j)(z_{j+1} - z_{j-1})} T_{j+1} \\ & - \frac{2}{z_{j+1} - z_{j-1}} \left(\frac{k_{j+1/2}}{z_{j+1} - z_j} + \frac{k_{j-1/2}}{z_j - z_{j-1}}\right) T_j \\ & + \frac{2k_{j-1/2}}{(z_j - z_{j-1})(z_{j+1} - z_{j-1})} T_{j-1} + \rho_j H\end{aligned} \tag{B.3}$$

We introduce:

$$\alpha_j = \frac{\Delta t}{(\rho c)_j} \frac{k_{j+1/2}}{(z_{j+1} - z_j)(z_{j+1} - z_{j-1})} \tag{B.4a}$$

$$\gamma_j = \frac{\Delta t}{(\rho c)_j} \frac{k_{j-1/2}}{(z_j - z_{j-1})(z_{j+1} - z_{j-1})} \tag{B.4b}$$

Equation B.3 thus becomes:

$$\Delta t \frac{\partial T_j}{\partial t} = 2\alpha_j T_{j+1} - 2(\alpha_j + \gamma_j)T_j + 2\gamma_j T_{j-1} + \frac{\Delta t H}{c_j} \tag{B.5}$$

Applying Crank-Nicolson, we get:

$$\begin{aligned} T_j^{n+1} - T_j^n =& \alpha_j T_{j+1}^{n+1} - (\alpha_j + \gamma_j)T_j^{n+1} + \gamma_j T_{j-1}^{n+1} \\ &+ \alpha_j T_{j+1}^n - (\alpha_j + \gamma_j)T_j^n + \gamma_j T_{j-1}^n + \frac{\Delta t H}{c_j} \end{aligned} \tag{B.6}$$

Rearranging the equation to isolate the different time-variables gives:

$$\begin{aligned} &- \alpha_j T_{j+1}^{n+1} + (1 + \alpha_j + \gamma_j)T_j^{n+1} - \gamma_j T_{j-1}^{n+1} \\ &= \alpha_j T_{j+1}^n + (1 - \alpha_j - \gamma_j)T_j^n + \gamma_j T_{j-1}^n + \frac{\Delta t H}{c_j} \end{aligned} \tag{B.7}$$

This system of linear equations is tridiagonal and can easily be solved at each time step by *LU* decomposition (see *tridag* routine from *Numerical Recipes* (Press et al., 1997), for instance). The thermal conductivity k is defined on half-points and $(\rho c)_j = \frac{(\rho c)_{j-1/2} + (\rho c)_{j+1/2}}{2}$ so that these parameters do not have to be determined at the interface of two layers with different thermal properties. The upper and lower boundary conditions are given by the surface temperature and the heat flow, respectively.

Lower boundary condition

If N is the total number of subsurface layers and assuming $z_{N+1} - z_N = z_N - z_{N-1}$, we can write:

$$k_{N+1/2}(T_{N+1} - T_N) = (z_{N+1} - z_N)F \tag{B.8}$$

and thus

$$T_{N+1} = T_N + \frac{(z_{N+1} - z_N)F}{k_{N+1/2}} \tag{B.9}$$

Using the above relation and the expression of α_N in Equation B.7 for $j = N$ leads to:

$$\begin{aligned}(1+\gamma_N)T_N^{n+1} - \gamma_N T_{N-1}^{n+1} =& (1-\gamma_N)T_N^n + \gamma_N T_{N-1}^n \\ &+ \frac{\Delta t F}{(\rho c)_N (z_N - z_{N-1})} + \frac{\Delta t H}{c_N}\end{aligned} \tag{B.10}$$