Numerical Modelling in Geosciences

Lecture 11

Conservation of heat

Heat conservation equation

Describes the balance of heat in a continuum and relates temperature changes due to internal heat generation, as well as with advective and conductive heat trasport.
Heat is the exchange of thermal energy among parts of the system that are at different temperatures. Temperature is an indicator of the thermal energy content (potential) of a system.

Amount of heat required for $\Delta T\,(K)$:

$$\Delta Q = m c_P \Delta T \quad (Joule)$$

Such amount of heat is given by the balance of all heat sources and sinks:

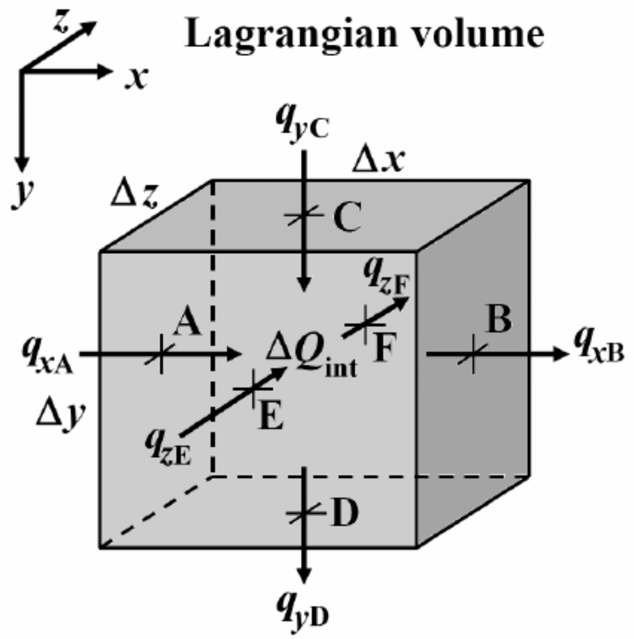
$$\Delta Q = \Delta Q_{\text{int}} + \Delta Q_A - \Delta Q_B + \Delta Q_C - \Delta Q_D + \Delta Q_E - \Delta Q_F$$

$$Ex:\ \Delta Q_A = q_{xA} \Delta y \Delta z \Delta t$$

$\Delta Q_{\text{int}} = H$ *is the rate of heat generated or consumed by different processes per unit volume* $(W\ m^{-3})$

Equating the above right hand sides and dividing by $V = \Delta x \Delta y \Delta z$ *and* Δt:

$$\rho c_P \frac{DT}{Dt} = -\nabla \cdot \vec{q} + H$$



Heat generation and consumption

$$H = H_r + H_r + H_r + H_r \ (W\,m^{-3})$$

$H_r = radioactive\ heat\ production,\ due\ to\ decay\ of\ radioactive\ elements$

$Granite \rightarrow 2\times10^{-6}\ W\,m^{-3}$

$Basalt \rightarrow 2\times10^{-7}\ W\,m^{-3}$

$Peridotite \rightarrow 2\times10^{-8}\ W\,m^{-3}$

$H_s = shear\ heat\ production,\ due\ to\ dissipation\ of\ mechanical\ energy\ during\ irreversible$

$non-elastic\ deformation$

$H_s = \sigma'_{ij}\dot{\varepsilon}'_{ij}\ where\ ij\ denotes\ summation$

$2D\ example: H_s = \sigma'_{xx}\dot{\varepsilon}'_{xx} + \sigma'_{yy}\dot{\varepsilon}'_{yy} + 2\sigma'_{xy}\dot{\varepsilon}'_{xy} = 2\sigma'_{xx}\dot{\varepsilon}'_{xx} + 2\sigma'_{xy}\dot{\varepsilon}'_{xy}$

$H_a = adiabatic\ heat\ production / consumption,\ due\ to\ adiabatic\ heating / cooling\ during$

$increase / decrease\ of\ pressure \Rightarrow H_a = T\alpha\frac{DP}{Dt}$

$H_L = latent\ heat\ production / consumption,\ due\ to\ phase\ transformations\ in\ rocks\ subjected$

$to\ changes\ in\ pressure\ and\ temperatures.$

$During\ melting\ H_L < 0,$

$During\ crystallization\ H_L > 0,$

Heat conservation equation

Describes the balance of heat in a continuum and relates temperature changes due to internal heat generation, as well as with advective and conductive heat trasport.

$$\rho c_P \frac{DT}{Dt} = -\nabla \cdot \vec{q} + H$$

$$\textit{Fourier's law}: q_i = -k\frac{\partial T}{\partial x_i} \;\; or \;\; \vec{q} = -k\nabla T$$

$$\rho c_P \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T \right) = \nabla \cdot \left(k \nabla T \right) + H$$

$$\rho c_P \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z} \right) + H$$

$$If \; k = const, \; no \; advection \;\; and \;\; H = 0$$

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_P}\Delta T \Rightarrow \boxed{\frac{\partial T}{\partial t} = \kappa \Delta T} \; (describes \; conduction \; of \; heat, \kappa \; is \; thermal \; diffusivity \; m^2 s^{-1})$$

$$If \; \frac{DT}{Dt} = 0 \Rightarrow \frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = 0 \; (temperature \; change \; at \; Eulerian \; points \; due \; to \; advection)$$

$$If \; \frac{DT}{Dt} = \frac{\partial T}{\partial t} = 0 \Rightarrow -\nabla \cdot \vec{q} + H = 0 \; (used \; to \; compute \; steady-state \; geotherms \rightarrow find \; analytical \; solution)$$

Heat diffusion

Heat diffusion is described by the Fourier's law, a constitutive relation stating that the flow of thermal energy along a given direction depends on the temperature gradient and thermal conductivity. Basically, thermal energy flows in order to elimate differences in potentials (temperature) and achieve equilibrium.
Diffusion (or conduction) of heat is due to propagation of kinetic energy among microscopic particles, without macroscopic displacement.
Characteristic timescale for diffusion of heat depends on the square of the width of the region where heat is produced and is inversely proportional to the material diffusivity

$$t_{diff} = \frac{L^2}{\kappa}$$

$$L = width\ of\ the\ region\ where\ the\ heat\ is\ generated$$

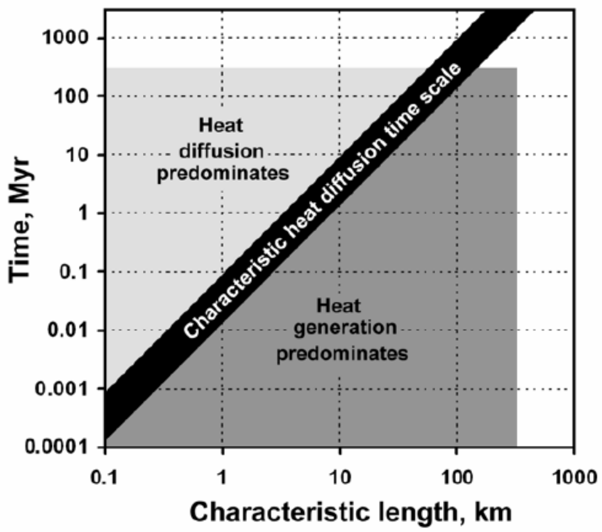


Fig. 9.2. Timescales for different thermal regimes calculated according to equation $t_{diff} = L^2/\kappa$ with $\kappa = 10^{-6}\ m^2 s^{-1}$. Shaded areas show length- and time-scales characteristic of collisional orogens (Burg and Gerya, 2005).

Thermal conductivity

It is the property of a material to conduct heat (W/m/°K)
Low k → thermal insulation
High k → heat sink

Heat transport in non-metals is by way of elastic vibrations of the lattice (phonons)

k in reality is a tensor → k_{ij}, because propagation of elastic vibrational waves depend on crystal structure and are limited by defects

Even if isotropic → **k=f(P,T,C)**

Typical values of thermal conductivity (in 0.001 calories per centimetre per second per degree Celsius)		
material	at 20 °C	at 200 °C
typical rocks	4–10	
granite	7.8	6.6
gneiss		
(perpendicular to banding)	5.9	5.5 (100 °C)
(parallel to banding)	8.2	7.4 (100 °C)
gabbro	5.1	5.0
basalt	4.0	4.0
dunite	12.0	8.1
marble	7.3	5.2
quartzite	15.0	9.0
limestone	6.0	
one sandstone		
(dry)	4.4	
(saturated)	5.4	
shale	3–4	
rock salt	12.8	
sand		
(dry)	0.65	
(30% water)	3.94	
water	1.34 (0 °C)	1.6 (80 °C)
ice	5.3 (0 °C)	9.6 (−130 °C)
magnetite	12.6	
quartz	20.0	
feldspars	5.0	

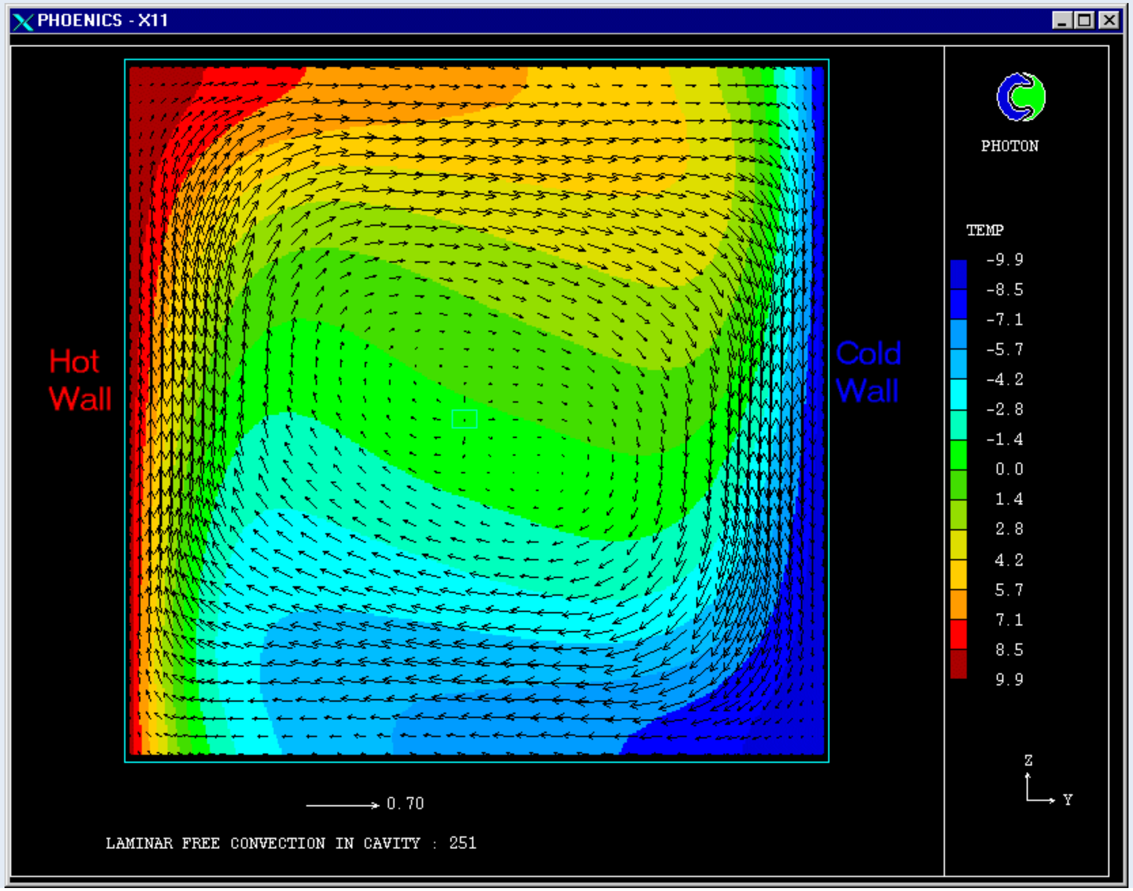
Diopside thermal conductivity

Heat advection

Heat advection occurs when there is macroscopic displacement of matter, which exchange places with other parcels of matter at a different temperature, so that internal energy is carried by the flow of matter.
In planetary bodies heat advection is due to internal temperature gradients generating buoyancy differences (through volume expansion/contraction). This is better known as thermal convection, occurring when the Rayleigh number:

$$Ra = \frac{g\alpha\rho_0 \Delta T D^3}{\mu\kappa} > Ra_C(10^3 - 10^4)$$

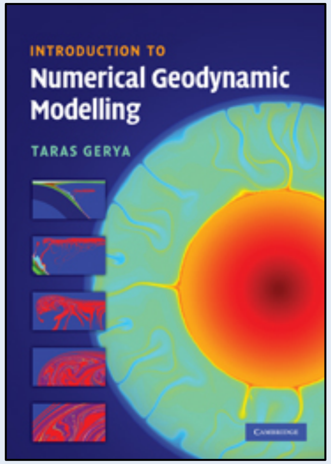
$$On\ \ Earth,\ Ra = 10^7$$



Homework

Read chapter 9 of textbook:

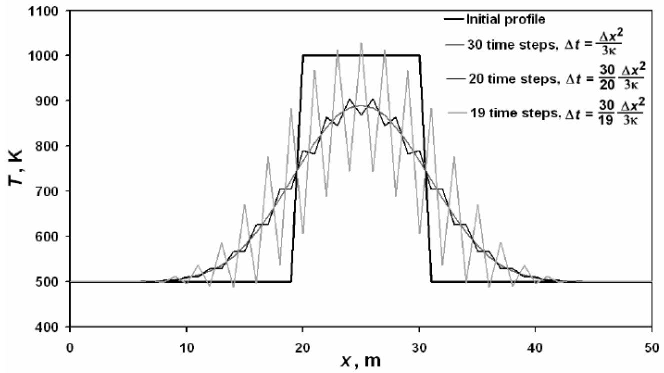
Gerya, T. *Introduction to numerical geodynamic modelling*. Cambridge University Press, 345 pp. (2010)



Solving heat equation: conduction

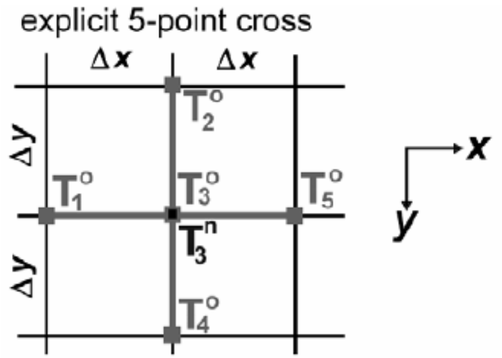
$$Constant\ \ k:$$

$$\rho c_P \frac{\partial T}{\partial t} = k\Delta T + H \Rightarrow \frac{\partial T}{\partial t} = \frac{k}{\rho c_P}\Delta T + \frac{H}{\rho c_P}$$



$$2D\,Explicit\ \ formulation:\ \Delta t < \frac{\Delta x^2}{3\kappa}\ \ !!!$$

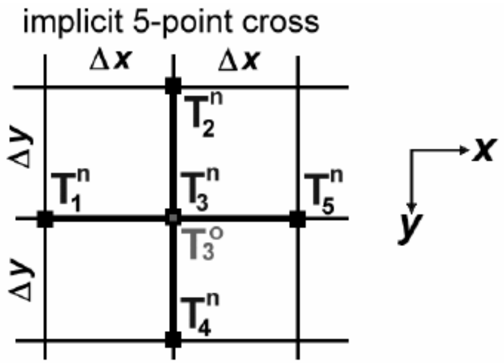
$$FD: T_3^n = T_3^0 + \frac{k\Delta t}{\rho c_P}\left(\frac{T_5^0 - 2T_3^0 + T_1^0}{\Delta x^2} + \frac{T_4^0 - 2T_3^0 + T_2^0}{\Delta y^2}\right) + \frac{H}{\rho c_P}\Delta t$$



$$2D\,Implicit\ \ formulation:$$

$$FD: \frac{T_3^n}{\Delta t} - \frac{k}{\rho c_P}\left(\frac{T_5^n - 2T_3^n + T_1^n}{\Delta x^2} + \frac{T_4^n - 2T_3^n + T_2^n}{\Delta y^2}\right) = \frac{T_3^0}{\Delta t} + \frac{H}{\rho c_P}$$

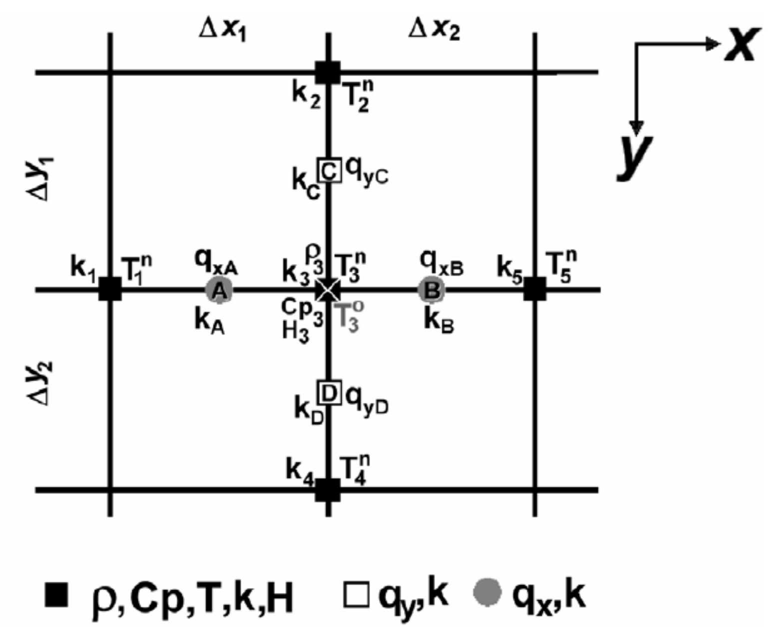
No limitation for Δt



Solving heat equation: conduction

General solution for variable grid and k

Implicit formulation:



$$\rho c_P \frac{\partial T}{\partial t} = -\nabla \cdot \vec{q} + H$$

$$\rho c_P \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T\right) + H$$

$$2D: \ \rho c_P \frac{\partial T}{\partial t} = -\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} + H = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + H$$

$$FD: \ \rho_3 c_{P_3} \frac{T_3^{t+\Delta t}}{\Delta t} + 2\frac{q_{xA} - q_{xB}}{\Delta x_1 + \Delta x_2} + 2\frac{q_{yD} - q_{yC}}{\Delta y_1 + \Delta y_2} = H_3 + \rho_3 c_{P_3} \frac{T_3^t}{\Delta t}$$

Solving heat equation: boundary conditions

Constant temperature:

$$T_1 = cnst$$

No heat flux (insulating or symmetric boundary):

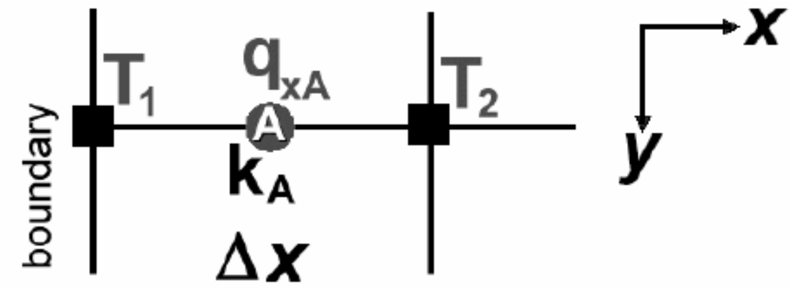
$$q_x = -k\frac{\partial T}{\partial x} = 0$$

$$T_1 - T_2 = 0$$

Constant heat flux:

$$q_x = -k\frac{\partial T}{\partial x} = cnst$$

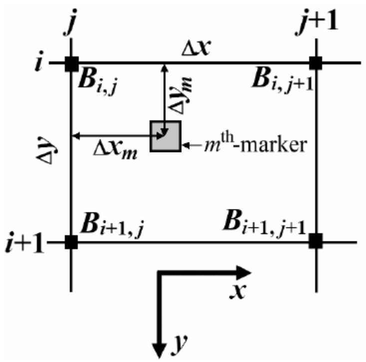
$$k_A \frac{T_1 - T_2}{\Delta x} = cnst$$



Solving heat equation: advection

In order to avoid numerical diffusion during advection (see Lecture 10), we can use the Lagrangian formulation of the heat equation and advect temperature with the marker-in-cell-technique. We must interpolate only temperature changes from the Eulerian nodes to the markers to minimize numerical diffusion during such interpolation.

$$\rho C_P \frac{DT}{Dt} = -\nabla \cdot \vec{q} + H$$



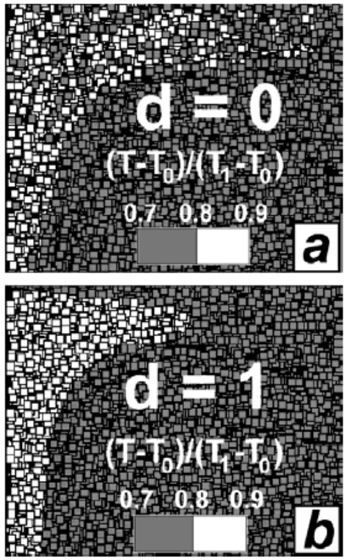
Changes in temperature for the Eulerian nodes:

$$\Delta T_{i,j} = T_{i,j}^{t+\Delta t} - T_{i,j}^{t}$$

are interpolated to get the marker temperature change ΔT_m :

$$T_m^{t+\Delta t} = T_m^{t} + \Delta T_m$$

This method, however, while preventing numerical diffusion, does not damp out small (subgrid) scale temperature differences between adjacent markers. In case of strong mixing due to thermal convection, numerical oscillations of the thermal field are produced. These oscillations do not damp out with time as would be the case if physical diffusion was active.



Solving heat equation: advection

In order to avoid numerical oscillations during advection, we must to introduce a consistent subgrid diffusion operation. We use part of the grid temperature change to apply subgrid temperature diffusion and thus remove non-physical subgrid oscillations.

1) *Changes in temperature for the Eulerian nodes are decomposed*:

$$\Delta T_{i,j} = \Delta T_{i,j}^{subgrid} + \Delta T_{i,j}^{remaining}$$

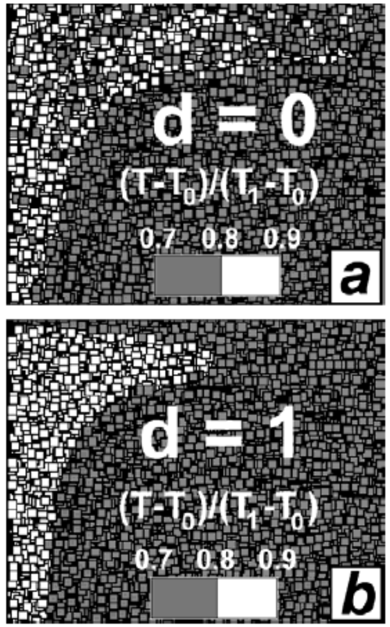
2) *Calculate subgrid* ΔT *for markers*:

$$\Delta T_m^{subgrid} = \left(T_{m(nodes)}^t - T_m^t\right)\left[1 - \exp\left(-d\frac{\Delta t}{\Delta t_{diff}}\right)\right]$$

$$\Delta t_{diff} = \frac{c_{P_m}\rho_m}{k_m\left(2/\Delta x^2 + 2/\Delta y^2\right)}$$ (*local heat diffusion timescale for a given cell*)

$0 \le d \le 1$ (*dimensionless numerical diffusion coefficient*)

$T_{m(nodes)}^t, c_{P_m}, \rho_m, k_m$ *are interpolated from* $T_{i,j}^t, c_{Pi,j}, \rho_{i,j}, k_{i,j}$



3) *Interpolate* $\Delta T_m^{subgrid}$ *to Eulerian nodes to get* $\Delta T_{i,j}^{subgrid}$

4) *Compute* $\Delta T_{i,j}^{remaining} = \Delta T_{i,j} - \Delta T_{i,j}^{subgrid}$

5) *Interpolate* $\Delta T_{i,j}^{remaining}$ *to markers to get* $\Delta T_m^{remaining}$

6) *Finally, compute new marker temperature*: $T_{m(corrected)}^t = T_m^t + \Delta T_m^{subgrid} + \Delta T_m^{remaining}$

Homework

Read chapter 10 of textbook:

Gerya, T. *Introduction to numerical geodynamic modelling*. Cambridge University Press, 345 pp. (2010)