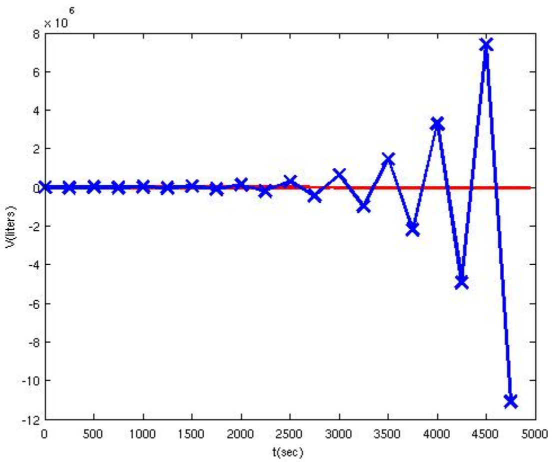
SUBITOP

Understanding subduction zone topography through modelling of coupled shallow and deep processes

- ❑ Heat diffusion equation
- ❑ Timestep stability criterion
- ❑ Essential versus natural boundary conditions



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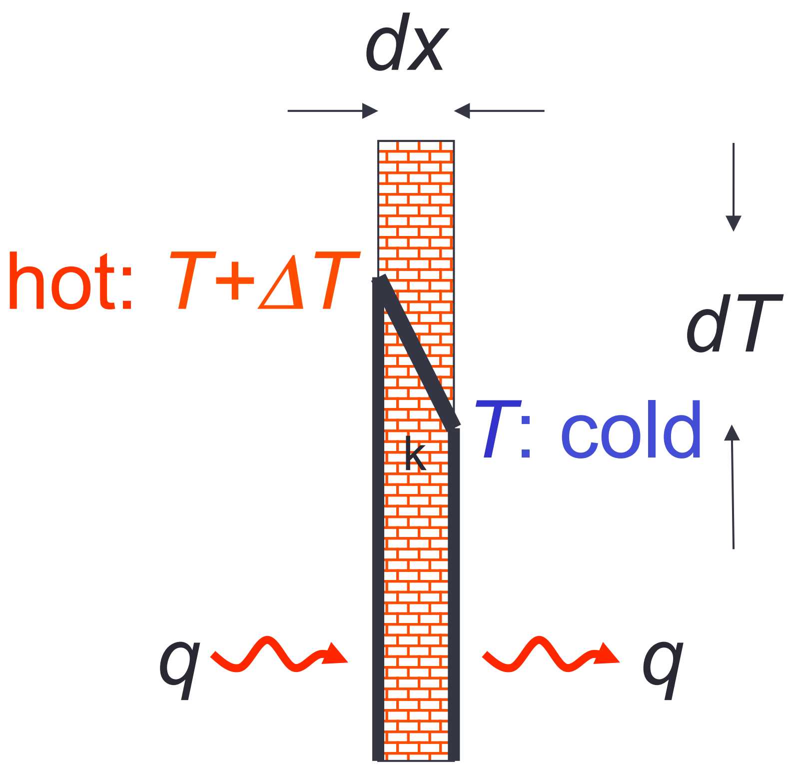
HORIZON 2020

Heat diffusion: Fourier's law



Joseph Fourier

$$q = -k \frac{dT}{dx}$$

'heat conductivity'

Conservation of heat (energy)

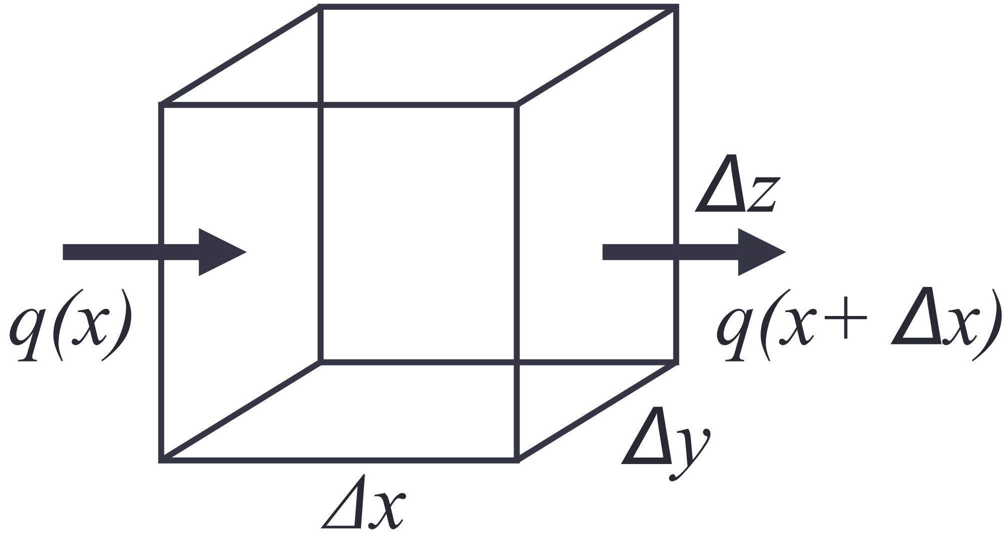
$$\frac{dE}{dt} = Q(x) - Q(x+\Delta x)$$

using:

$$E = MC_pT = \rho \Delta x \Delta y \Delta z C_p T$$

$$Q = q \Delta y \Delta z$$

$$\rho C_p \frac{dT}{dt} = \frac{q(x) - q(x+\Delta x)}{\Delta x}$$



Heat conservation and Fourier's law

$$\rho C_p \frac{dT}{dt} = \frac{q(x) - q(x+\Delta x)}{\Delta x}$$

$$q = -k \frac{dT}{dx}$$

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

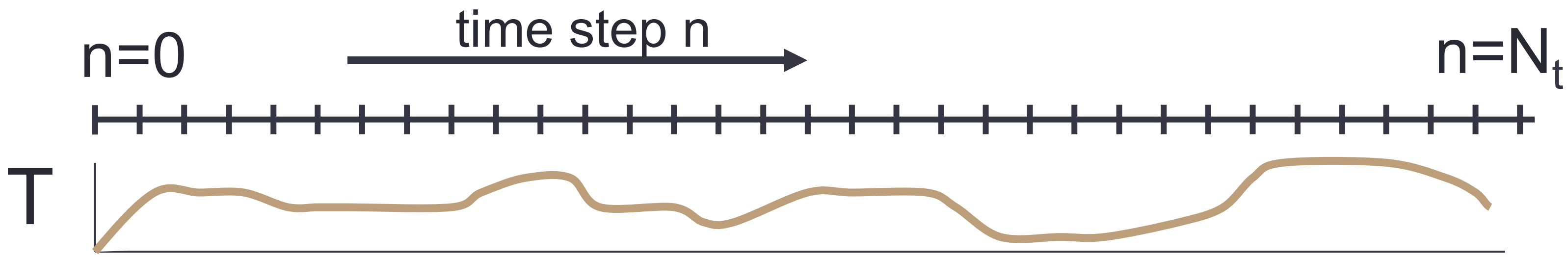
if $\kappa = \dfrac{k}{\rho C_p}$ is constant

'heat diffusivity'

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

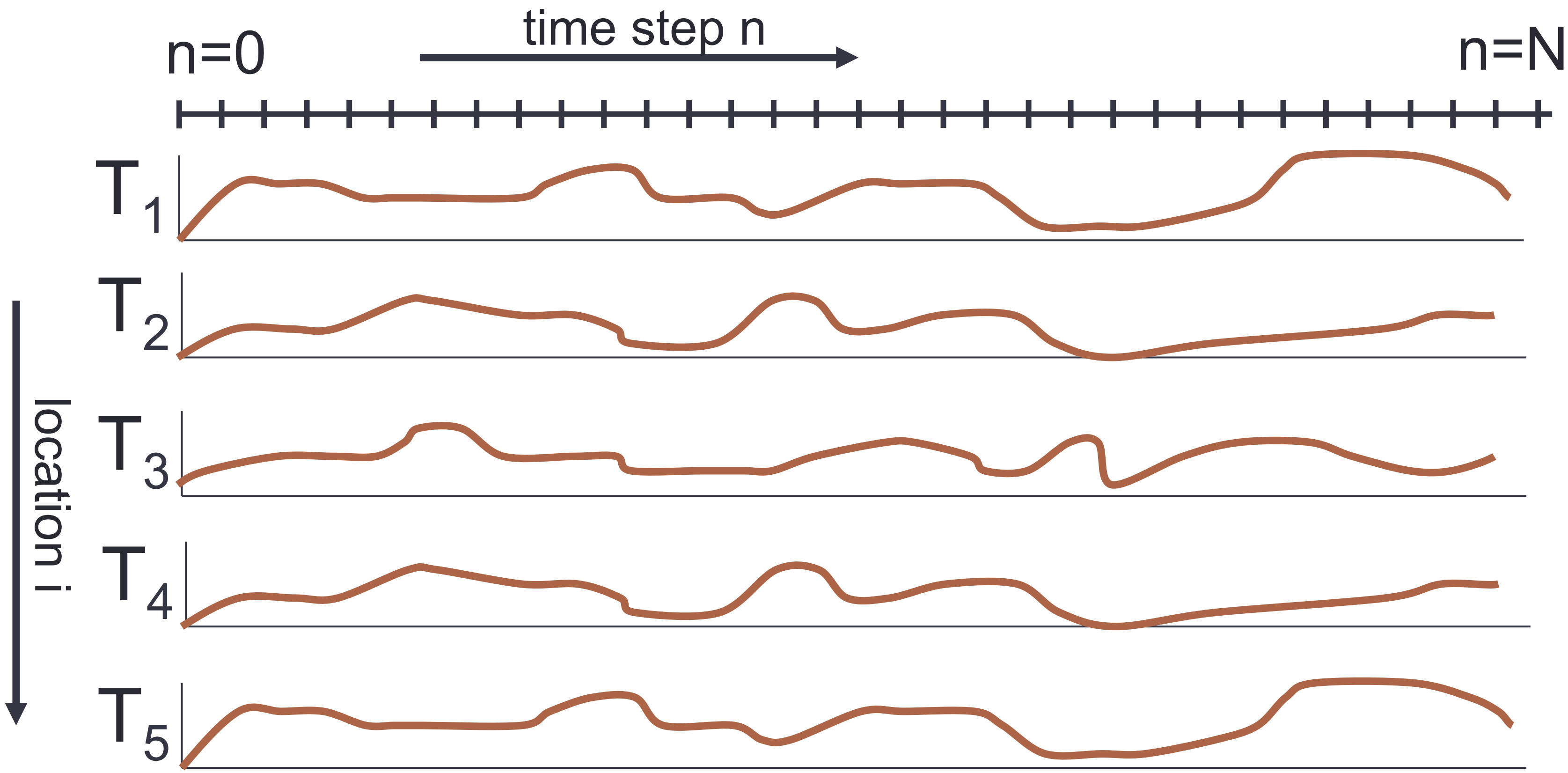
From Physics to Model

- Modelling one point/parameter through time:



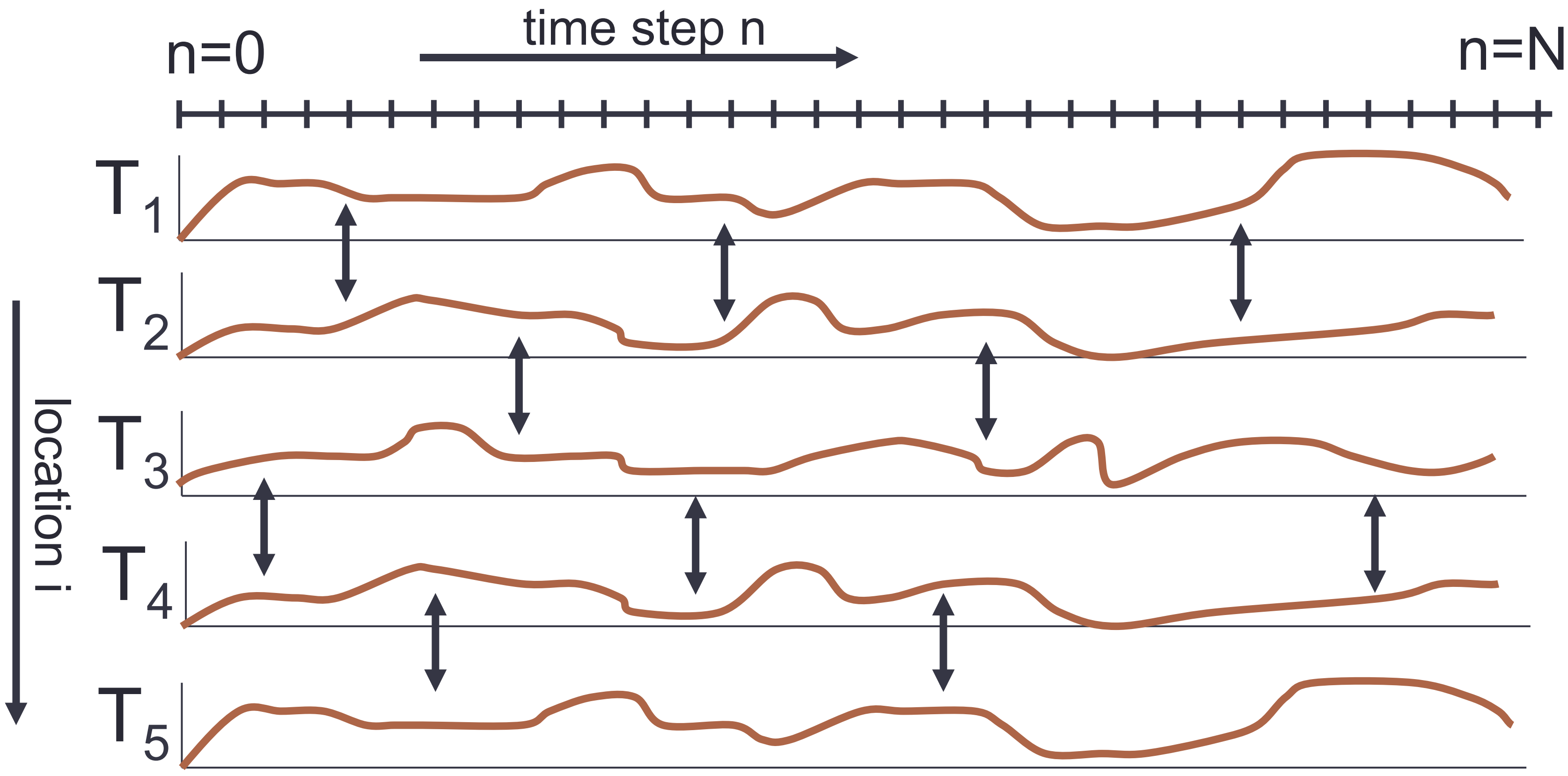
From Physics to Model

- Modelling *N* independent points through time:



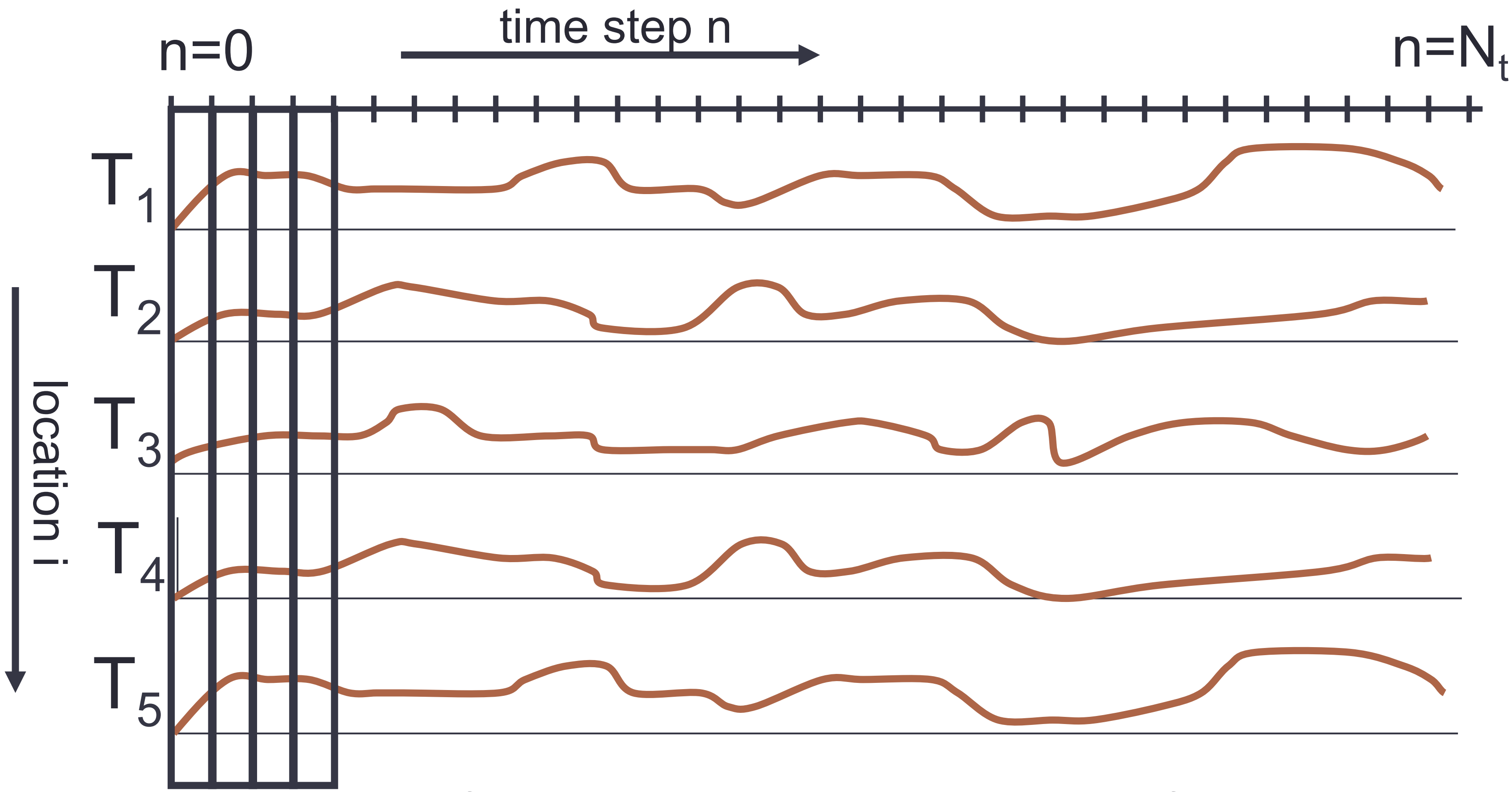
From Physics to Model

- Modelling *N dependent* points through time:



From Physics to Model

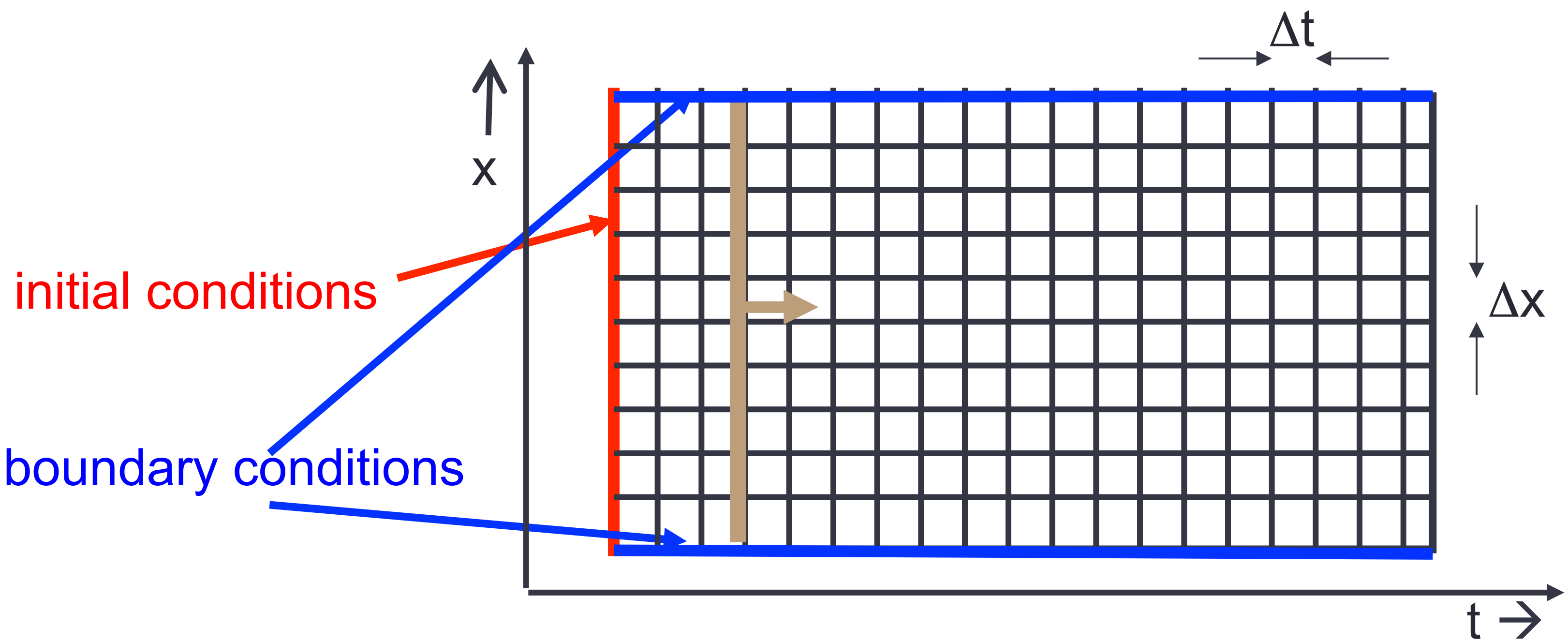
- Modelling *N dependent* points through time:



Model an array of data at time *t*, rather than a bunch of independent points

Initial and boundary conditions

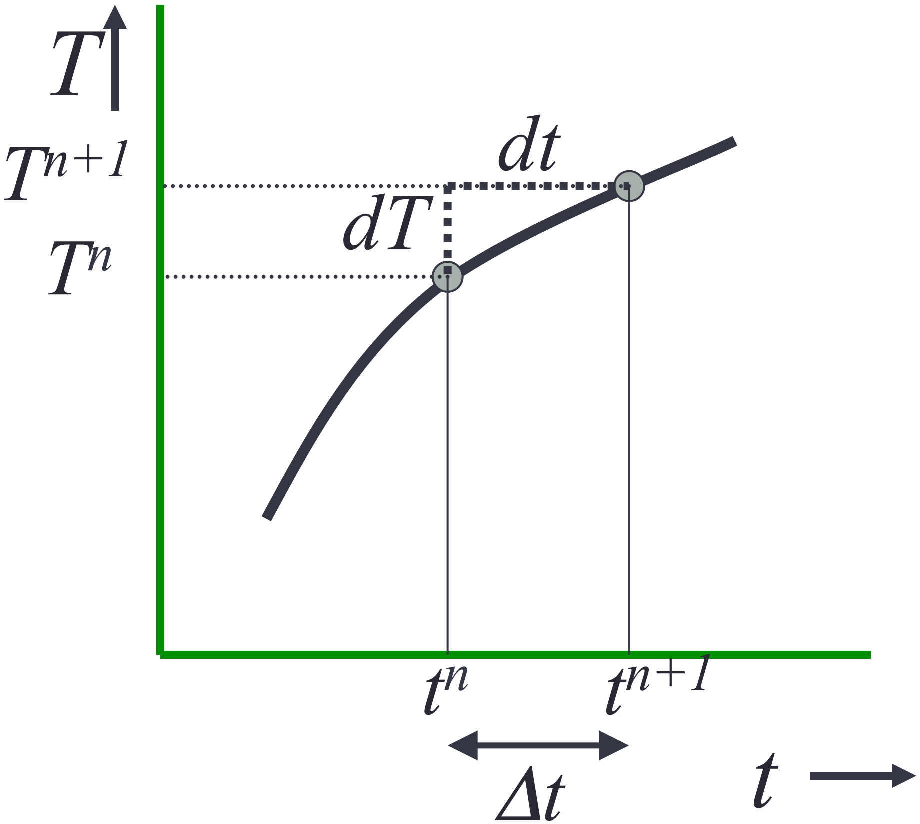
- Initial conditions need to be provided for every grid point (only at *t=0*).
- Boundary conditions need to be provided for every time step (only at first and last grid point).



Time derivative → finite difference

$$\frac{dT}{dt} = \frac{T(t+\Delta t) - T(t)}{\Delta t}$$

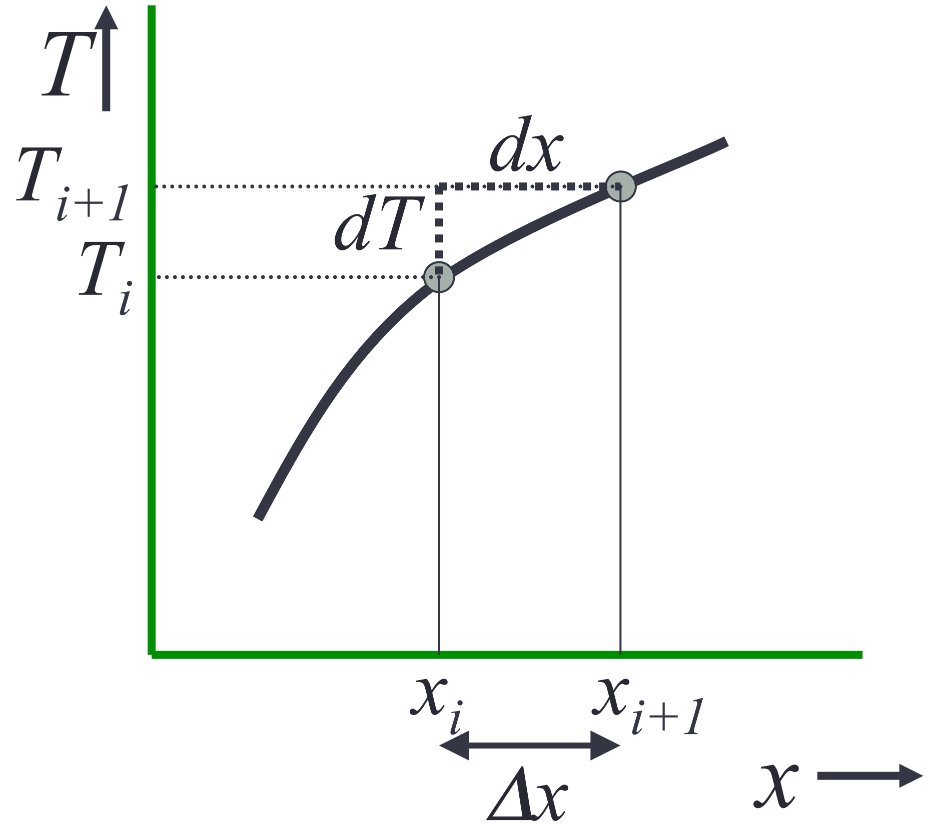
$$\frac{dT}{dt} = \frac{T^{n+1} - T^{n}}{\Delta t}$$



Spatial derivative → finite difference

$$\frac{dT}{dx} = \frac{T_{i+1} - T_i}{\Delta x}$$

→



Other ways to calculate derivative:

$$\frac{dT}{dx} = \frac{T_i - T_{i-1}}{\Delta x}$$

$$\frac{dT}{dx} = \frac{T_{i+1} - T_{i-1}}{2\Delta x}$$

$$\frac{dT}{dx} = \frac{T_{i+1/2} - T_{i-1/2}}{\Delta x}$$

The second-order derivative

$$\frac{\partial T_i^n}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{\Delta t}$$

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

$$\frac{\partial^2 T_i^n}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial T_i^n}{\partial x}\right) = \frac{\partial}{\partial x}\left(S_i^n\right)$$

$$\approx \frac{S_{i+1/2}^n - S_{i-1/2}^n}{\Delta x}$$

$$\approx \frac{\frac{T_{i+1}^n - T_i^n}{\Delta x} - \frac{T_i^n - T_{i-1}^n}{\Delta x}}{\Delta x}$$

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

The second-order derivative

$$\frac{\partial T_i^n}{\partial t} \approx \frac{T_i^{n+1} - T_i^n}{\Delta t}$$

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

$$\frac{\partial^2 T_i^n}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial T_i^n}{\partial x}\right) = \frac{\partial}{\partial x}\left(S_i^n\right)$$

$$\approx \frac{S_{i+1/2}^n - S_{i-1/2}^n}{\Delta x}$$

$$\approx \frac{\dfrac{T_{i+1}^n - T_i^n}{\Delta x} - \dfrac{T_i^n - T_{i-1}^n}{\Delta x}}{\Delta x}$$

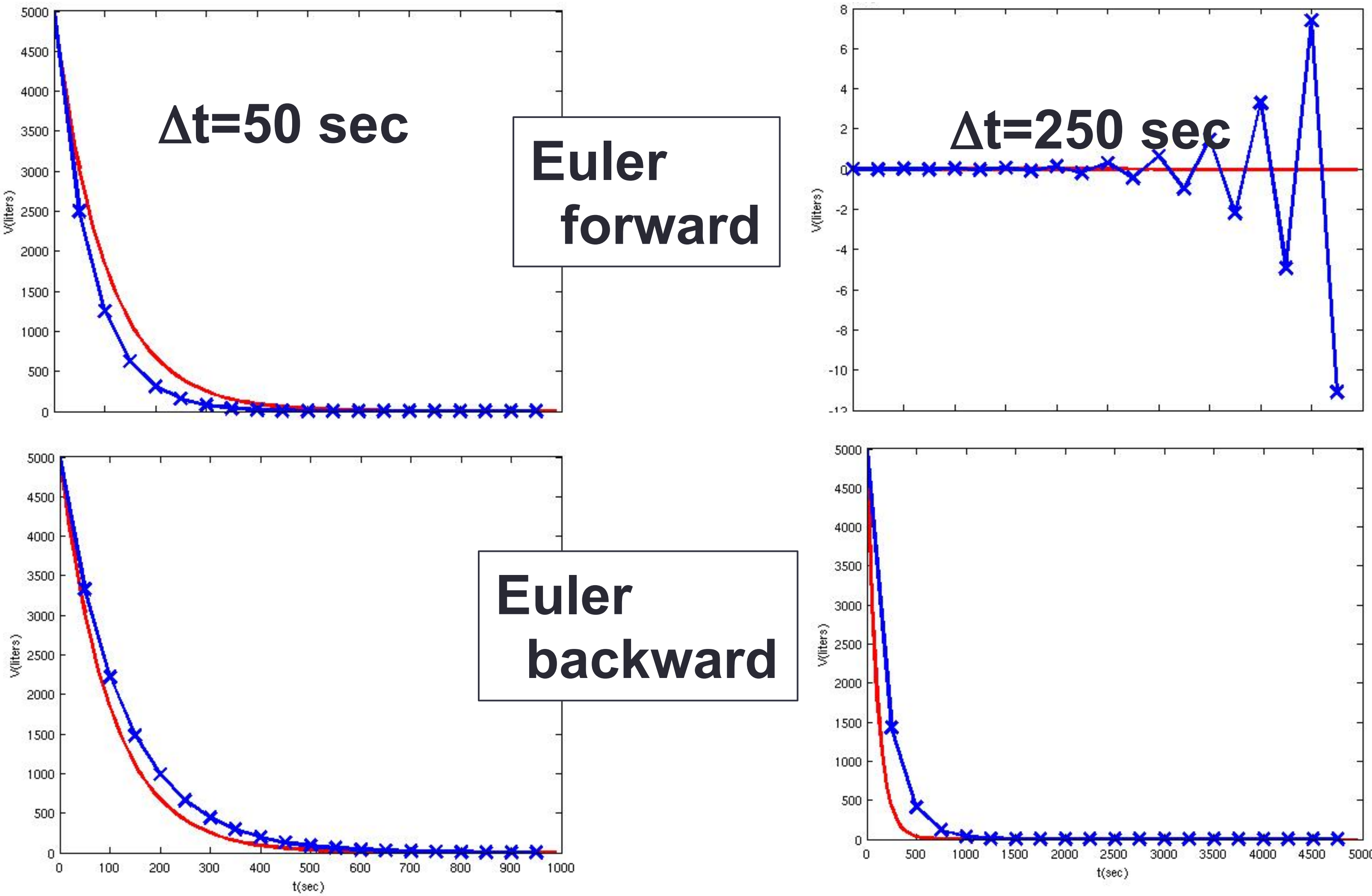
$$= \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

Notation !

Practical 2, part 1:

- Modelling a cooling ocean lithosphere:
  - Familiarise yourself with the model and equations using a simple scenario and paper and pencil
  - Complete the model in Python by adding your own subfunction for diffusion
  - Explore how numerical and analytical solutions compare and the effect of different discretisation steps in time and space
  - If time permits, calculate the growth of the lithosphere with time

Stability criterion: exp. decay function

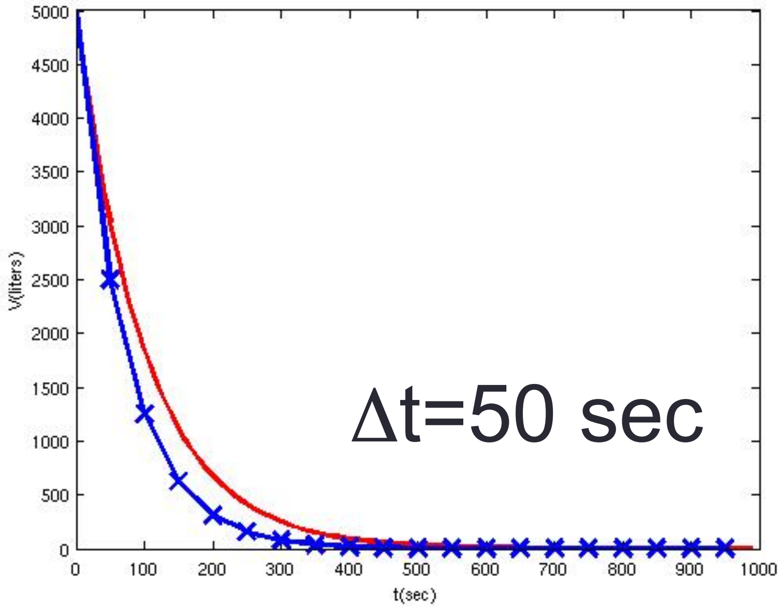


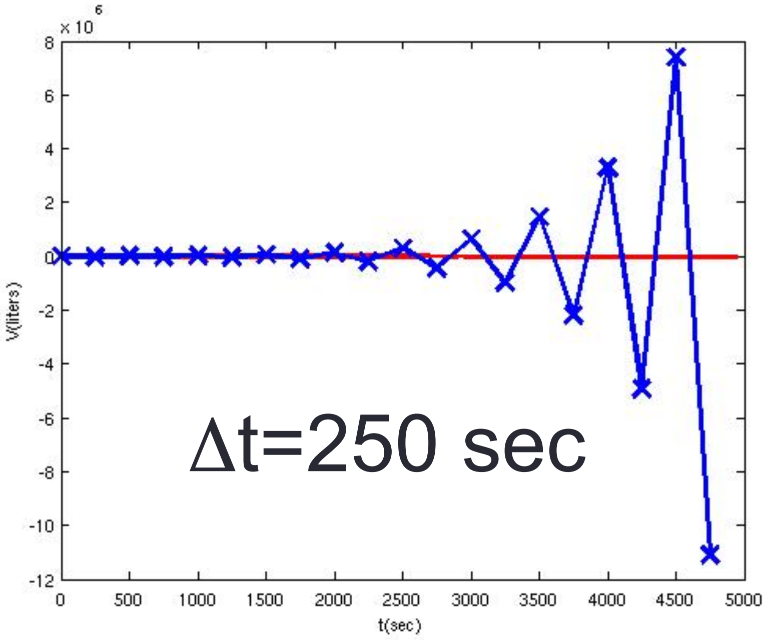
Stability criterion for Euler forward

- Differential equation: $$\frac{dV}{dt} = -aV$$
- Discretized solution with error: $$V^{new} + \varepsilon^{new} = (V^{old} + \varepsilon^{old})(1 - a\Delta t)$$
- Subtract solution w/out error: $$V^{new} = V^{old}(1 - a\Delta t)$$
- Error in solution: $$\varepsilon^{new} = \varepsilon^{old}(1 - a\Delta t)$$
- To keep error from growing: $$-1 < \left(1 - a\Delta t\right) < 1$$
- This restricts time step: $$\Delta t < \frac{2}{a}$$

Stability criterion

- a=0.01
- so $\Delta t_{crit} = 2/a = 200$ sec.





Stability criterion for Euler backward

- differential equation: $$\frac{dV}{dt} = -aV$$
- discretized solution: $$V^{new} = \frac{V^{old}}{1 + a\Delta t}$$
- So error in solution: $$\varepsilon^{new} = \frac{\varepsilon^{old}}{1 + a\Delta t}$$
- To keep error from growing: $$-1 < \frac{1}{1 + a\Delta t} < 1$$
- Criterion always met!

Practical 2, Part 2

Try for yourself:

- Use your radiogenic heating code:
  - Calculate Δt_{crit}
  - Increase t_{max} to 100 Gyrs
  - Try different Δt
- Use your heat diffusion code:
  - Increase timestep and see what happens

Stability criterion for heat diffusion

- Forward Euler time stepping method:

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

- So error propagates as:

$$\frac{\varepsilon_i^{new} - \varepsilon_i^{old}}{\Delta t} = \kappa \left(\frac{\varepsilon_{i+1}^{old} - 2\varepsilon_i^{old} + \varepsilon_{i-1}^{old}}{\Delta x^2} \right)$$

Stability criterion for heat diffusion

$$\varepsilon_i^{new} = \varepsilon_i^{old} + \frac{\kappa \Delta t}{\Delta x^2}\left(\varepsilon_{i+1}^{old} - 2\varepsilon_i^{old} + \varepsilon_{i-1}^{old}\right)$$

or

$$\varepsilon_i^{new} = r\varepsilon_{i+1}^{old} + (1-2r)\varepsilon_i^{old} + r\varepsilon_{i-1}^{old}$$

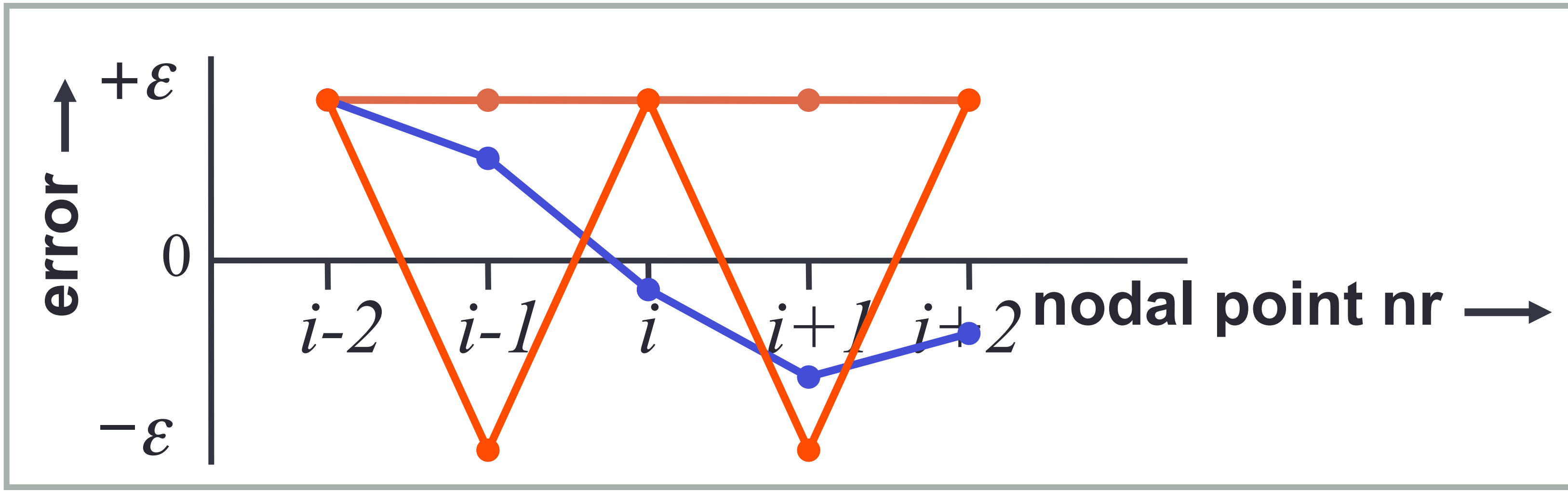
with $r = \frac{\kappa \Delta t}{\Delta x^2}$

- New error ε_i^{new} depends on ε_i^{old}, ε_{i+1}^{old}, and ε_{i-1}^{old}
- These ε^{old} can cancel out or amplify each other.

Stability criterion for heat diffusion

$$\varepsilon_i^{new} = r\varepsilon_{i+1}^{old} + (1-2r)\varepsilon_i^{old} + r\varepsilon_{i-1}^{old}$$ with $r = \frac{\kappa \Delta t}{\Delta x^2}$

- Let's look at 3 different error scenarios:



- — $\varepsilon_i^{old} = \varepsilon_{i-1}^{old} = \varepsilon_{i+1}^{old}$ so that $\varepsilon_i^{new} = \varepsilon_i^{old}$
- — $\varepsilon_i^{old} = -\varepsilon_{i-1}^{old} = -\varepsilon_{i+1}^{old}$ so that $\varepsilon_i^{new} = (1-4r)\varepsilon_i^{old}$

Stability criterion for heat diffusion

- $\varepsilon_i^{new} = (1-4r)\varepsilon_i^{old}$
- Avoiding amplification: $|1-4r| < 1$
- i.e.: $-1 < 1-4r$ or $r < \frac{1}{2}$ or $\frac{\kappa \Delta t}{\Delta x^2} < \frac{1}{2}$
- So $$\frac{T_i^{new} - T_i^{old}}{\Delta t} = \kappa \left(\frac{T_{i+1}^{old} - 2T_i^{old} + T_{i-1}^{old}}{\Delta x^2} \right)$$

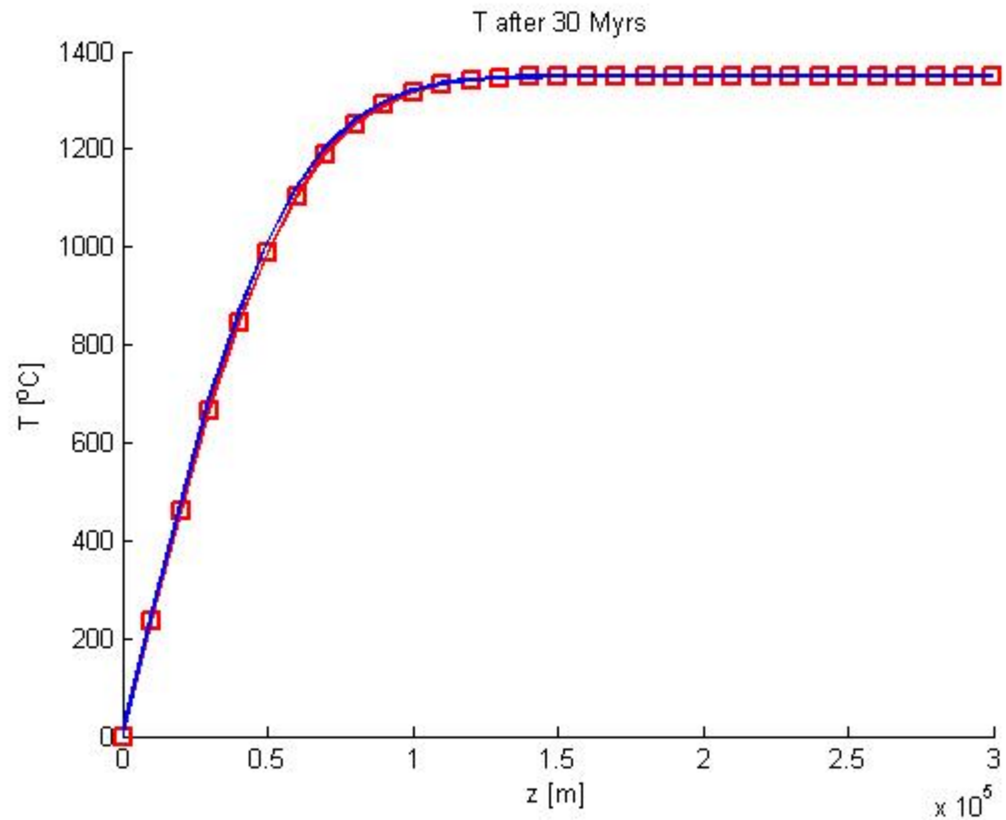
  has following stability criterion: $\Delta t < \frac{\Delta x^2}{2\kappa}$
- This is a simplified analysis.

  The full Fourier analysis referred to as the von Neumann stability criterion.

Example cooling oceanic plate

- Δx = 10 km, $\kappa = 10^{-6}$ m^2/s, so Δt < 1.58 Myr
- Results after 20 time steps of Δt = 1.5 Myr

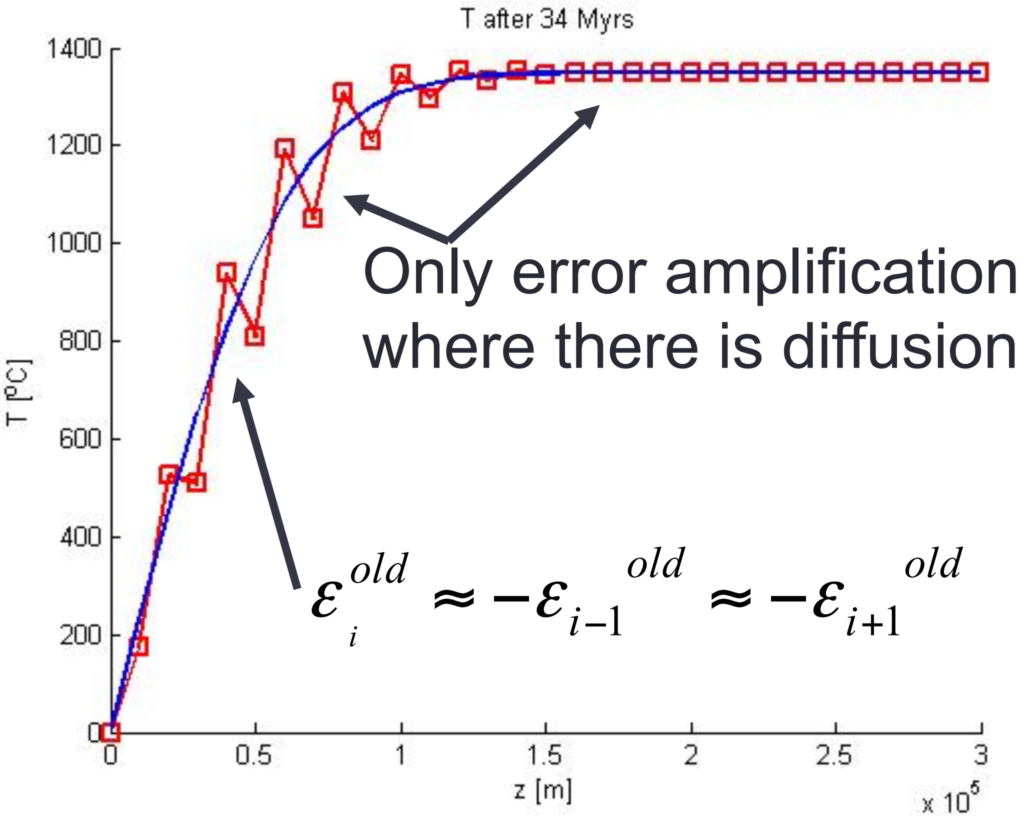
$$\Delta t < \frac{\Delta x^2}{2\kappa}$$



Example cooling oceanic plate

$$\Delta t < \frac{\Delta x^2}{2\kappa}$$

- Δx = 10 km, $\kappa = 10^{-6}$ m²/s, so Δt < 1.58 Myr
- Results after 20 time steps of Δt = 1.7 Myr



$$\varepsilon_i^{old} \approx -\varepsilon_{i-1}^{old} \approx -\varepsilon_{i+1}^{old}$$

Boundary conditions

Possible boundary conditions:

1. essential-, or Dirichlet boundary condition:

   f = given *(this is what we used so far)*

2. natural-, flux-, or Neumann boundary condition:

   gradient is given or $\frac{df}{dx}$ = given

3. periodic boundary condition: link ends together

Implementation of natural boundary conditions for the heat equation

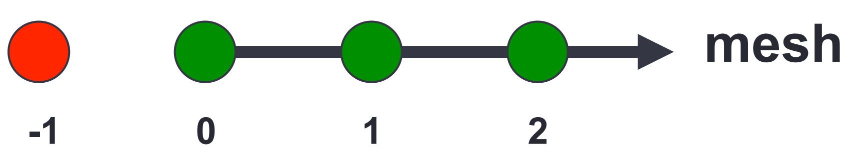
- Flux b.c. at nodal point 0: $q = -k\dfrac{dT}{dx} = -kc$ or $\dfrac{dT}{dx} = c$
- Since T_0 is not explicitly given as b.c., the usual d.e.

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

- Discretize (e.g. with Forward Euler) for $i=0$:

$$T_0^{new} - T_0^{old} = r\left(T_{-1}^{old} - 2T_0^{old} + T_1^{old}\right) \quad \text{with} \quad r = \frac{\kappa \Delta t}{\Delta x^2}$$

- What to do with T_{-1}?



Implementation of natural boundary conditions for the heat equation

- Discretization of $\frac{dT}{dx} = c$ at end points:

$$\frac{T_1 - T_{-1}}{2\Delta x} = c \qquad \text{or} \qquad T_{-1} = T_1 - 2\Delta x c$$

- So now the d.e. becomes:

$$T_0^{new} - T_0^{old} = r\left(T_1^{old} - 2\Delta x c - 2T_0^{old} + T_1^{old}\right)$$

or

$$T_0^{new} = T_0^{old} + r\left(2T_1^{old} - 2T_0^{old} - 2\Delta x c\right)$$

Practical 2, Part 3

Natural boundary conditions

- Apply to your oceanic lithosphere cooling model
- Replace given T at base of model with given heat flux from mantle into the lithosphere
- Zero heat flux is simplest: insulating base of the lithosphere