Numerical Simulation Methods in Geophysics, Part 3: Time-stepping

1. MGPY+MGIN, 3. MDRS+MGEX-CMG

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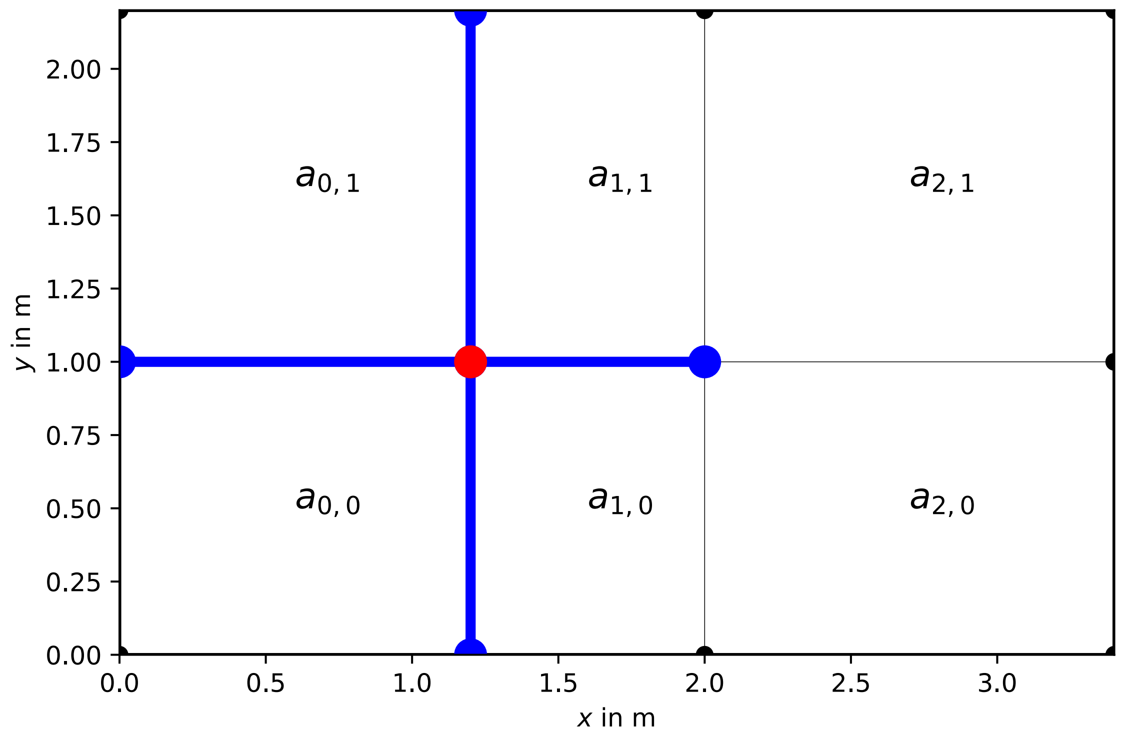
Recap

- Poisson's equation, solved with FD in 1D
- boundary conditions determine shift (Dirichlet) and flow (Neumann)
- no sources: linear potential (constant flow)
- sources: positive curvature (max), continuous: parabola
- slope changes with conductivity (a contrasts act like source)

FD in 2D: discretization



Simple 2D conductivity grid with FD stencil

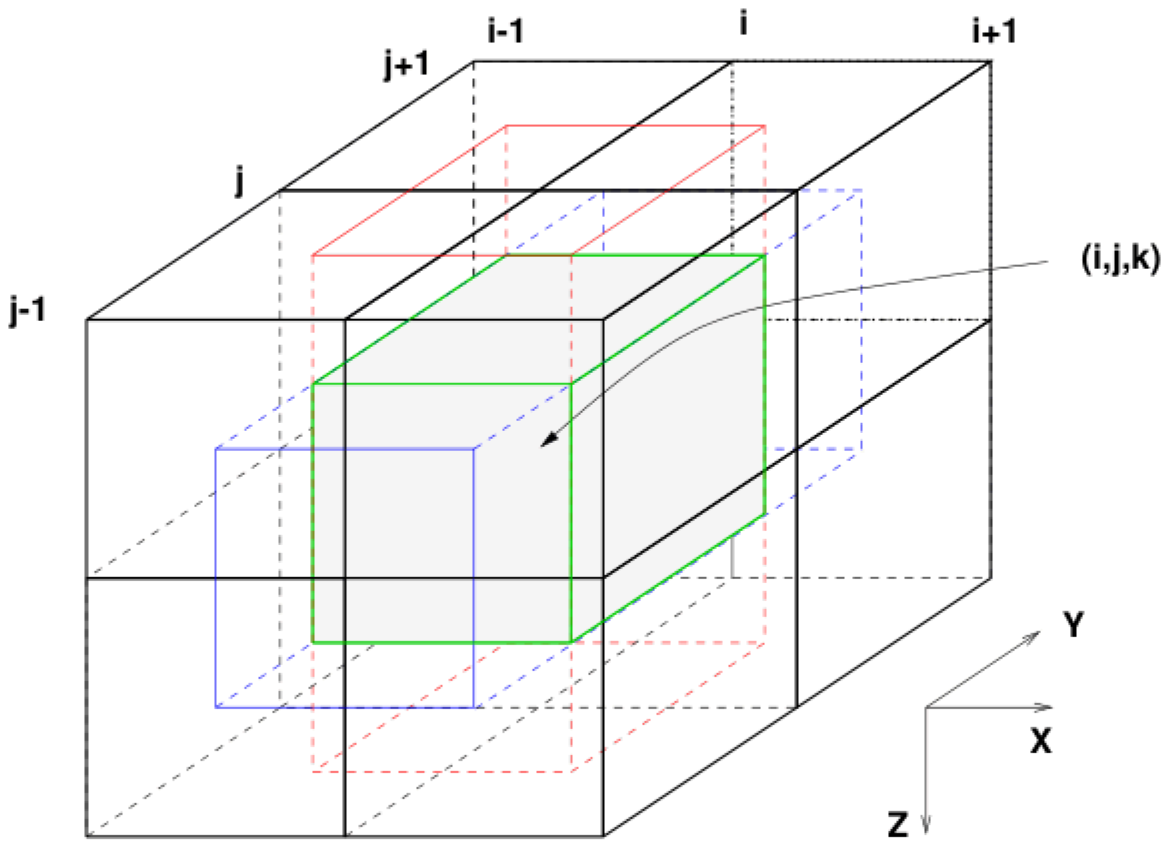
$$C_{i,j}^{right} = a_{i,j-½}/(x_{i+1} - x_i)^2$$

$$a_{i,j-½} = (a_{i,j-1} + a_{i,j})/2 \text{ ?}$$

harmonic, geometric? weighting?

$$a_{i,j-½} = \frac{a_{i,j-1}\Delta y_{j-1} + a_{i,j}\Delta y_j}{y_j + 1 - y_{j-1}} \text{ ?}$$

FD in 3D: discretization



3D discretization

$$C_{top} = -\frac{1}{\Delta z_{k-1}}\left(\sigma_{i-1,j,k-1}\frac{\Delta x_{i-1}\Delta y_j}{4} + \sigma_{i,j,k-1}\frac{\Delta x_i \Delta y_j}{4} + \right.$$

$$\left. + \sigma_{i-1,j-1,k-1}\frac{\Delta x_{i-1}\Delta y_{j-1}}{4} + \sigma_{i,j,k-1}\frac{\Delta x_i \Delta y_j}{4}\right)$$

coupling coefficient

Solution of Poisson's equation in 1D/2D/3D

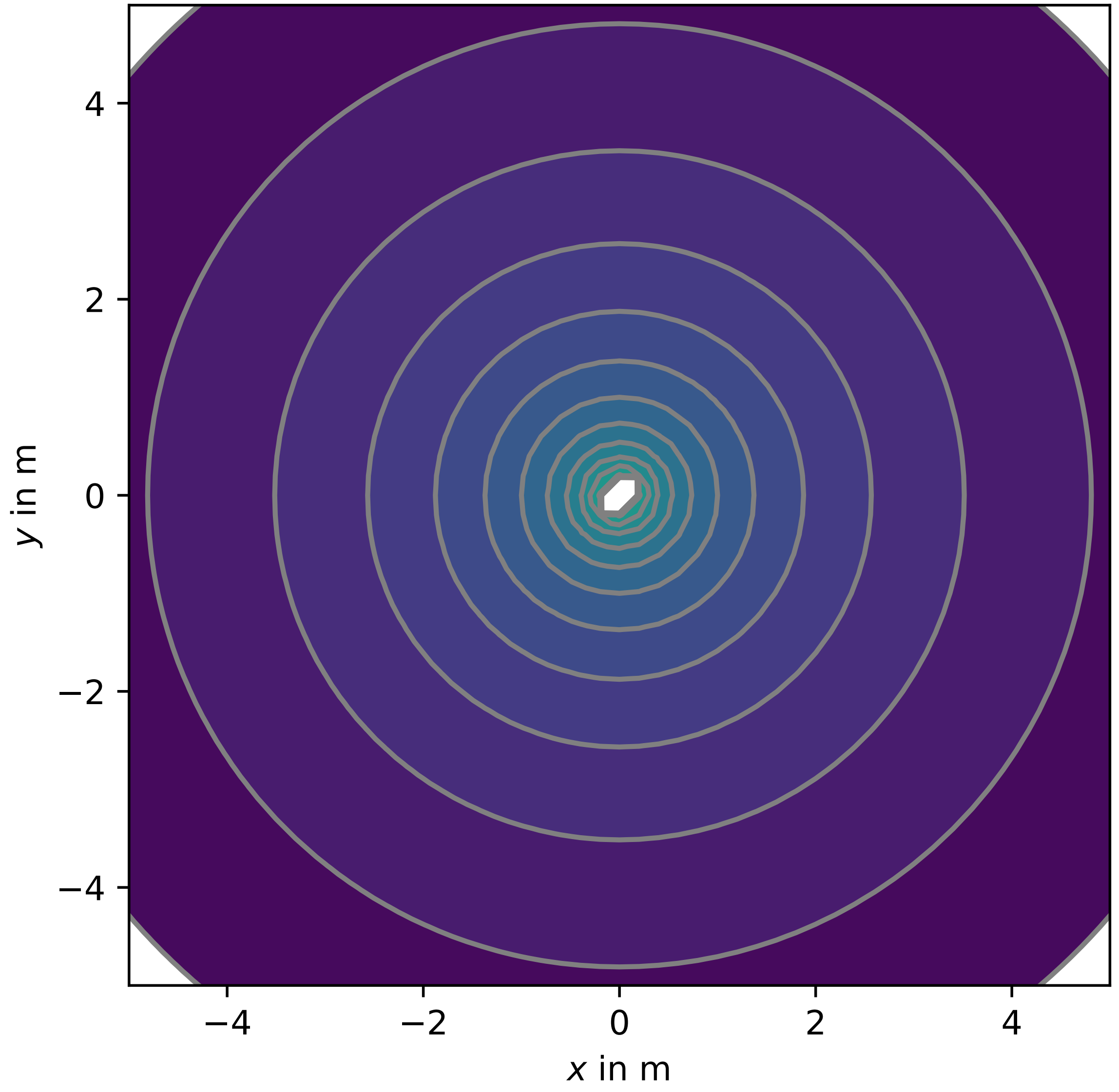
- point source (fundamental solution = Greens function)
- 1D: flow is constant (cannot spread)
- 2D: flow distributes on circle circumference (constant a)

$$q(r) = \frac{Q}{2\pi r} \quad \Rightarrow \quad u = -\frac{Q\rho}{2\pi} \ln r$$

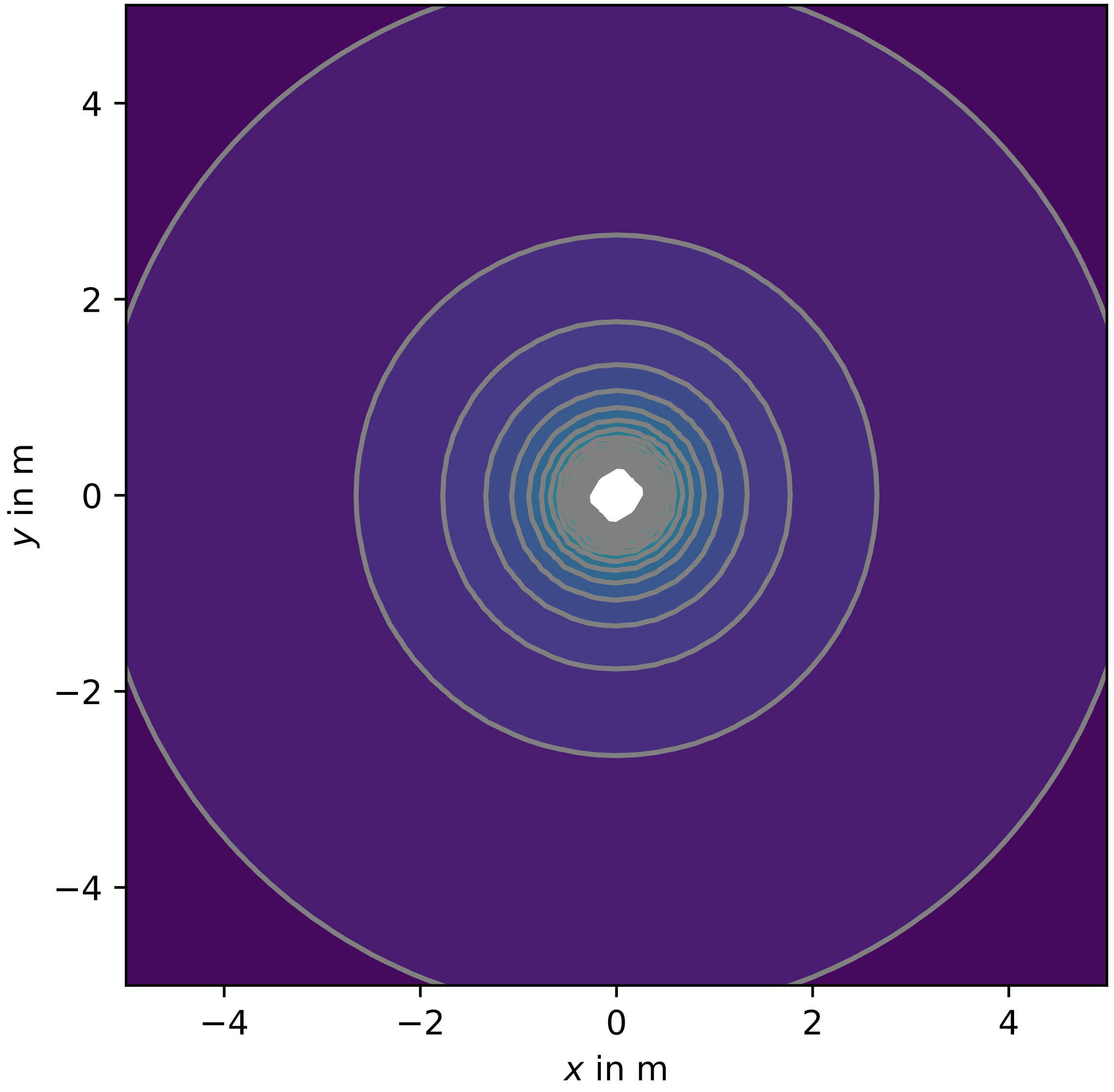
- 3D: flow distributes on sphere surface

$$j(r) = \frac{I}{4\pi r^2} \quad \Rightarrow \quad u = \frac{I\rho}{4\pi r}$$

Spatial 2D and 3D solutions

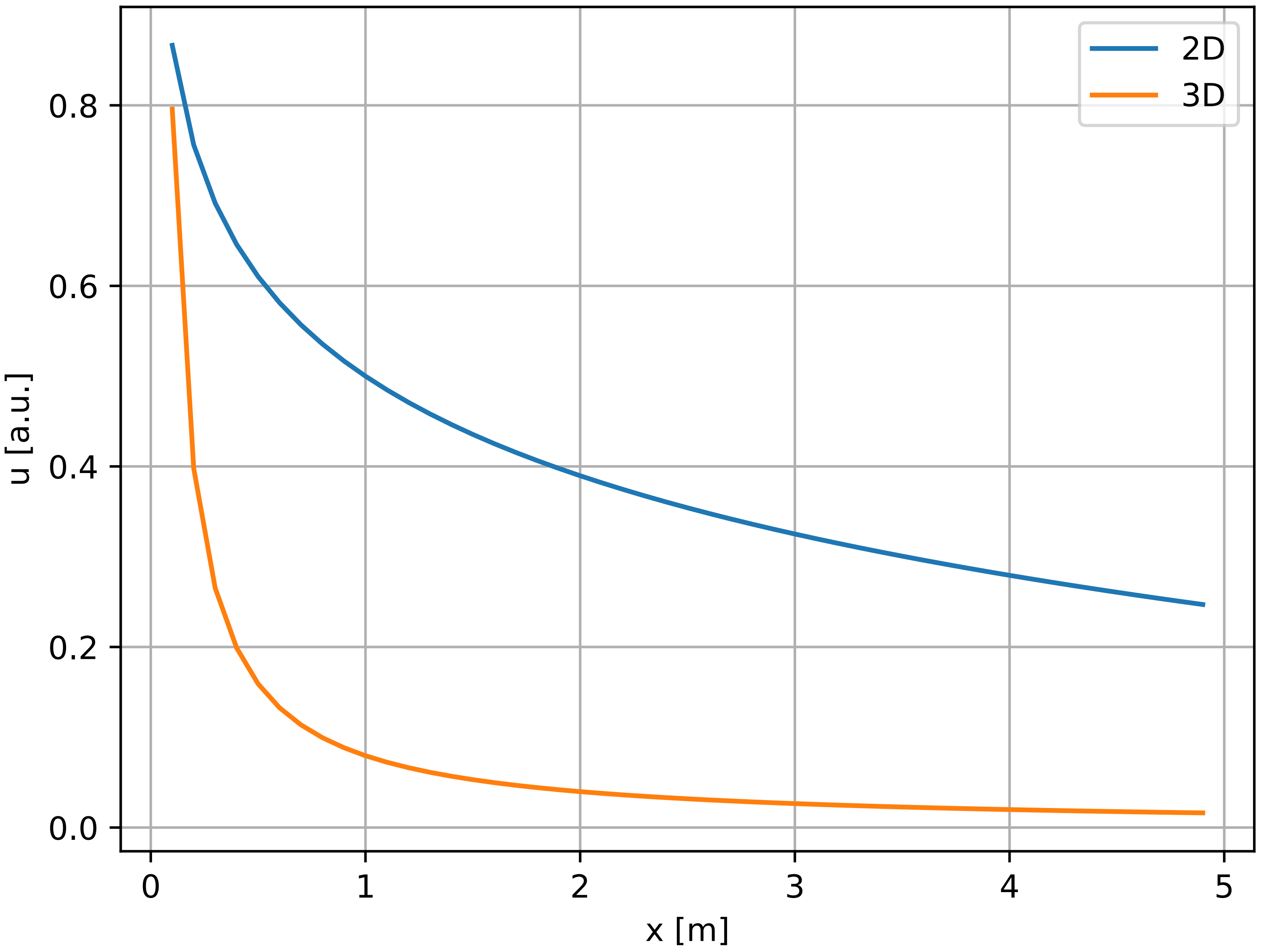


2D solution (-ln r)



3D solution (1/r)

Comparison of 2D and 3D solutions



Parabolic PDEs

- describe diffusion problems (of potential fields)
- second spatial and first temporal derivative, e.g. in 1D

$$\frac{\partial T}{\partial t} - a\frac{\partial^2 T}{\partial z^2} = \boldsymbol{\nabla} \cdot \mathbf{q_s}$$

Heat flow in 1D

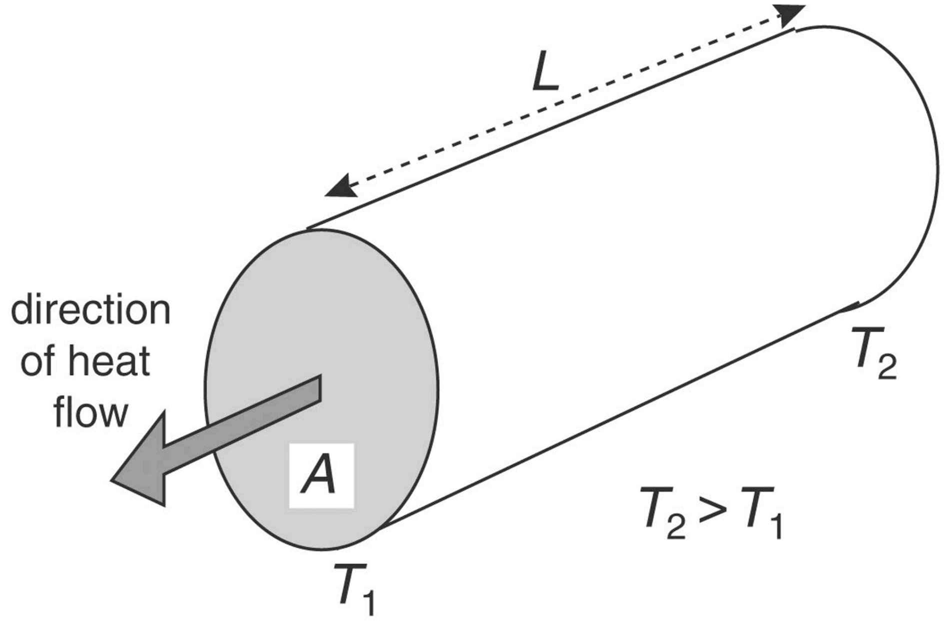
temperature gradient $\Delta T \Rightarrow$ heat flow

$$Q/\Delta t = \frac{kA}{L}\Delta T$$

$$\mathbf{q} = -\frac{1}{A}\frac{\partial Q}{\partial t} = -k\frac{\partial T}{\partial z}$$

cannot disappear (divergence 0)

$$\boldsymbol{\nabla}\cdot\mathbf{q} = -\boldsymbol{\nabla}\cdot(k\boldsymbol{\nabla}T) = \boldsymbol{\nabla}\cdot\mathbf{q}_s$$



- T [K], A [m²], L [m]
- Q [J/m/K], q [W/m²]
- k [W/m] thermal conduct.

Heat conduction equation

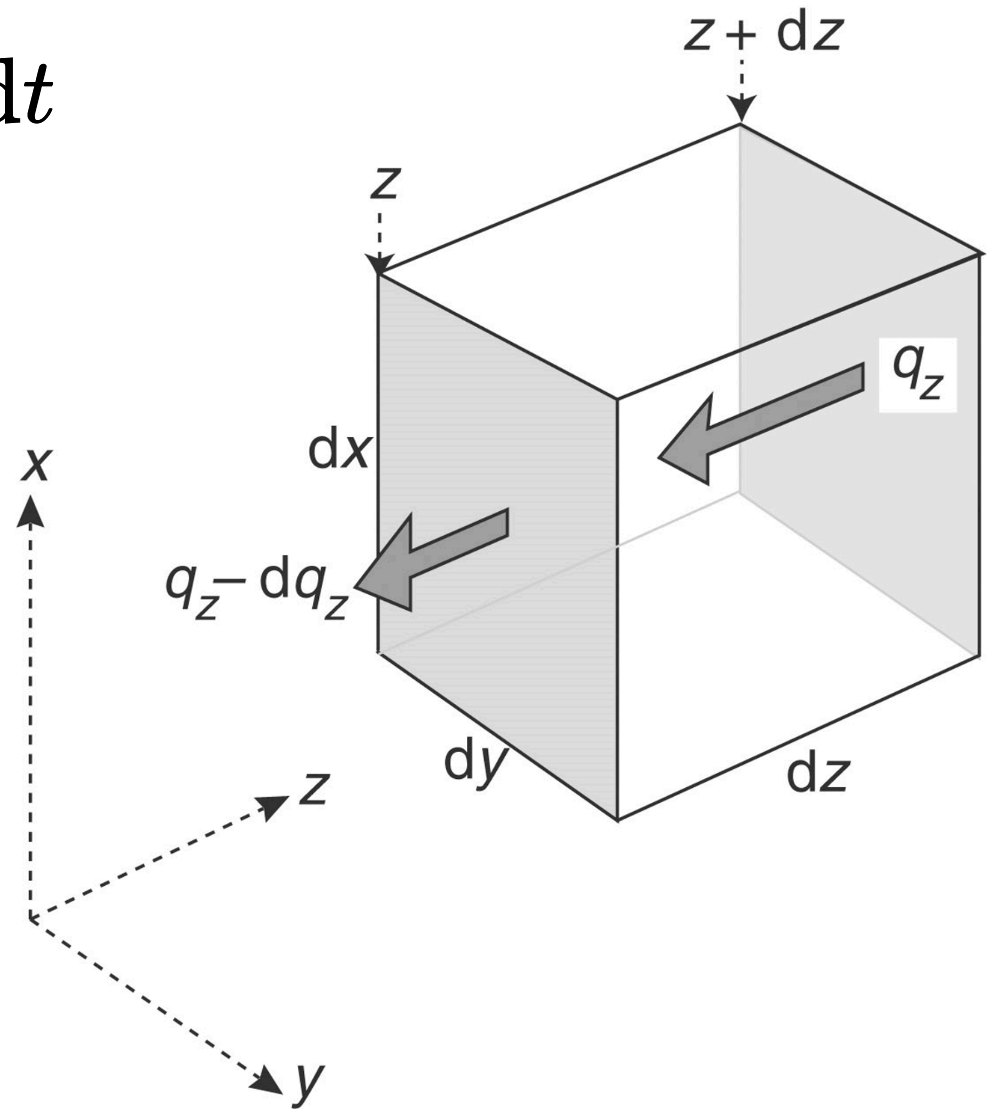
$$\frac{\mathrm{d}Q_z}{\mathrm{d}z}\mathrm{d}z = \frac{\mathrm{d}q_z}{\mathrm{d}z}\mathrm{d}z\mathrm{d}x\mathrm{d}y\mathrm{d}t = k\frac{\mathrm{d}^2T}{\mathrm{d}z^2}\mathrm{d}V\mathrm{d}t$$

with the heat capacity c_p [W/kg/K]

$$c_p m\mathrm{d}T = c_p\rho\mathrm{d}V\mathrm{d}T$$

$\Rightarrow$ heat conduction equation

$$\frac{\mathrm{d}T}{\mathrm{d}t} - \frac{k}{\rho c_p}\frac{\mathrm{d}^2T}{\mathrm{d}z^2} = Q_s$$



Instationary heat flow in 3D

$$\frac{\partial T}{\partial t} - \nabla \cdot a \nabla T = \nabla \cdot q_s$$

- $a = \frac{k}{\rho c_p}$ [m²/s] thermal diffusivity - measure of heat transfer
- k [W/m/K] thermal conductivity - measure of temperature transfer
- c_p [J/kg/K] - heat capacity - measure of heat storage per mass
- ρ (kg/m³) density

Water k=0.6 W/m/K, ρ=1000 kg/m³, c=4180 J/kg/K $\Rightarrow$ a=1.43e-7 m²/s

Our first case: temperature diffusion into the Earth

Periodic boundary conditions

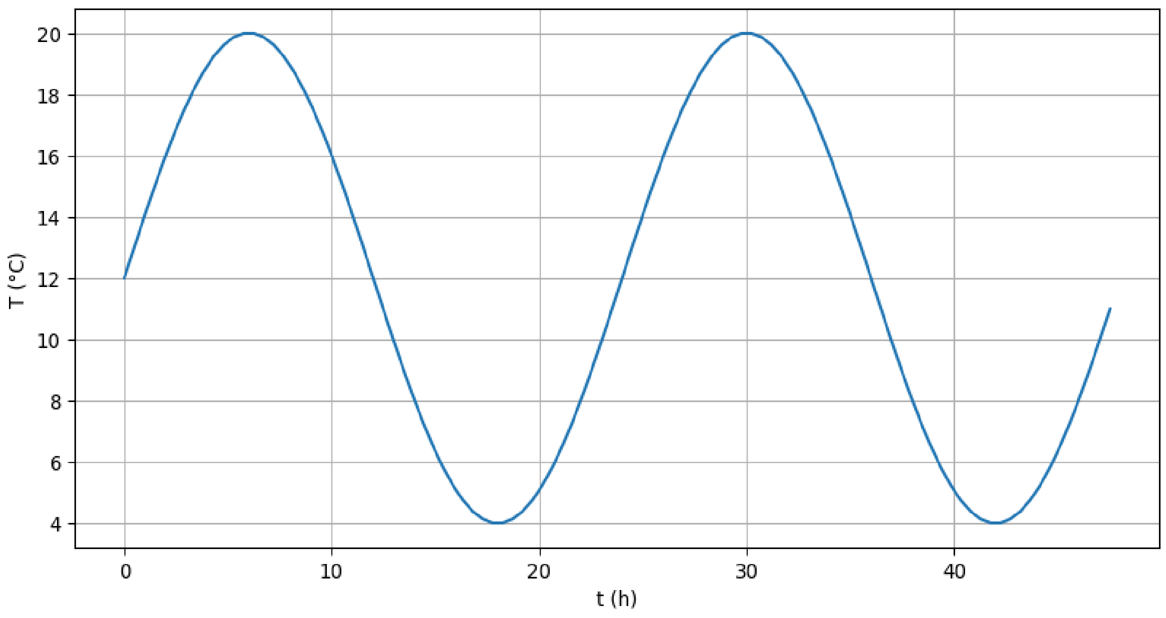
Upper boundary: daily/yearly variation

$$T(z=0) = T_0 + \Delta T \sin \omega t$$

T_0 mean temperature (e.g. 12°C), ΔT variation, e.g. 8°C

$\omega = 2\pi/\tau$ daily (τ_d=3600*24s) or yearly ($\tau_y = 365\tau_d$) cycle

```
day = 3600 * 24
T0, dT = 12, 8
t = np.arange(100) / 50 * day
T = T0+dT*np.sin(t/day*2*np.pi)
plt.plot(t/day*24, T)
plt.xlabel("t (h)")
plt.ylabel("T (°C)")
plt.grid()
```



Analytical solution

$$\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial z^2}$$

$T = T_0 + \Delta t\hat{T}$ (shift and scale) $\Rightarrow$ same equation for $\hat{T}$

Separation of variables: $\hat{T}(t, z) = \theta(t)Z(z)$$

$$Z\frac{\partial \theta}{\partial t} = a\theta\frac{\partial^2 Z}{\partial z^2} \quad \Rightarrow \quad \frac{1}{\theta}\frac{\partial \theta}{\partial t} = C = a\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}$$

Solution

regarding the BC $e^{\imath\omega t}$ leads to $C = \imath\omega$ and thus $\theta = \theta_0 e^{\imath\omega t}$

$$\frac{\partial^2 Z}{\partial z^2} - \imath\frac{\omega}{a}Z = \frac{\partial^2 Z}{\partial z^2} + n^2 Z = 0$$

Helmholtz equation with solution $Z = Z_0 e^{\imath nz}$ $(n^2 = \imath\omega/a)$

$$Z = Z_0 e^{\imath nz} = Z_0 e^{\sqrt{\imath\omega/a}z} = Z_0 e^{\sqrt{\omega/2a}(1+\imath)z}$$

$$T(t,z)/\Delta T + T_0 = Z(z)\theta(t) = Z_0\theta_0 e^{-\sqrt{\omega/2a}z} e^{i(\omega t - \sqrt{\omega/2a}z)}$$

Interpretation

replacing the term $\sqrt{2a/\omega} = \sqrt{a\tau/\pi} = d$ leads to

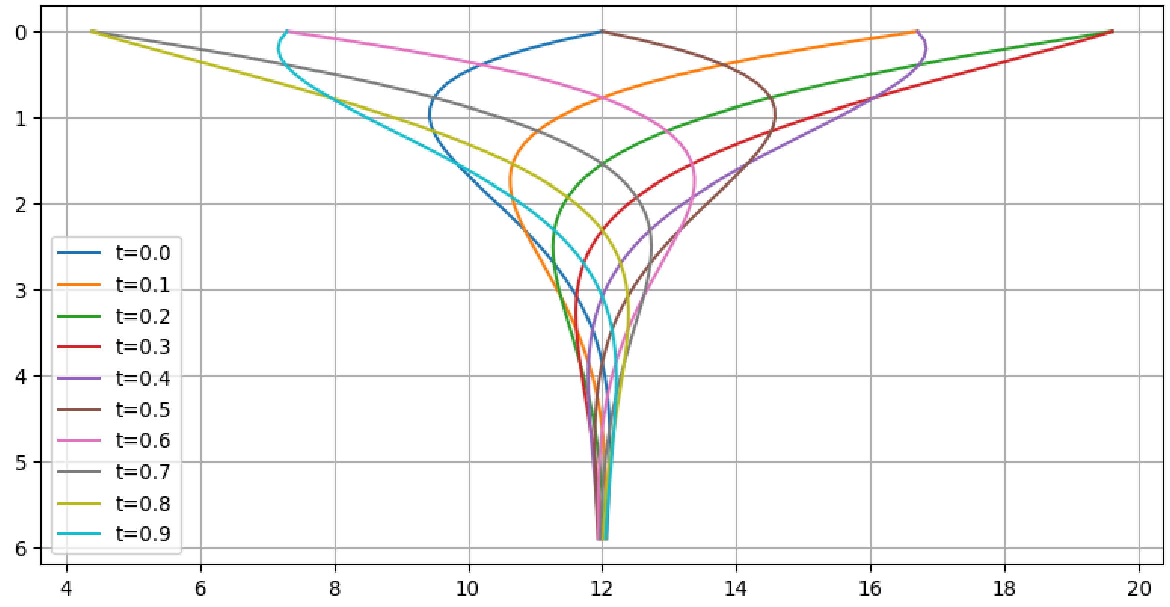
$$T(z,t) = T_0 + \Delta T e^{-z/d} \sin(\omega t - z/d)$$

- exponential damping of the temperature variation with decay depth d
- phase lag z/d increases with depth, $z_\pi = \sqrt{2a/\omega}\pi = \sqrt{a\tau\pi}$

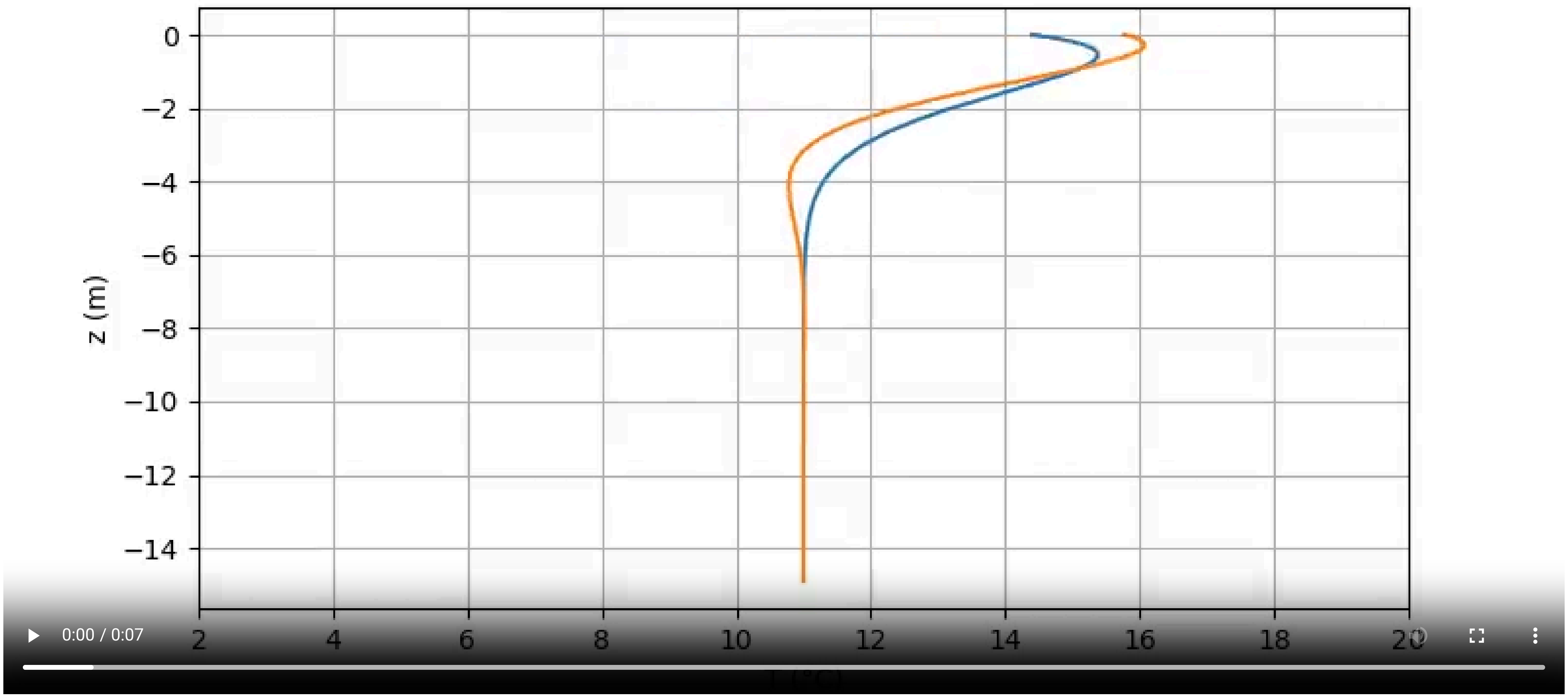
1. Daily cycle: decay depth d=6cm, minimum depth=20cm
2. Yearly cycle: decay depth d=1.2m, minimum depth=4m

Depth profiles

```
a = 1.5e-7
year = day*365
d = sqrt(a*year/pi)
t = np.arange(0, 1, 0.1) * year
z = np.arange(0, 6, 0.1)
fig, ax = plt.subplots()
for ti in t:
    Tz = np.exp(-z/d)*np.sin(ti*2*pi/year-
                                   z/d) * dT + T0
    ax.plot(Tz, z, label="t={:.1f}".format(
        ti/year))

ax.invert_yaxis()
ax.legend()
ax.grid()
```

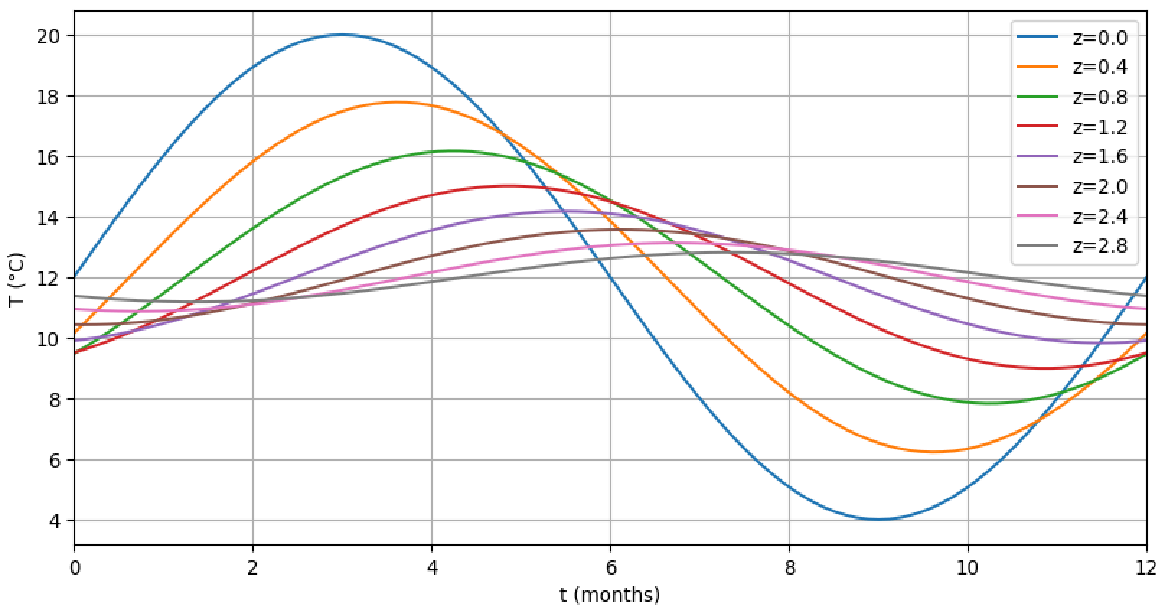


Animation

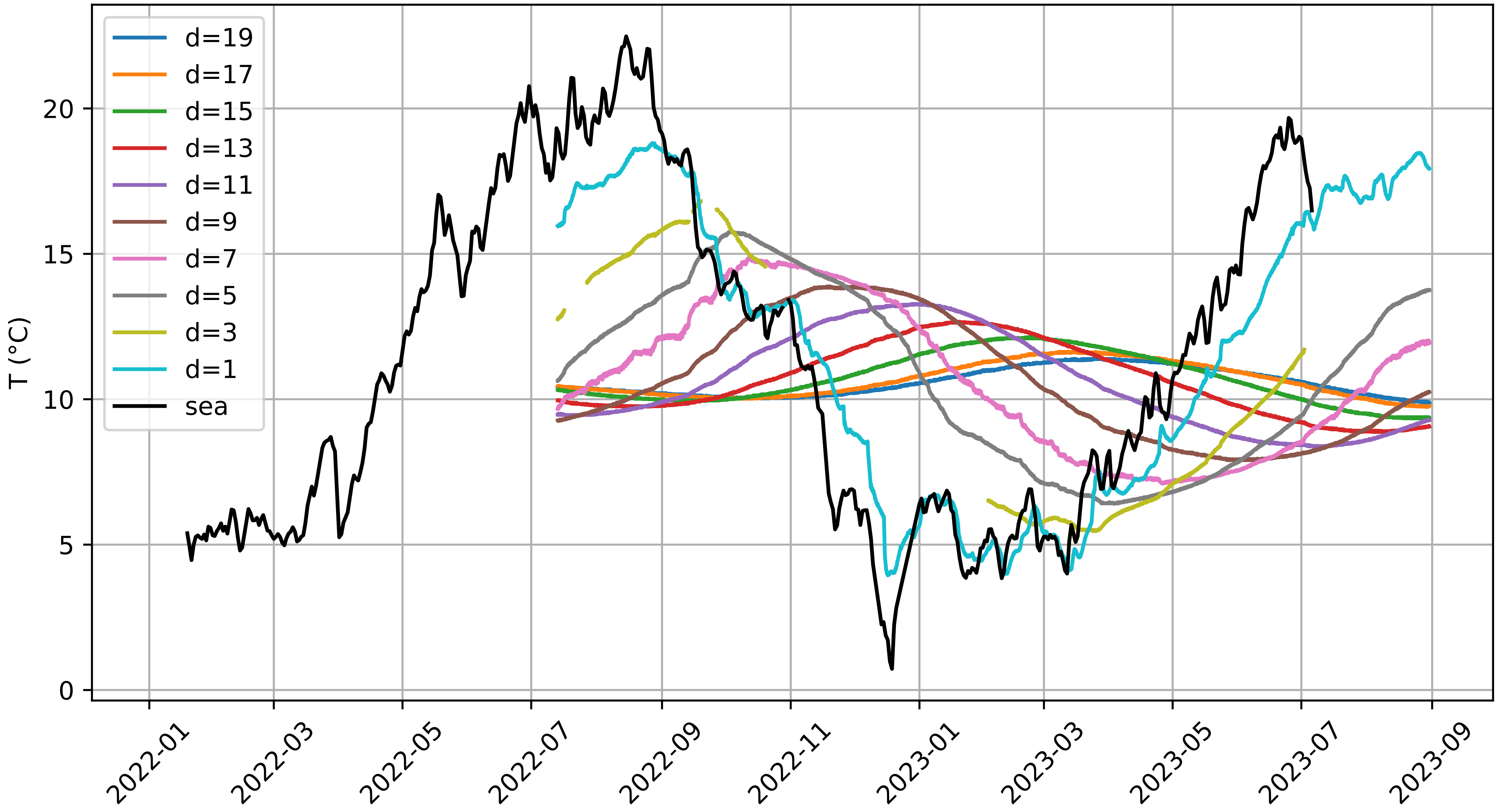


Temporal behaviour

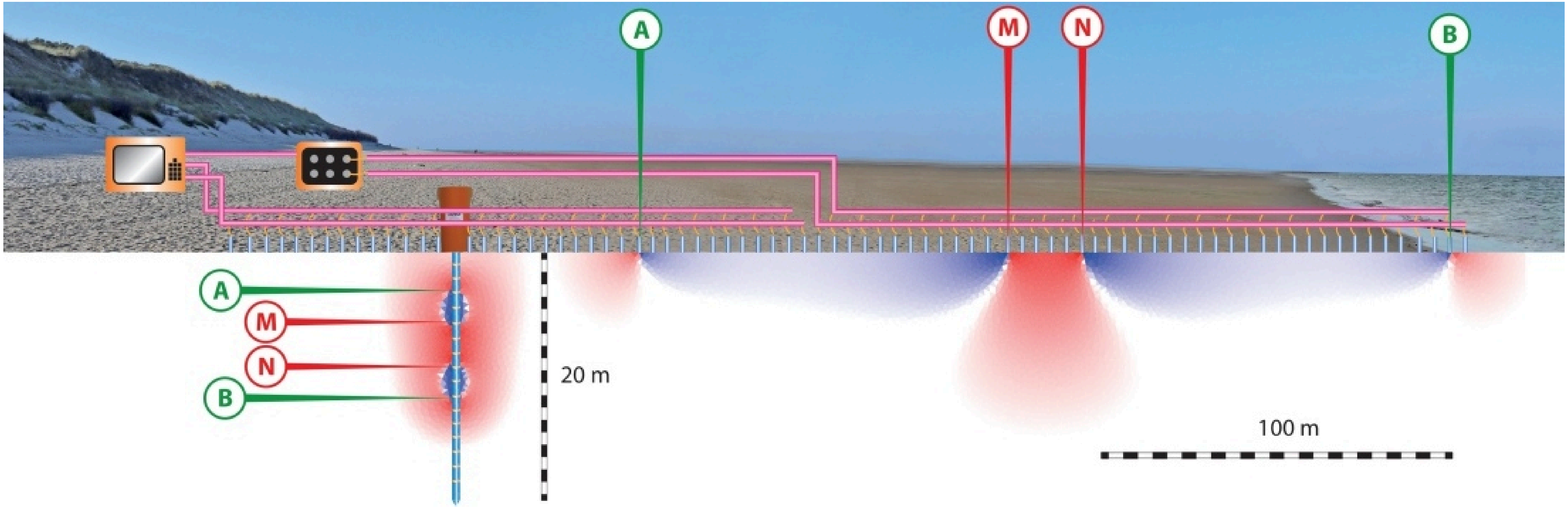
```
t = np.arange(0, 1.01, 0.01) * year
z = np.arange(0, 3, 0.4)
fig, ax = plt.subplots()
for zi in z:
    Tt = np.exp(-zi/d)*np.sin(t*2*pi/year-
                              zi/d) * dT + T0
    ax.plot(t/year*12, Tt, label=f"z={zi:.1f}")

ax.set_xlim(0, 12)
ax.set_xlabel("t (months)")
ax.set_ylabel("T (°C)")
ax.legend()
ax.grid()
```



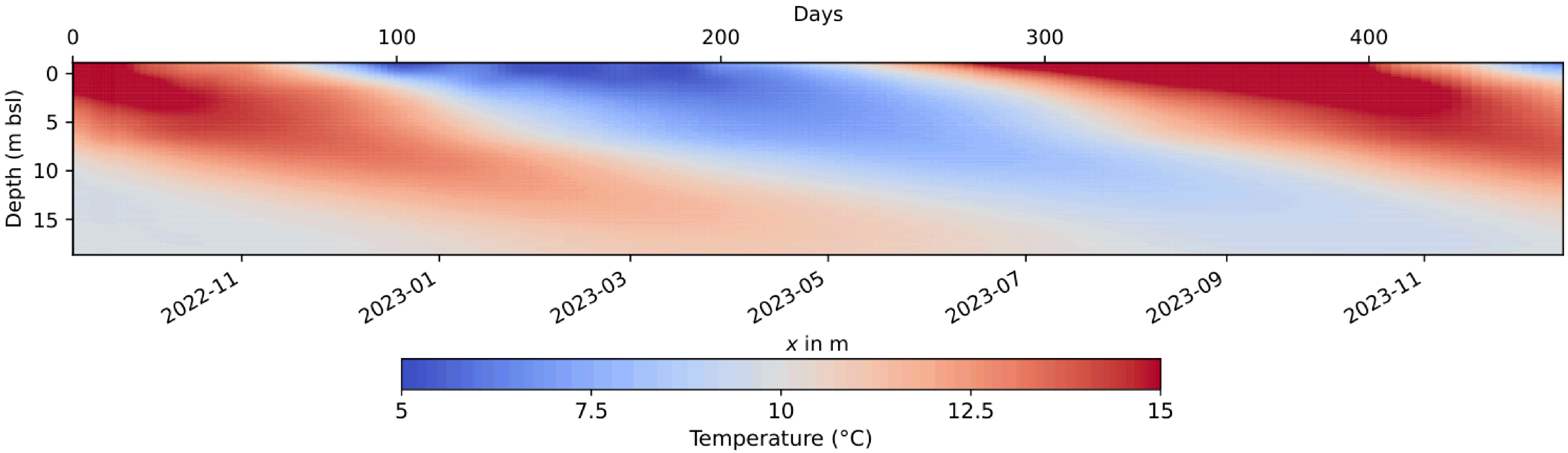
Experimental temperature curves



The DynaDeep project - measuring scheme



The DynaDeep project - temperature over time



Time-stepping with FD

$$\frac{\partial u}{\partial t} - a\frac{\partial^2 u}{\partial z^2} = 0$$

Finite-difference approximation (^{n} means time step n)

$$\frac{\partial u}{\partial t}^n \approx \frac{u^{n+1} - u^n}{\Delta t} = a\frac{\partial^2 u^n}{\partial z^2}$$

Explicit (forward) Euler method

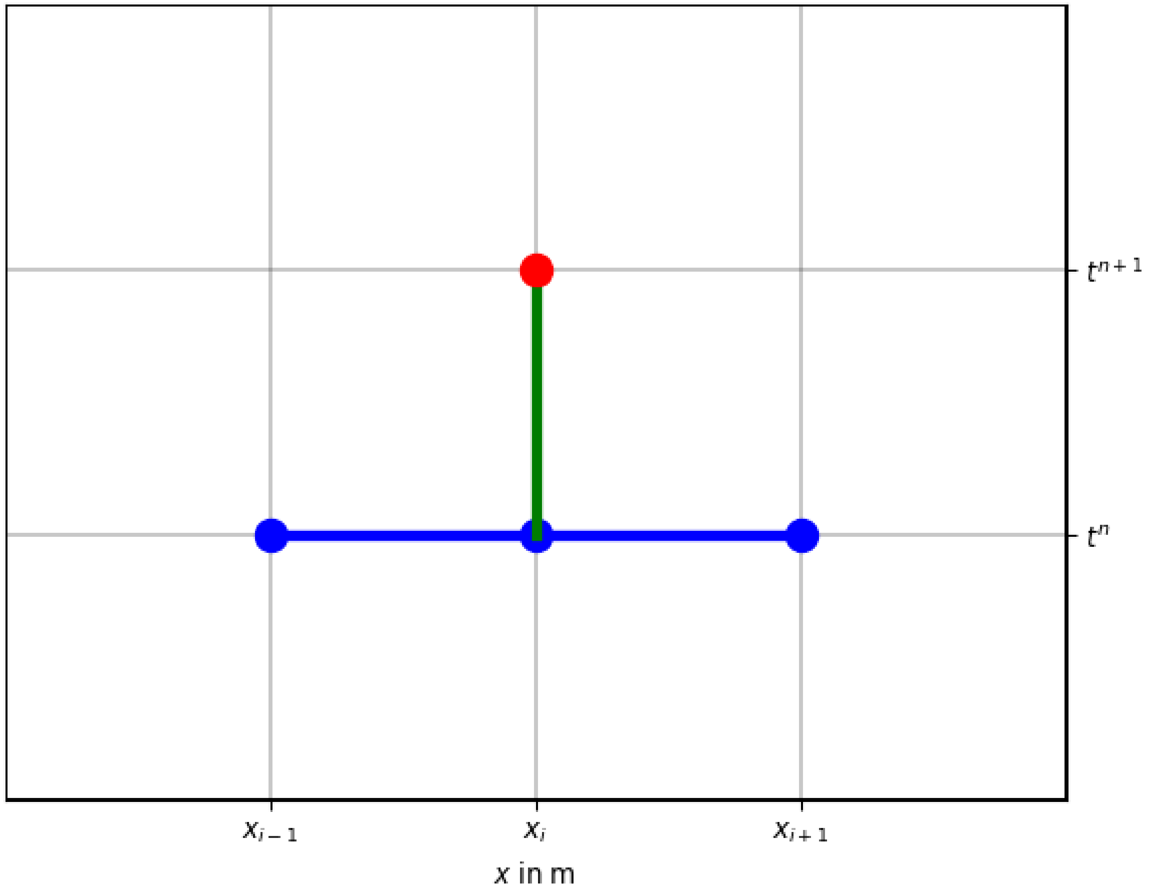
Start T^0 with initial condition

Update field by

$$u^{n+1} = u^n + a\frac{\partial^2 u^n}{\partial z^2} \cdot \Delta t$$

E.g. by using the matrix $\mathbf{A}$:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \mathbf{A} \mathbf{u}^n = (\mathbf{I} - \Delta t \mathbf{A})\mathbf{u}^n$$

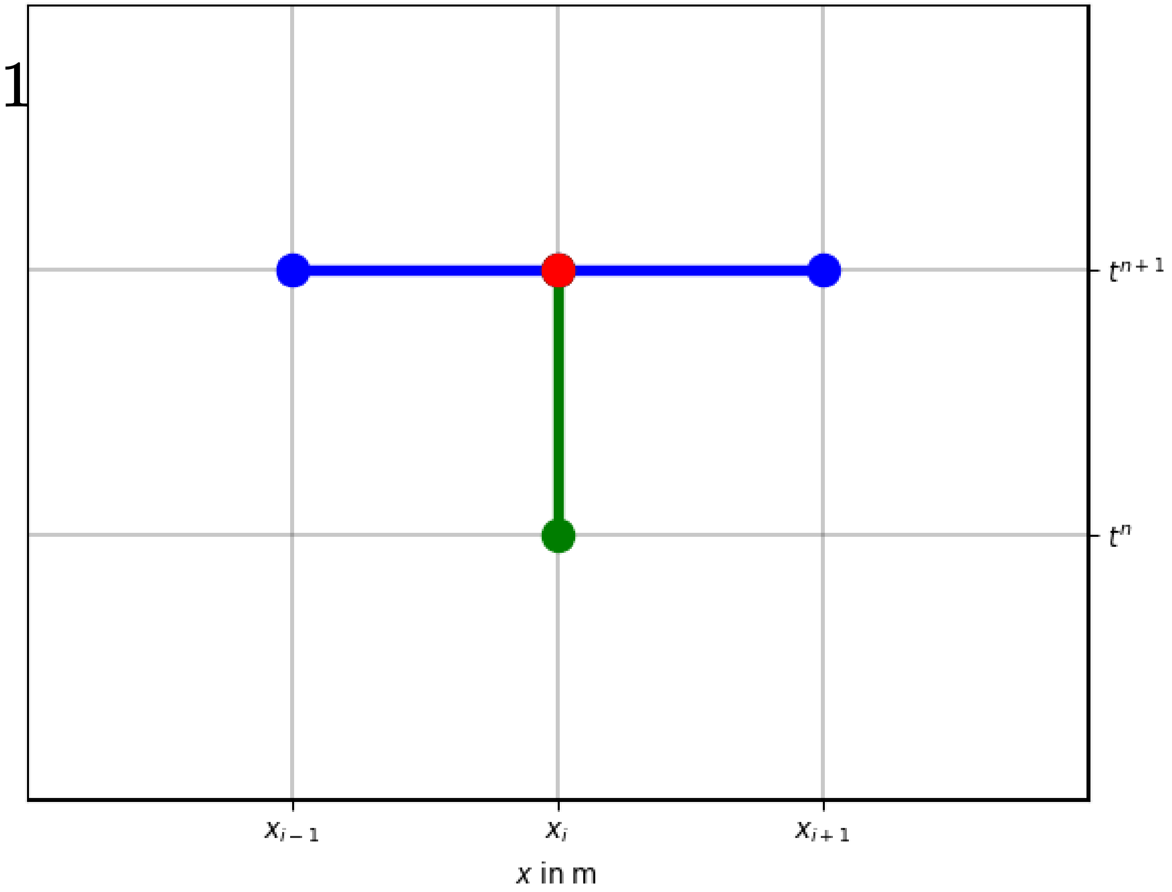


Implicit (backward) Euler method

$$\frac{\partial u}{\partial t}^{n+1} \approx \frac{u^{n+1} - u^n}{\Delta t} = a \frac{\partial^2 u}{\partial z^2}^{n+1}$$

$$\frac{1}{\Delta t} u^{n+1} - a \frac{\partial^2 u}{\partial z^2}^{n+1} = \frac{1}{\Delta t} u^n$$

$$(\mathbf{I} + \Delta t \mathbf{A})\mathbf{u}^{n+1} = \mathbf{u}^n$$



Solving an equation system

Mixed (Crank-Nicholson) method

$$\frac{\partial u}{\partial t}^{n+½} \approx \frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2} a \frac{\partial^2 u}{\partial z^2}^{n} + \frac{1}{2} a \frac{\partial^2 u}{\partial z^2}^{n+1}$$

$$\frac{2}{\Delta t} u^{n+1} - a \frac{\partial^2 u^{n+1}}{\partial z^2} = \frac{2}{\Delta t} u^n + a \frac{\partial^2 u^n}{\partial z^2}$$

$$(2\mathbf{I} + \Delta t \mathbf{A})\mathbf{u}^{n+1} = (2\mathbf{I} - \Delta t \mathbf{A})\mathbf{u}^n$$