Numerical Simulation Methods in Geophysics, Part 5: Timestepping

1. MGPY+MGIN

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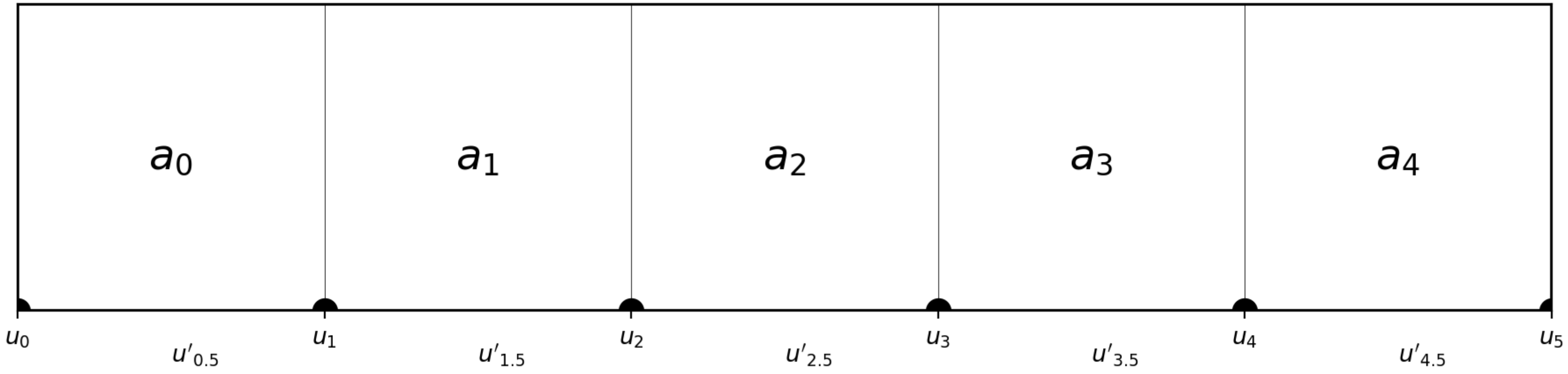
Recap last lessons & exercises

The general case

$$\Delta x \neq 1 \;\&\; a \neq 1 \Rightarrow a\frac{\partial u}{\partial x} \approx a_i \frac{u_{i+1}-u_i}{x_{i+1}-x_i}$$



$$\frac{\mathrm{d}}{\mathrm{d}x}\left(a\frac{\partial u}{\partial x}\right) \approx \left(a_i \frac{u_{i+1}-u_i}{x_{i+1}-x_i} - a_{i-1}\frac{u_i-u_{i-1}}{x_i-x_{i-1}}\right)/(x_{i+1}-x_{i-1}) \cdot 2$$

$$A_{i,i-1} = a_{i-1}/(x_i - x_{i-1})/(x_{i+1}-x_{i-1}) \cdot 2$$

The coupling coefficients

$$A_{i,i-1} = C_i^{left} = a_{i-1}/(x_i - x_{i-1})/(x_{i+1} - x_{i-1}) \cdot 2$$

$$A_{i,i+1} = C_i^{right} = a_i/(x_{i+1} - x_i)/(x_{i+1} - x_{i-1}) \cdot 2$$

$$\begin{bmatrix} +1 & 0 & 0 & \dots & & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots & \\ \vdots & \vdots & \ddots & \vdots & & \\ \dots & \dots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \dots & \dots & & 0 & -1 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} u_B \\ f_1 \\ \vdots \\ f_N \\ g_B\Delta \end{bmatrix}$$

Symmetry

$$A_{i+1,i} = C_{i+1}^{left} = a_i/(x_{i+1} - x_i)/(x_{i+2} - x_i) \cdot 2$$

$$A_{i,i+1} = C_i^{right} = a_i/(x_{i+1} - x_i)/(x_{i+1} - x_{i-1}) \cdot 2$$

only symmetric if Δx is constant around x_i, better take $a_i/(\Delta x_i)^2$

$$A_{i,i-1} = C_i^{left} = a_{i-1}/(x_i - x_{i-1})^2$$

$$A_{i,i+1} = C_i^{right} = a_i/(x_{i+1} - x_i)^2$$

$\Rightarrow$ inaccuracies expected for non-equidistant discretization

A closer look at the Dirichlet boundary

$$\begin{bmatrix} +1 & 0 & 0 & \dots & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots \end{bmatrix} \begin{bmatrix} u_B \\ f_1 \end{bmatrix}$$

1. C can be differently scaled from 1 $\Rightarrow$ multiply with C_i^L
2. Matrix is non-symmetric

$$\begin{bmatrix} C_1^L & 0 & 0 & \dots & \\ C_1^L & -(C_1^L + C_1^R) & C_1^R & 0 & \dots \end{bmatrix} \begin{bmatrix} u_B C_i^L \\ f_1 \end{bmatrix}$$

A closer look at the Neumann boundary

$$\begin{bmatrix} \dots & \dots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \dots & \dots & & 0 & -1 & +1 \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_N \\ g_B \Delta x_N \end{bmatrix}$$

1. C can be differently scaled from 1 $\Rightarrow$ multiply with C_N^R
2. Matrix is non-symmetric $\Rightarrow$ multiply with -1

$$\begin{bmatrix} \dots & \dots & 0 & C_N^L & -(C_N^L + C_N^R) & C_N^R \\ \dots & \dots & & 0 & C_N^R & -C_N^R \end{bmatrix} \cdot \mathbf{u} = \begin{bmatrix} f_N \\ -g_B \Delta x_N C_N^R \end{bmatrix}$$

Accuracy

How can we prove the accuracy of our solution?

- compare with analytical solutions
- single (Point) f lead to piece-wise linear u (correct)
- what about continuous source terms?
  (e.g. radioactive elements in the Earth's crust)

Analytical solution

a=1, $f(x)$=1 $\Rightarrow$ double integration $\Rightarrow$ quadratic function

$$u(x) = C_0 + C_1 x - 1/2x^2$$

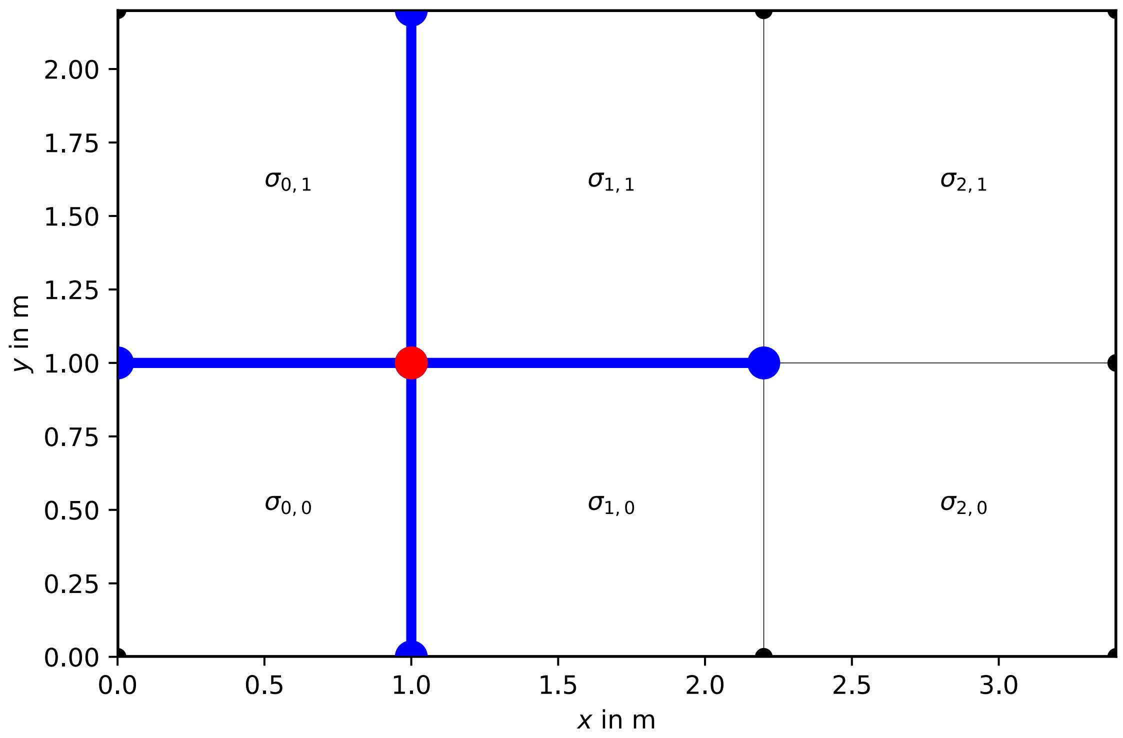
Left BC	Right BC	C_0	C_1
Dirichlet	Dirichlet	u_L	$L/2 + (u_R - u_L)/L$
Dirichlet	Neumann	u_L	$g_R + L$
Neumann	Dirichlet	$u_R - g_L L + L^2/2$	g_L

with $L = (x_N - x_0)$

Tasks stationary heat equation

- finish your implementation so that it can work with any x, a and f, and at least D-D or D-N boundary conditions
- make sure you achieve the same (phenomenological) results like in the “collection notebook” (variation of, a, x, f)
- simulate the two different cases (D-D, D-N) with some choices of uL and uR or gR
- make sure the N-D case is analog to D-N
- compute analytical solution and plot it with numerical solution
- change the discretization and improve the solution

Next spatial dimension



Simple 2D conductivity grid with FD stencil

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

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

harmonic, geometric? weighting?

$$a_{i,j-1/2} = \frac{a_{i,j-1}\Delta y_{j-1} + a_{i,j}\Delta y_j}{y_j + 1 - y_{j-1}} \text{ ?}$$

Parabolic PDEs

Instationary heat flow in 3D

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

- $a = \frac{k}{\rho c_p}$ [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

Periodic boundary conditions

Separation of variables

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

$$T(t,z)/\Delta T - T_0 = \theta(t)Z(z)$$

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

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

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 $Z = Z_0 e^{\imath n z}$ $(n^2 = \imath\omega/a)$

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

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

Interpretation

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

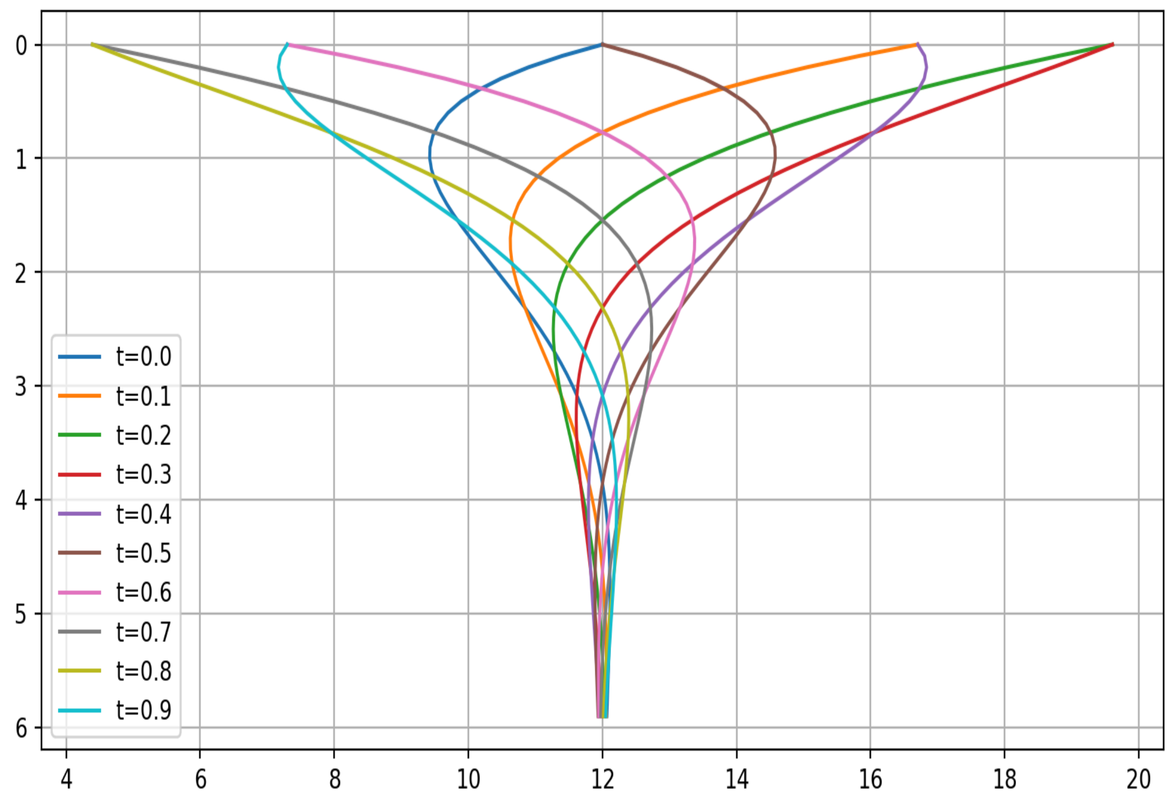
$$T(z,t) = T_0 + \Delta T e^{-z/d} \sin(\omega t - z/d)$$

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

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

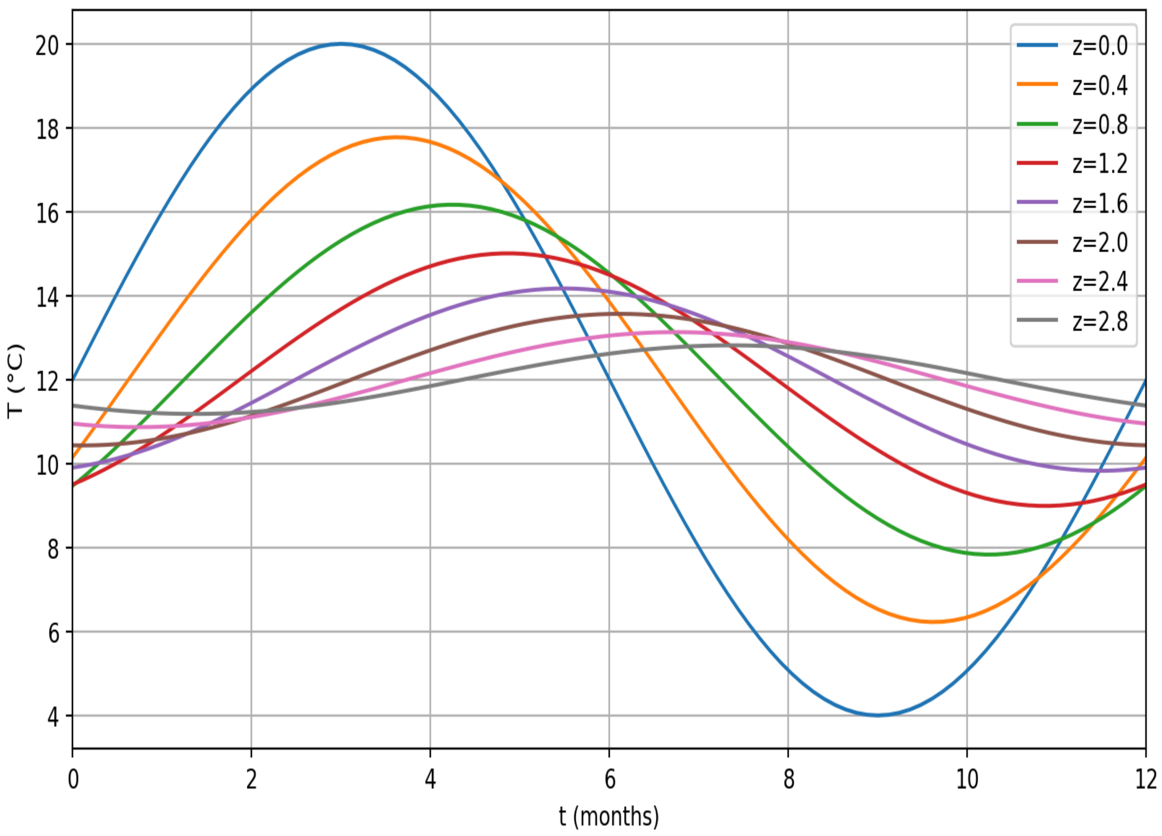
Depth profiles

```
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()
```



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()
```



Time stepping - explicit method

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

Finite-difference approximation

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

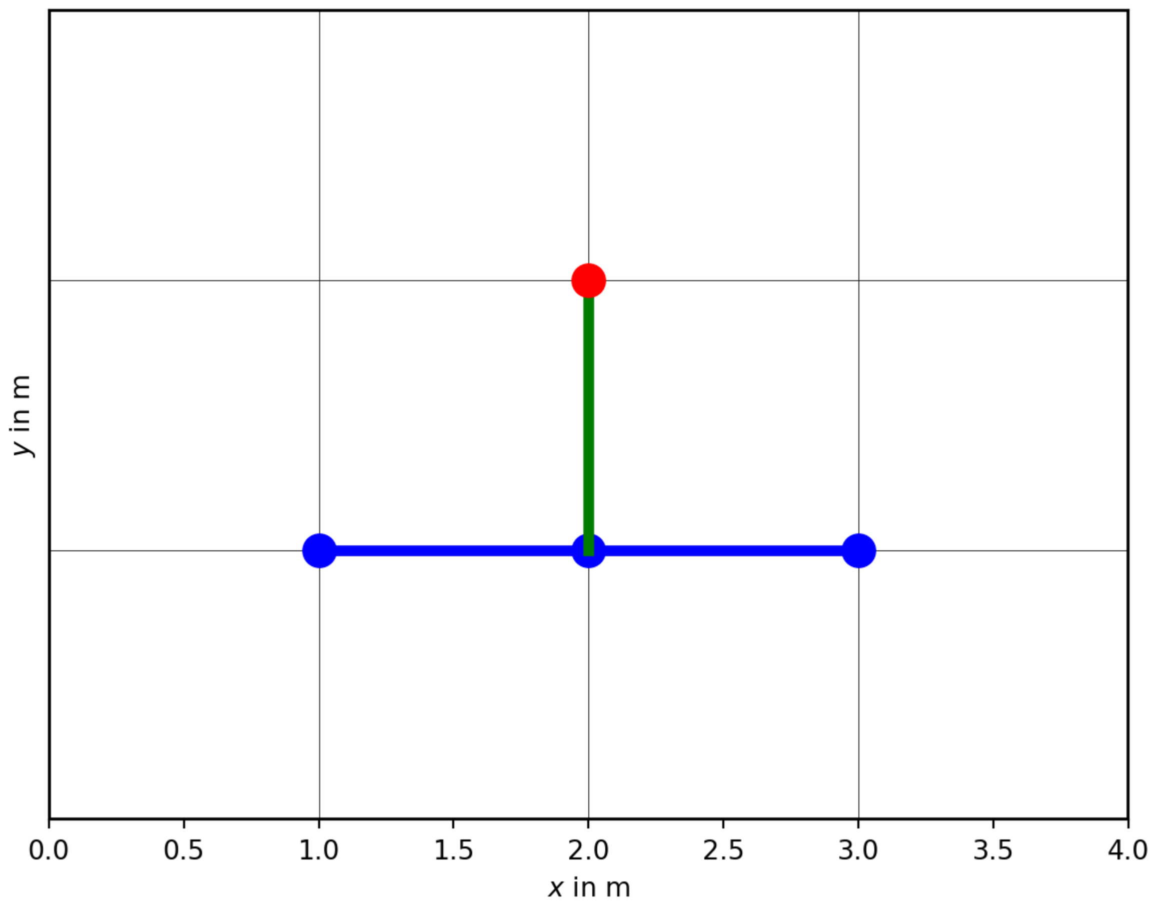
Explicit

Start T^0 with initial condition (e.g. 0)

Update field by

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

E.g. by using the matrix A

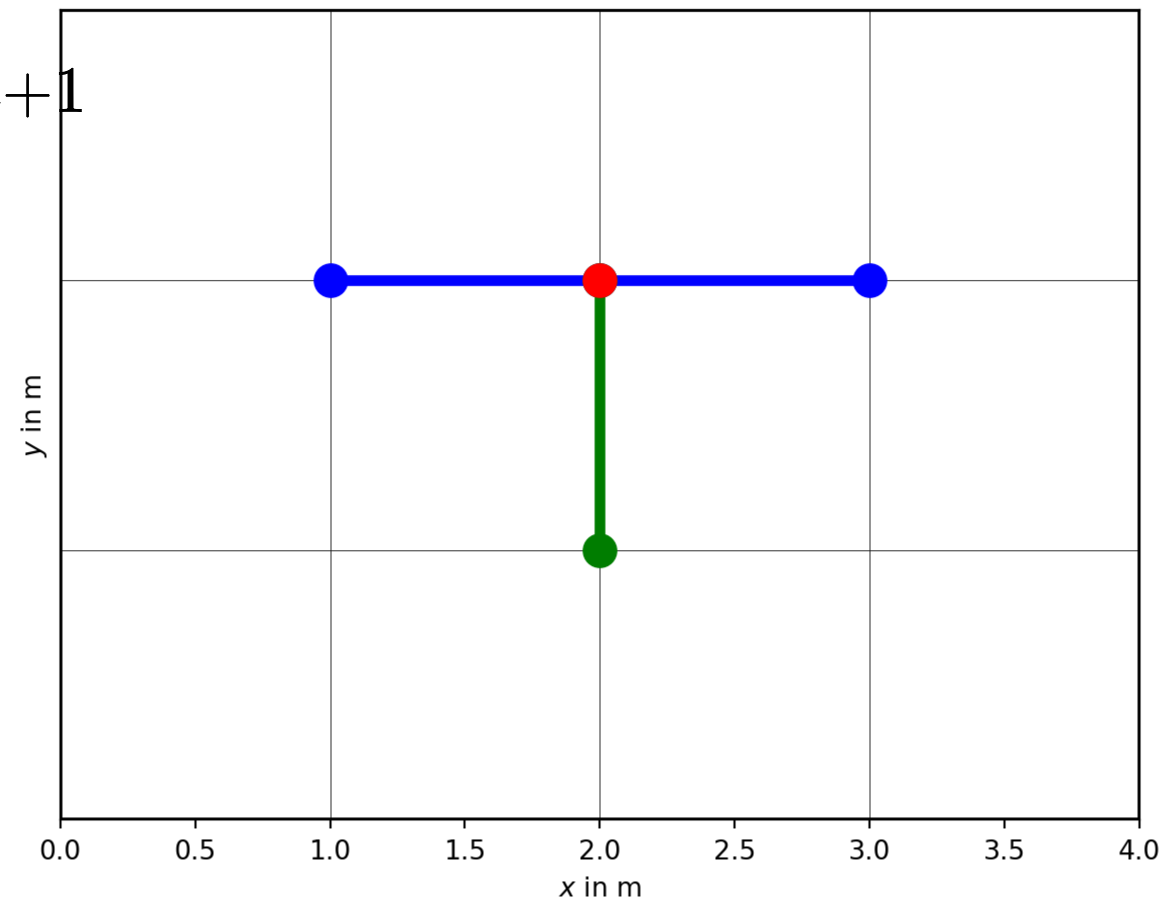


Implicit methods

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

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

$$(\mathbf{M} - \mathbf{A})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^n$$



$\mathbf{M}$ - mass matrix

Mixed - Crank-Nicholson method

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

Tasks instationary heat equation

- setup a discretization and compute the stiffness matrix A for some a
- choose an initial condition (e.g. homogeneous)
- choose a time step Δt and perform the explicit method using the surface temperature
- change the spatial/temporal discretization and observe the solution
- setup mass matrix and implement the implicit method for diff. Δt
- implement the Crank-Nicholson method and compare all three
- compare the solutions with the analytical solution