Linear equations 3

Iterative methods

Dr.ir. Ivo Roghair, Prof.dr.ir. Martin van Sint Annaland

Chemical Process Intensification group
Eindhoven University of Technology

Numerical Methods (6E5X0), 2023-2024

Today's outline

- Introduction
- Sparse matrices
- Laplace's equation
- Creating a sparse system
- Iterative methods
- Summary

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Sparse matrices

- In many engineering cases, we deal with sparse matrices (as opposed to dense matrices)
- A matrix is sparse when it mostly consists of zeros
- Linear systems where equations depend on a limited number of variables (e.g. spatial discretization)
- Storing zeros is not very efficient:

```python
import numpy as np
from scipy.sparse import csr_matrix

A = np.eye(10000)
print(A.nbytes)

S = csr_matrix(A)
print(S.data.nbytes)
```

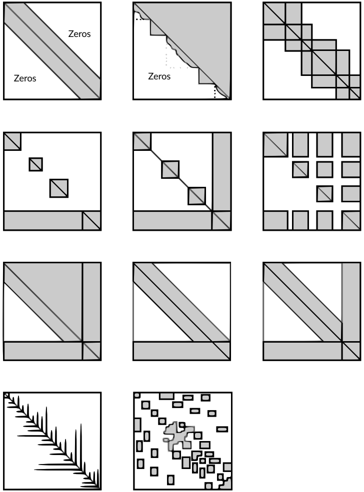
- Can you think of a way to achieve this?
- Sparse matrix formats: Yale, CRS, CCS

Sparse matrix storage format

- Example: Yale storage format, storing 3 vectors:
  - `A = [5 8 3 6]`
  - `IA = [0 1 2 3 4]`
  - `JA = [0 1 2 1]`
  - `A` stores the non-zero values
  - `IA` stores the index in A of the first non-zero in row i
  - `JA` stores the column index

$$A = \begin{bmatrix} 5 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 6 & 0 & 0 \end{bmatrix}$$

Sparse matrix layout examples



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Today's outline

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Laplace's equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$$T = \text{Temperature}$$

$$\alpha = \text{Thermal diffusivity}$$

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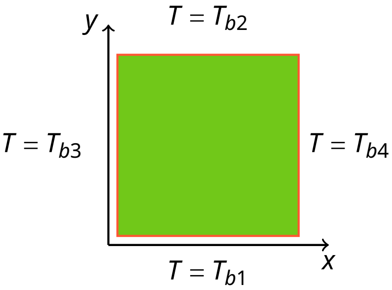


Laplace's equation

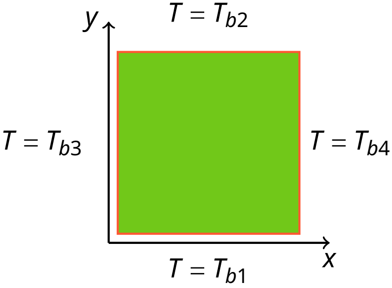
$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

T = Temperature

α = Thermal diffusivity

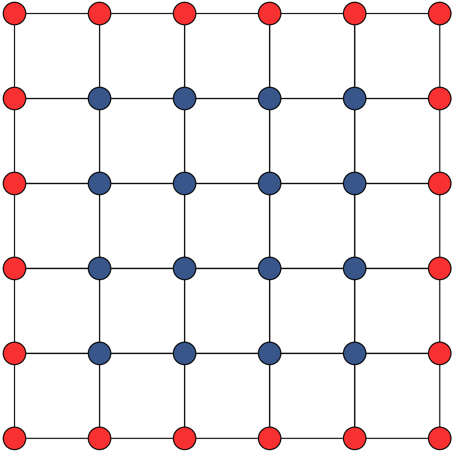
In steady state:

$$\nabla^2 T = 0$$



$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Discretization of Laplace's equation (I)



- Define a grid of points in x and y

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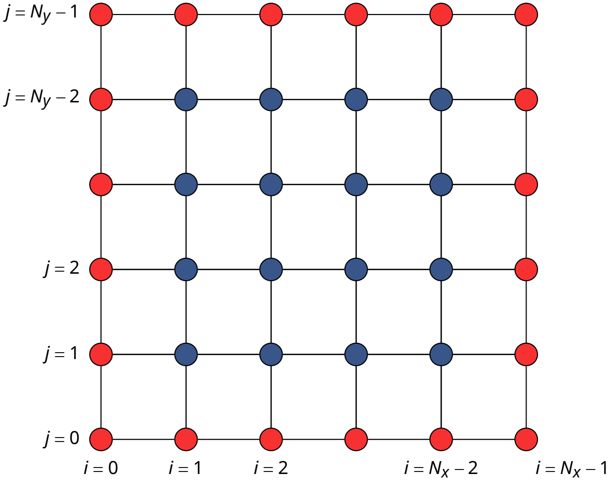

- Define a grid of points in x and y
- Index of the grid points using 2D coordinates i and j

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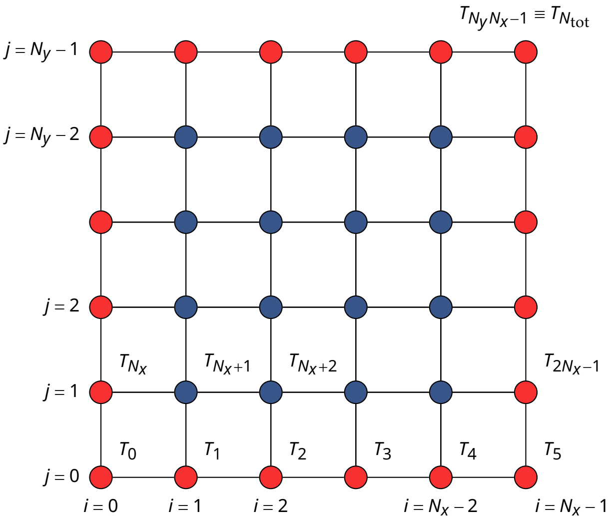
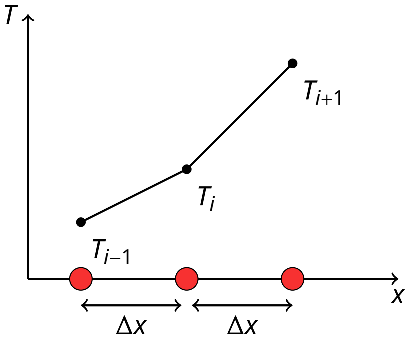


- Define a grid of points in x and y
- Index of the grid points using 2D coordinates i and j
- Set up the equations using a 1D index system: $T_{i,j} \to T_{i+jNx}$

Discretization of Laplace's equation (II)

Estimate the second-order differentials: assume a piece-wise linear profile in the temperature:



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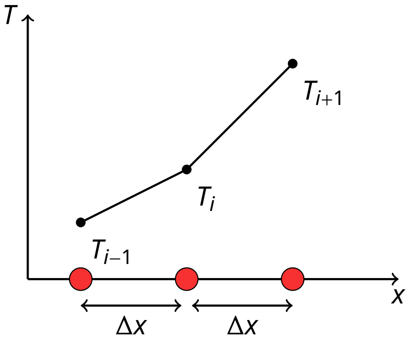

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2}}}{\Delta x}$$

$$\approx \frac{\frac{(T_{i+1,j}-T_{i,j})}{\Delta x} - \frac{(T_{i,j}-T_{i-1,j})}{\Delta x}}{\Delta x}$$

$$= \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2}$$

Discretization of Laplace's equation (III)

The y-direction is derived analogously, so that the 2D Laplace's equation is discretized as:

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0$$

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Use a single index counter $k = i + N_x(j-1)$, so that the equation becomes:

$$\frac{T_{k+1} - 2T_k + T_{k-1}}{(\Delta x)^2} + \frac{T_{k+N_x} - 2T_k + T_{k-N_x}}{(\Delta y)^2} = 0$$

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For an equal spaced grid $\Delta x = \Delta y = 1$:

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

$$\Rightarrow AT = b$$

Today's outline

Creating the linear system

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

Create a *banded* matrix A: the main diagonal k contains -4, whereas the bands at $k-1$, $k+1$, $k-N_x$ and $k+N_x$ contain a 1. Boundary cells just contain a 1 on the main diagonal so that the temperature is equal to T_b (e.g. $T_1 = 1T_b$).

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \ddots & 0 \\ 0 & \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_k \\ T_k + 1 \\ \vdots \\ T_{N_y N_x - 2} \\ T_{N_y N_x - 1} \end{bmatrix} = \begin{bmatrix} T_b \\ T_b \\ \vdots \\ 0 \\ 0 \\ \vdots \\ T_b \\ T_b \end{bmatrix}$$

Creating the linear system

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

Create a *banded* matrix A in Python, by setting the coefficients for the internal cells:

```
import numpy as np
from scipy.sparse import diags

Nx,Ny = 50,50 # Number of grid points along x,y direction
Nc = Nx*Ny    # Total number of points

e = np.ones(Nc)
A = diags([e, e, -4*e, e, e], [-Nx, -1, 0, 1, Nx], shape=(Nc,Nc))
b = np.zeros(Nc)
```

The function `diags` uses the following arguments:

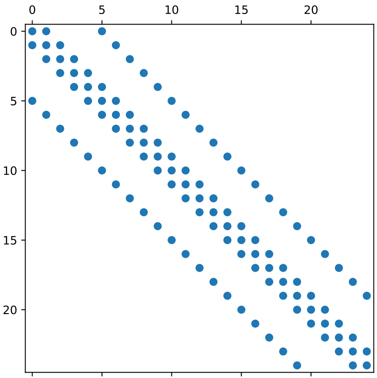
- The coefficients that have to be put on the diagonals arranged as columns in a matrix
- The position of the bands with respect to the main diagonal
- Size of the resulting matrix (in our case square $N_xN_y \times N_xN_y$)

Matrix sparsity

- Let's check the matrix layout by adding:

```
print(A)
plt.spy(A, marker='o',markersize=6)
```

- The *sparse* structure stores/prints only the nonzero elements
- `spy` shows the location of the nonzero values in the matrix
- Apart from the main diagonal, there are offset bands!



About boundary conditions

- For the nodes on the boundary, we have a simple equation:

$$T_{k,\text{boundary}} = \text{Some fixed value}$$

- However, we have set all nodes to be a function of their neighbors
- Solution: Determine the boundary node indices k and set the coefficients accordingly

```
bnd_bottom = np.arange(Nx)
bnd_left = np.arange(Ny) * Nx
bnd_right = bnd_left + Nx - 1
bnd_top = bnd_bottom + Nx*(Ny-1)
```

- Reset each row k in A to zeros, then set element $A_{kk} = 1$
- Set values in rhs: $b_k = T_\text{boundary}$
- Boundary conditions are often more elaborate to implement!

Implementation of the boundary conditions

A (shortened) version of the `set_boundary_conditions(A,b,Tb,Nx,Ny)` function:

```
def set_boundary_conditions(A, b, Tb, Nx, Ny):

    A = lil_matrix(A) # Required for efficient modification of the sparsity

    # Select nodes that lie at the boundaries
    bnd_bottom = np.arange(Nx)
    bnd_left = np.arange(Ny) * Nx
    bnd_right = bnd_left + Nx - 1
    bnd_top = bnd_bottom + Nx*(Ny-1)

    bnd_all = np.unique(np.concatenate((bnd_bottom,bnd_left,bnd_right,bnd_top)))

    # Reset the coefficient row to zero, add a 1 only on the main diagonal
    A[bnd_all,:] = 0
    A[bnd_all,bnd_all] = 1

    b[bnd_bottom] = Tb['bottom']
    b[bnd_left] = Tb['left']
    b[bnd_right] = Tb['right']
    b[bnd_top] = Tb['top']

    return A.tocsr(), b
```

How applying boundary conditions affects the linear system

Using the functions provided in `laplace_demo.py`:

```
Nx = Ny = 5 # number of internal grid cells over x/y-direction

T_boundary = {'bottom': 300, 'left': 1000, 'right': 1000, 'top': 500}

A,b = create_laplace_coefficient_matrix(Nx,Ny)
A,b = set_boundary_conditions(A, b, T_boundary, Nx, Ny)
```

How applying boundary conditions affects the linear system

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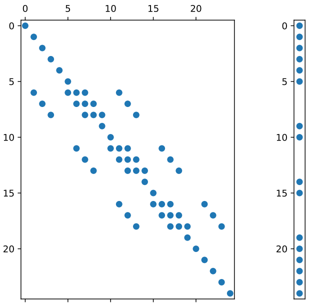
```

Check the new structure of the matrix and the right hand side:

```
plt.subplot(121); plt.spy(A2);
plt.subplot(122); plt.spy(b[:,None]);
```



A full program, including solver

The program and auxiliary functions are on Canvas (`laplace_demo.py`)

```
import numpy as np
from scipy.sparse.linalg import spsolve
from matplotlib import cm
import matplotlib.pyplot as plt

Nx = Ny = 20

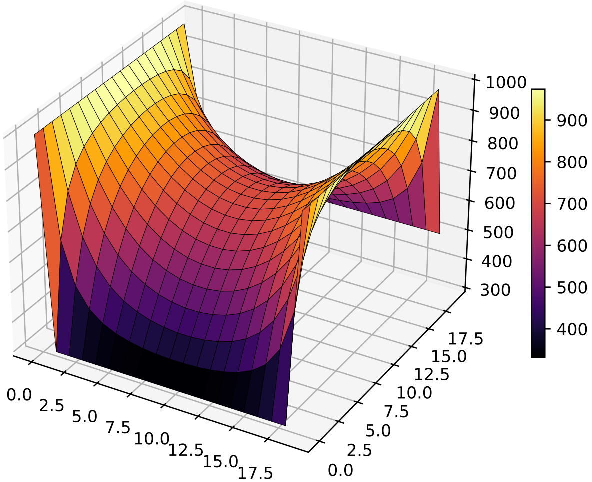
T_boundary = {'bottom': 300, 'left': 1000, 'right': 1000, 'top': 500}

A,b = create_laplace_coefficient_matrix(Nx,Ny)
A,b = set_boundary_conditions(A, b, T_boundary, Nx, Ny)

T = spsolve(A,b).reshape((Nx,Ny))

fig, ax = plt.subplots(subplot_kw={"projection": "3d"})
x,y = np.meshgrid(np.arange(Nx),np.arange(Ny))
surf = ax.plot_surface(x,y,T,cmap=cm.inferno)
fig.colorbar(surf, shrink=0.5)
plt.show()
```

Sample results



Exercise: Verify the numerical solution using Fourier-series

A Fourier-series expansion for the steady-state heat conduction in a flat plate is given for a domain: $x, y \in [0, 1]$, with fixed-temperature boundaries $T\big|_{x=0} = T\big|_{x=1} = T\big|_{y=0} = 0$ and $T\big|_{y=1} = 1$:

$$T = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin(m\pi x)\sinh(m\pi y)}{m \sinh(m\pi)} \quad \text{with} \quad m = 2n - 1$$

Compute and plot the exact temperature profile in the 2D plate, and compare it with the numerical solution:

Hints:

- Use meshgrid to create a mesh in x and y
- Compute the temperature using the Fourier series, use vectorised computations over x and y so that only 1 loop (over n) is required.
- Solve the numerics for the same problem (note the boundary conditions)
- Compare the numerical and exact solutions (e.g. a plot).

Exercise: Verify the numerical solution using Fourier-series

Full script in `solveLaplaceEqAndFourier.py`

```python
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.cm as cm

Nx = Ny = 20

xf,yf = np.meshgrid(np.linspace(0,1,Nx),np.linspace(0,1,Ny))
term = np.zeros_like(x)
N = 100

for m in range(1,N,2):
    term = term + (np.sin(m*np.pi*xf)*np.sinh(m*np.pi*yf)) / (m*np.sinh(m*np.pi))

sol = term * 4 / np.pi
fig, ax = plt.subplots(subplot_kw={"projection": "3d"})
surf = ax.plot_surface(x,y,sol,cmap=cm.inferno)
fig.colorbar(surf, shrink=0.5)
plt.show()
```

LU decomposition of a sparse matrix

```
import numpy as np
from scipy.linalg import lu
import matplotlib.pyplot as plt
from laplace_demo import
        create_laplace_coefficient_matrix

A,b = create_laplace_coefficient_matrix(5,5)

# Perform LU decomposition
# Note: lu does not work on sparse arrays,
# so we map to a full array
P,L,U = lu(A.toarray())

# Plot the sparsity patterns of L and U
plt.subplot(121)
plt.spy(L)
plt.title('L')
plt.subplot(122)
plt.spy(U)
plt.title('U')
plt.tight_layout()
```

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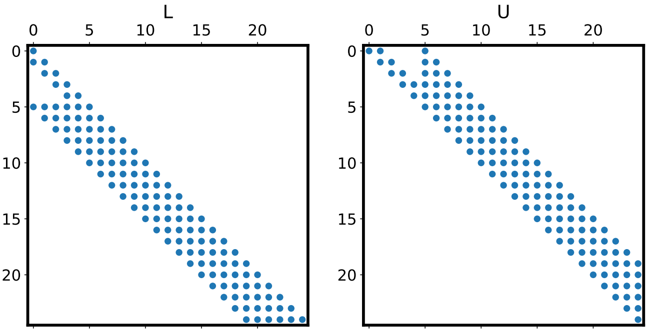
```

- With LU decomposition we produce matrices that are less sparse than the original matrix.
- Sparse storage often required, and also numerical techniques that fully utilizes this!



LU decomposition

- LU decomposition and Gaussian elimination on a matrix like A requires more memory (with 3D problems, the offset in the diagonal would even be bigger!)
- In general extra memory allocation will not be a problem for Python
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Alternatives for elimination methods

- Use iterative methods when systems are large and sparse.
- Often such systems are encountered when we want to solve PDE's of higher dimensions

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Examples of iterative methods

- Jacobi method
- Gauss-Seidel method
- Succesive over relaxation

- `bicg` — Bi-conjugate gradient method
- `pcg` — preconditioned conjugate gradient method
- `gmres` — generalized minimum residuals method
- `bicgstab` — Bi-conjugate gradient method

The Jacobi method

- In our example we derived the following equation:

$$T_{k-N_x} + T_{k-1} - 4T_k + T_{k+1} + T_{k+N_x} = 0$$

- Rearranging gives:

$$T_k = \frac{T_{k-N_x} + T_{k-1} + T_{k+1} + T_{k+N_x}}{4}$$

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  1. Start with an initial guess for the values of T at each node
  2. Compute updated values and store a new vector:

$$T_k^{\text{new}} = \frac{T_{k-N_x}^{\text{old}} + T_{k-1}^{\text{old}} + T_{k+1}^{\text{old}} + T_{k+N_x}^{\text{old}}}{4}$$

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  3. Do this for all nodes
  4. Repeat the procedure until converged

Jacobi method for Laplace's equation

See `laplace_jacobi.py` for animation included (from Canvas)

```python
import numpy as np
import matplotlib.pyplot as plt

# Set grid resolution
nx = 40
ny = 40

# Set old solution array
T = np.zeros((nx,ny))

# Set boundary conditions
T[0,:] = 40 # Left
T[nx-1,:] = 60 # Right
T[:,0] = 20 # Bottom
T[:,ny-1] = 30 # Top

# Set new solution array (inc bnd conditions)
Tnew = T.copy()
```

```python
# Create grid for plotting
x,y = np.meshgrid(np.arange(1,nx+1), np.arange(1,ny+1))

# Perform iterations
for iter in range(1,1001):
    for i in range(1,nx-1):
        for j in range(1,ny-1):
            # Calculate new solution
            Tnew[i,j] =  \
                (T[i-1,j]+T[i+1,j]+T[i,j-1]+T[i,j+1])/4.0
    T = Tnew.copy()
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    T = Tnew.copy()
```

→ Try to modify this script so that 1 cell/block of cells in the center is kept at 100 degrees

About the straightforward implementation

- The method as implemented works fine for a simple Laplace equation
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- For generic systems of linear equations, the implementation cannot be used.

> We will now introduce the Jacobi method so it can be used for generic systems of linear equations.

The Jacobi method with matrices

We can split our (banded) matrix A into a diagonal matrix D and a remainder R:

$$A \quad = \quad D \quad + \quad R$$

$$\begin{bmatrix}
\times & \times & & & & & \times & & \\
\times & \times & \times & & & & & \times & \\
& \times & \times & \times & & & & & \times \\
& & \times & \times & \times & & & & \\
& & & \times & \times & \times & & & \\
& & & & \times & \times & \times & & \\
\times & & & & & \times & \times & \times & \\
& \times & & & & & \times & \times & \times \\
& & \times & & & & & \times & \times
\end{bmatrix} = \begin{bmatrix}
\times & & & & & & & & \\
& \times & & & & & & & \\
& & \times & & & & & & \\
& & & \times & & & & & \\
& & & & \times & & & & \\
& & & & & \times & & & \\
& & & & & & \times & & \\
& & & & & & & \times & \\
& & & & & & & & \times
\end{bmatrix} + \begin{bmatrix}
& \times & & & & & \times & & \\
\times & & \times & & & & & \times & \\
& \times & & \times & & & & & \times \\
& & \times & & \times & & & & \\
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& & & & \times & & \times & & \\
\times & & & & & \times & & \times & \\
& \times & & & & & \times & & \times \\
& & \times & & & & & \times &
\end{bmatrix}$$

Jacobi method: solving a system

- We can solve $AT = b$, now written generally as $Ax = b$, by:

$$\begin{aligned}
Ax &= b \\
(D+R)x &= b \\
Dx &= b - Rx \\
Dx^{\text{new}} &= b - Rx^{\text{old}} \\
x^{\text{new}} &= D^{-1}(b - Rx^{\text{old}})
\end{aligned}$$

- Using the n and $n+1$ notation for old and new time steps, we find in general:

$$x^{n+1} = D^{-1}\left(b - Rx^{n}\right)$$

$$x_i^{n+1} = \frac{1}{A_{ii}}\left(b_i - \sum_{j\neq i} A_{ij}x_j^{n}\right)$$

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Diagram of the Jacobi method

Set T^{old} = a guess

Diagram of the Jacobi method

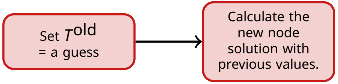
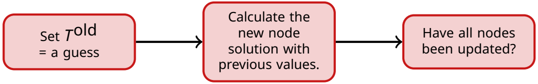


Diagram of the Jacobi method



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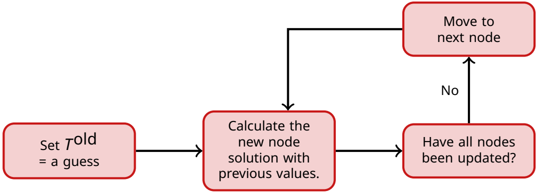

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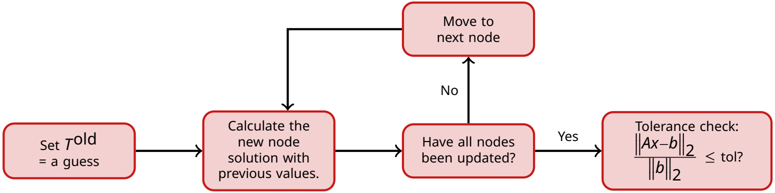

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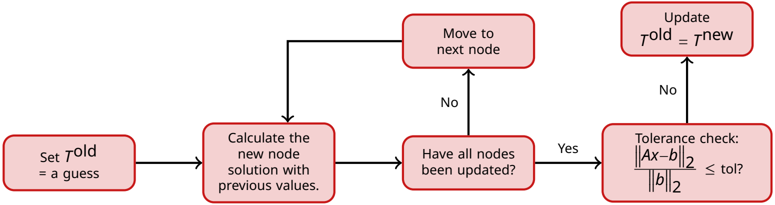

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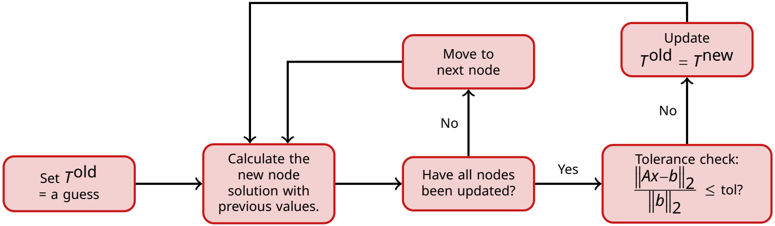

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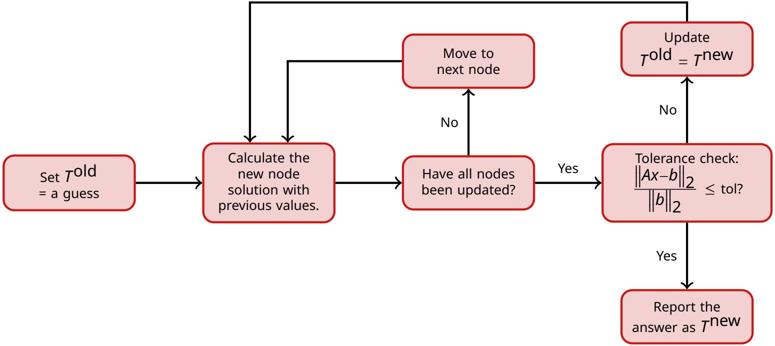

The core of the solver

The full function `jacobi(A, b, tol=1e-2)` is on Canvas, see `it_methods.py`. The gist is:

```
# While not converged or max_it not reached
while (x_diff > tol and it_jac < 1000):
    x_old = x.copy()
    for i in range(N):
        s = 0
        for j in range(N):
            if j != i:
                # Sum off-diagonal*x_old
                s += A[i,j] * x_old[j]
        # Compute new x value
        x[i] = (b[i] - s) / A[i,i]

    # Increase number of iterations
    it_jac += 1
    x_diff = norm(A@x - b)/norm(b)
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Try to call it from the `laplace_demo.py` file, instead of using `spsolve`.

A few details on this algorithm

- The while loop holds two aspects
  - A convergence criterion (`norm(A@x - b)/norm(b)> tol`). Some considerations are:
    - L_1-norm (sum)
    - L_2-norm (Euclidian distance)
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- Start vector x is not shown in the example, but should be there!
- It can have huge impact on performance!
- The for-loops also have a large performance penalty!

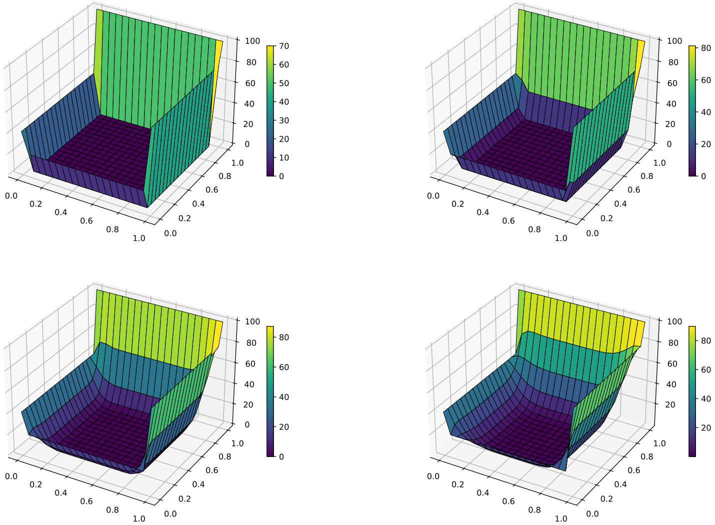
The solver using array indices

Make a copy of the Jacobian solver, and replace the for-loop on `j` by a vector-operation in a new function `jacobi_vec(A, b, tol=1e-2)`:

```
# While not converged or max_it not reached
while (x_diff > tol and it_jac < 1000):
    x_old = x.copy()
    for i in range(N):
        j = np.r_[np.arange(i),np.arange(i+1,N)]
        # Sum off-diagonal*x_old
        s = A[i,j] @ x_old[j]
        # Compute new x value
        x[i] = (b[i] - s) / A[i,i]

    # Increase number of iterations
    it_jac += 1
    x_diff = norm(A@x - b)/norm(b)
```

Iterations 1, 2, 5 and 10



Gauss-Seidel method

The Gauss-Seidel method is quite similar to Jacobi method

- The only difference is that the new estimate x^{new} is returned to the solution x^{old} as soon as it is completed
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- Our straightforward script (from the Jacobi method) is therefore changed easily:
  - Do not create a `Tnew` array (save memory!)
  - Do not store the solution in `Tnew`, but simply in `T`
  - Do not perform the update step `T=Tnew`
  - See `gaussseidel(A, b, tol=1e-2)` for the algorithm.

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  - Do not perform the update step `T=Tnew`
  - See `gaussseidel(A, b, tol=1e-2)` for the algorithm.
- The straightforward script works well for the current Laplace equation, but we define the generic Gauss-Seidel algorithm on the following slides.

Gauss-Seidel method

- Define a lower and strictly upper triangular matrix, such that $A = L + U$
- Now we can solve AT=b by:

$$\begin{aligned}(L+U)T &= b\\ LT &= b - UT\\ LT^{\text{new}} &= b - UT^{\text{old}}\\ T^{\text{new}} &= L^{-1}(b - UT^{\text{old}})\end{aligned}$$

- Using the n and $n+1$ notation for old and new time steps, we find in for the general Gauss-Seidel method:

$$x^{n+1} = L^{-1}\left(b - Ux^{n}\right)$$

$$x_i^{n+1} = \frac{1}{A_{ii}}\left(b_i - \sum_{j<i} A_{ij}x_j^{n+1} - \sum_{j>i} A_{ij}x_j^{n}\right)$$

Create yourself: Gauss-Seidel method

- Create a copy of the `jacobi` method and rename it to `gaussseidel`
- Rework the inner algorithm to reflect the changes for the Gauss-Seidel method
- Test! Perform a timing check and check if the solution is correct.
- Next, create a new copy of the just created method and vectorize it, analogous to our vectorized Jacobi method

Today's outline

- Introduction
- Sparse matrices
- Laplace's equation
- Creating a sparse system
- Iterative methods
- Summary

Summary

- Partial differential equations can be discretized into sparse systems of linear equations
- Sparse matrices can be stored in memory efficiently using specialised formats (e.g. compressed row storage)
- The Jacobi and Gauss–Seidel methods were introduced as iterative methods; other methods are based on the same principle (successive over-relaxation method, for example)
- Various implementation issues were discussed, e.g. vectorised computing, convergence tolerances

Direct methods vs. Iterative methods

- Iterative methods converge *gradually* to a solution while direct methods (possibly with partial pivoting) factorise a (set of) matrix(ces) which allow to compute the solution by *substitution*.
- Direct methods generally use more memory, since they need to store also the result matrices.
- A strictly (or irreducibly) diagonally dominant matrix is a prerequisite for convergence of the Jacobi and Gauss-Seidel method.
- For real-life situations; 1D problems are generally solved with direct methods (LU decomposition). If you have systems of more than 1 dimension, a direct method still can be used, if there are no memory issues, otherwise an iterative method would be more attractive.