Linear equation solvers

Iterative methods

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Today's outline

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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:

```
>> A = eye(10000);
>> whos A
>> S = sparse(A);
>> whos S
```

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

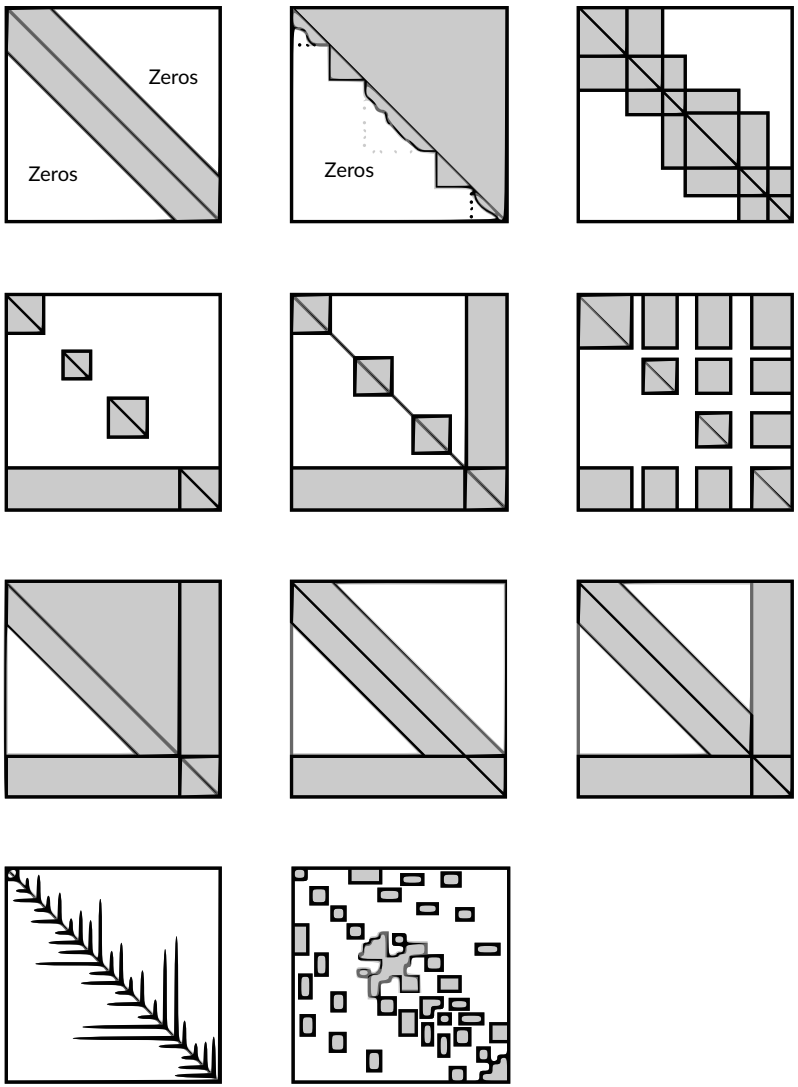
Sparse matrix storage format

- Example: Yale storage format, storing 3 vectors:
  - `A = [5 8 3 6]`
  - `IA = [0 0 2 3 4]`
  - `JA = [0 1 2 1]`

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

- `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
- Note: zero-based indices are used here!

Sparse matrix layout examples



Today's outline

Laplace's equation

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

T = Temperature

α = Thermal diffusivity

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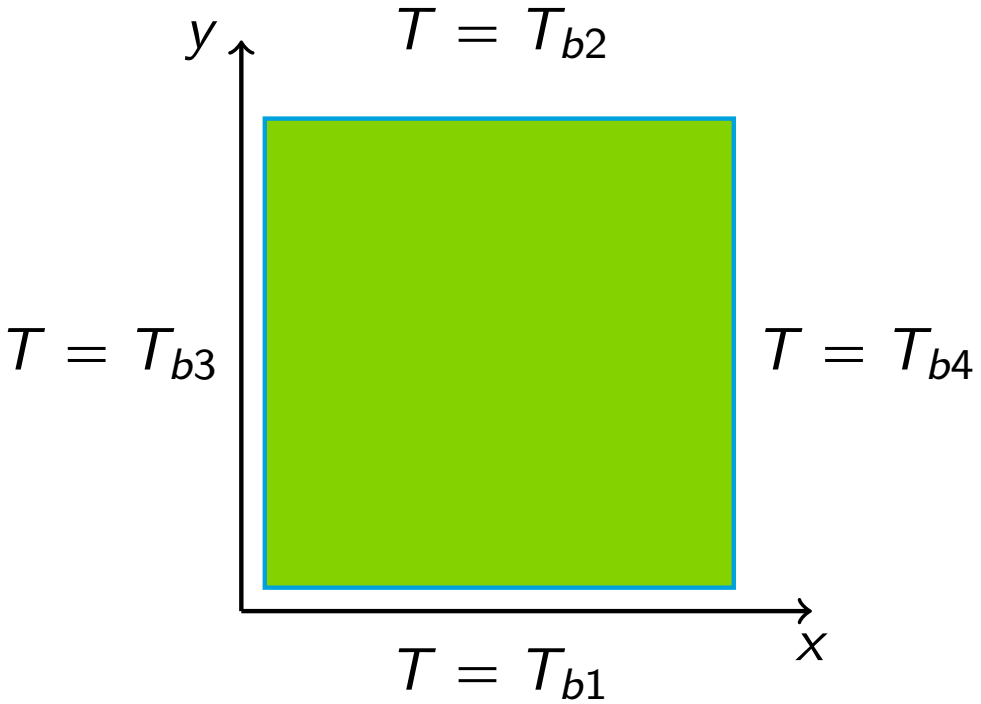

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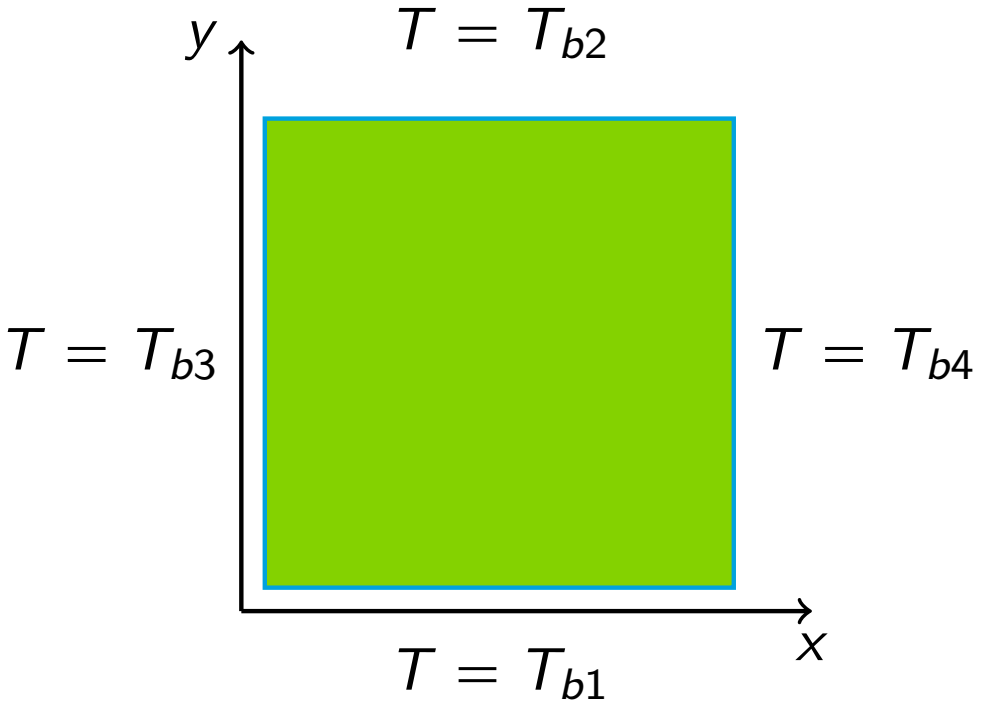
T = Temperature

α = Thermal diffusivity

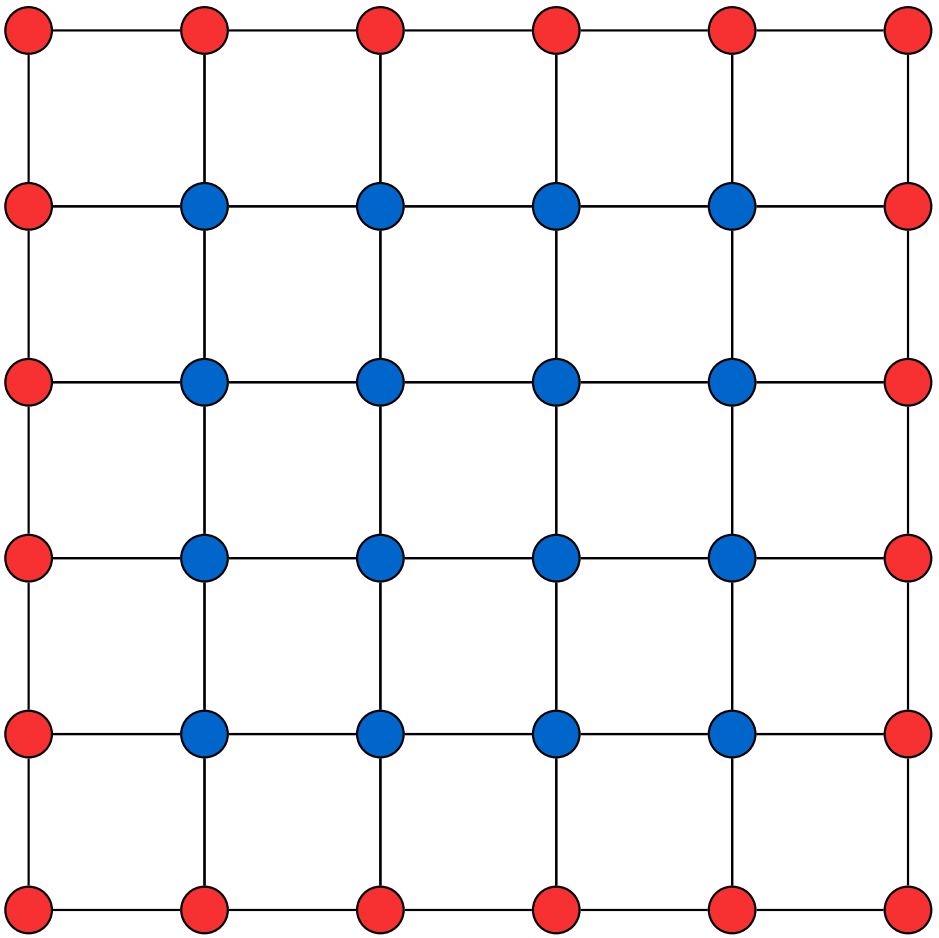
In steady state:

$$\nabla^2 T = 0$$



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

Discretization of Laplace's equation (I)



- Define a grid of points in x and y

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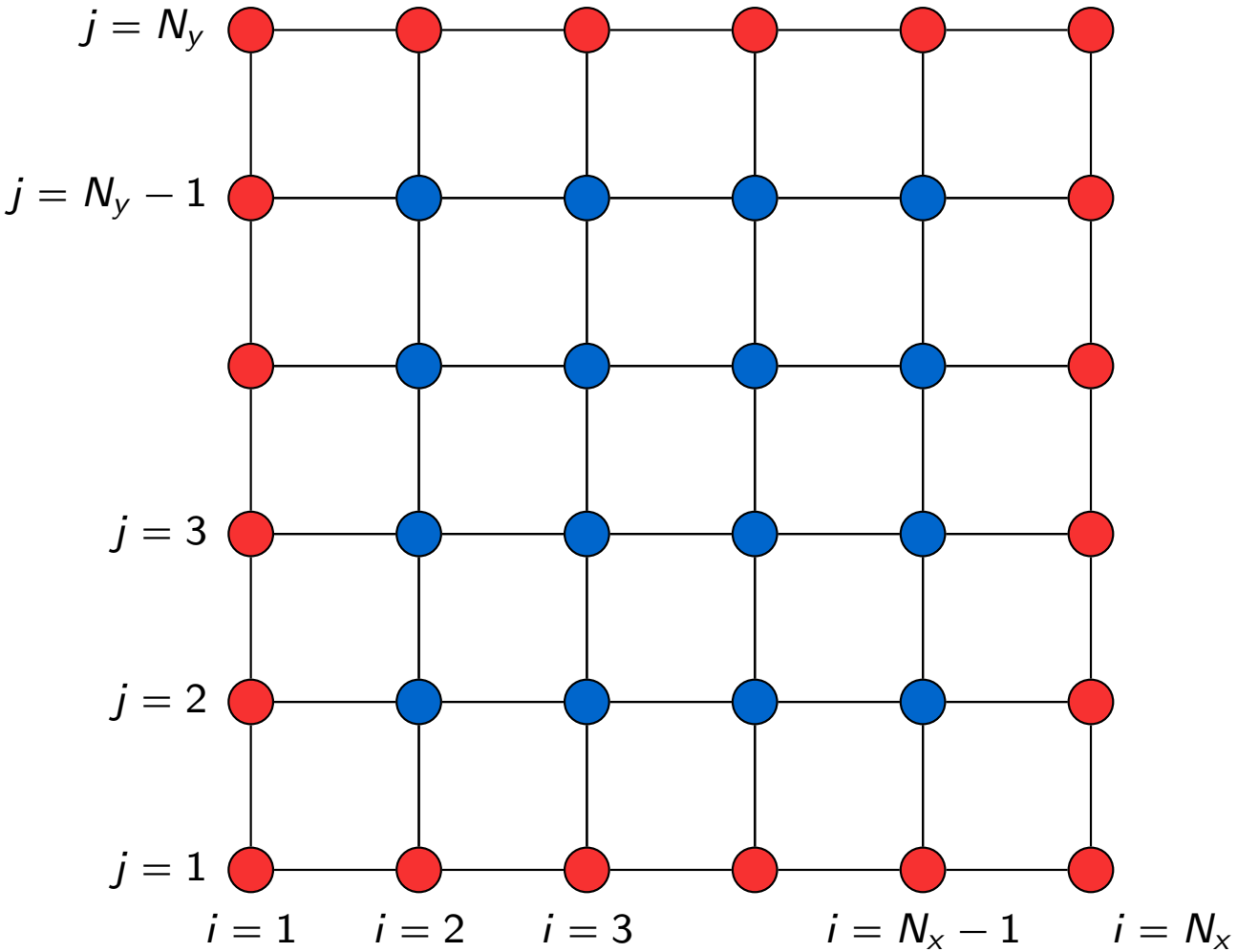

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- Index of the grid points using 2D coordinates i and j

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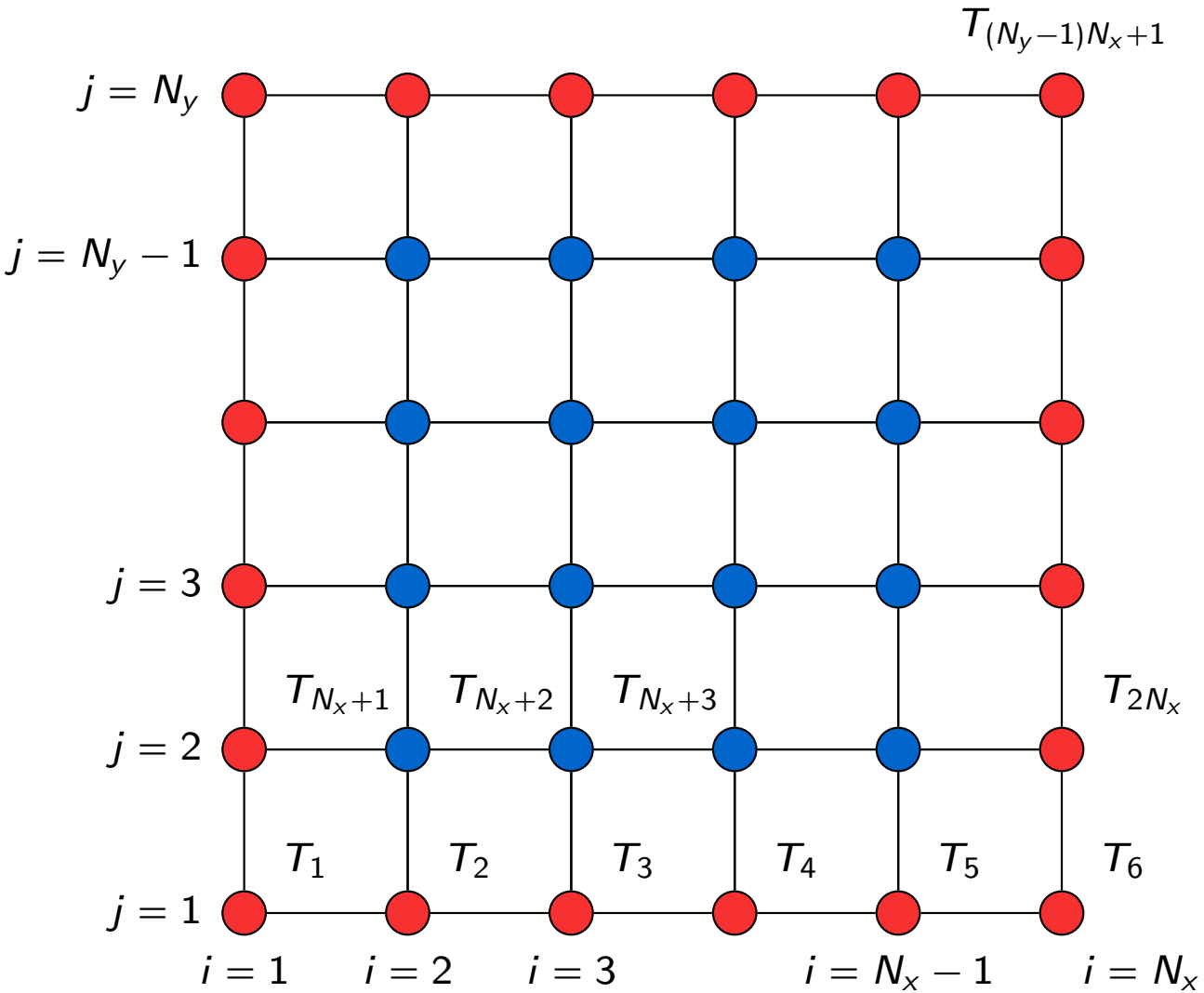
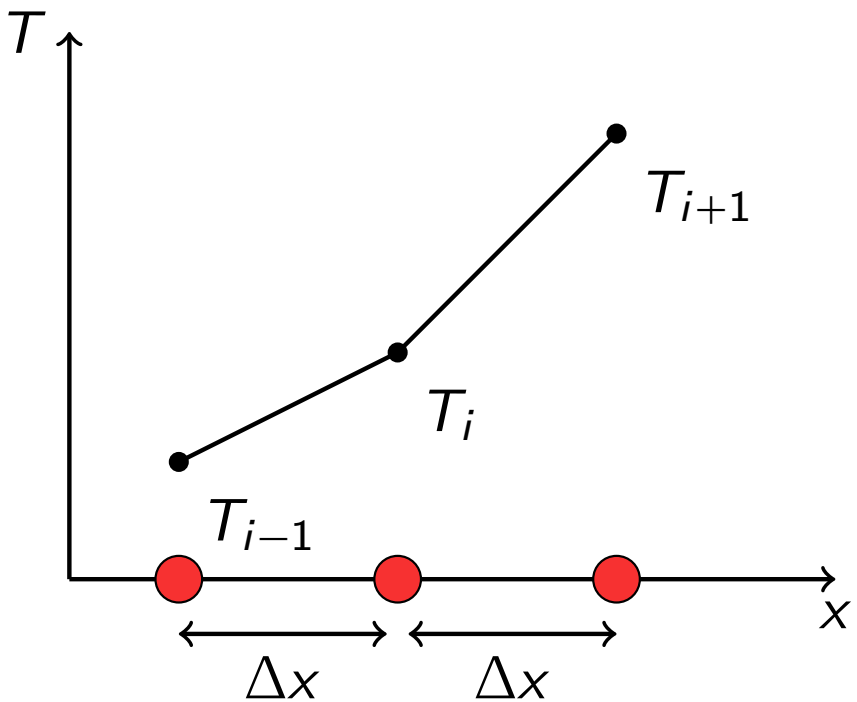


- Define a grid of points in x and y
- Index of the grid points using 2D coordinates i and j
- Set up the equations using a 1D index system: $T_{i,j} = T_{i+N_x(j-1)}$

Discretization of Laplace's equation (II)

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



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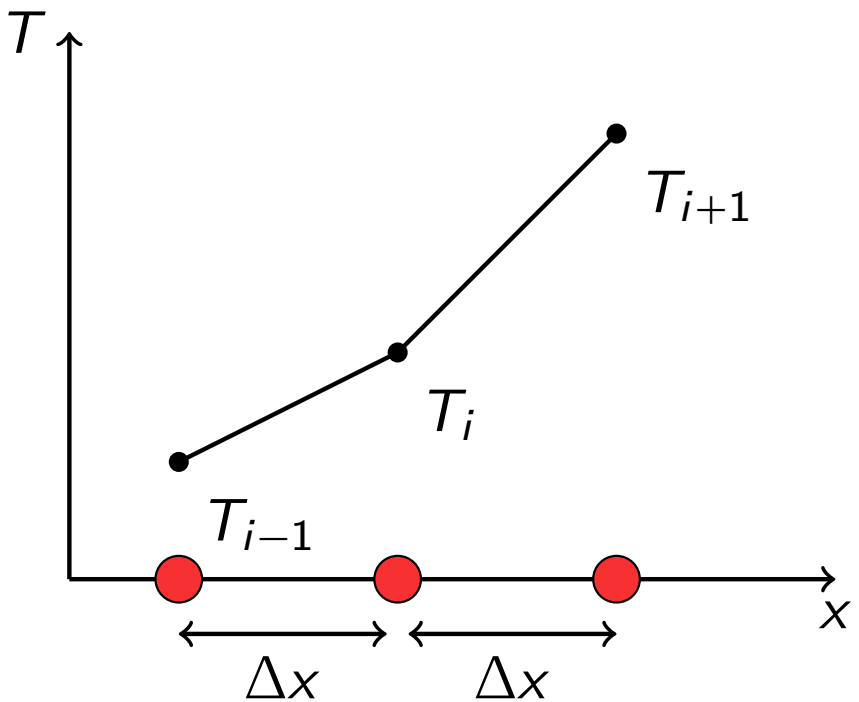

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2}}}{\Delta x}$$

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

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

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. $T_1 = 1T_b$).

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \ddots & 0 \\ 0 & \cdots & 1 & \cdots & 1 & -4 & 1 & \cdots & 1 & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_k \\ T_k + 1 \\ \vdots \\ T_{(N_y-1)N_x} \\ T_{(N_y-1)N_x+1} \end{bmatrix} = \begin{bmatrix} T_b \\ T_b \\ \vdots \\ 0 \\ 0 \\ \vdots \\ T_b \\ T_b \end{bmatrix}$$

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 Matlab, by setting the coefficients for the internal cells:

```
Nx=5;  %number of points along x direction
Ny=5;  %number of points in the y direction
Nc=Nx*Ny; % Total number of points

e = ones(Nc,1);
A = spdiags([e,e,-4*e,e,e],[-Nx,-1,0,1,Nx],Nc,Nc);
b = zeros(Nc,1);
```

The function `spdiags` uses the following arguments:

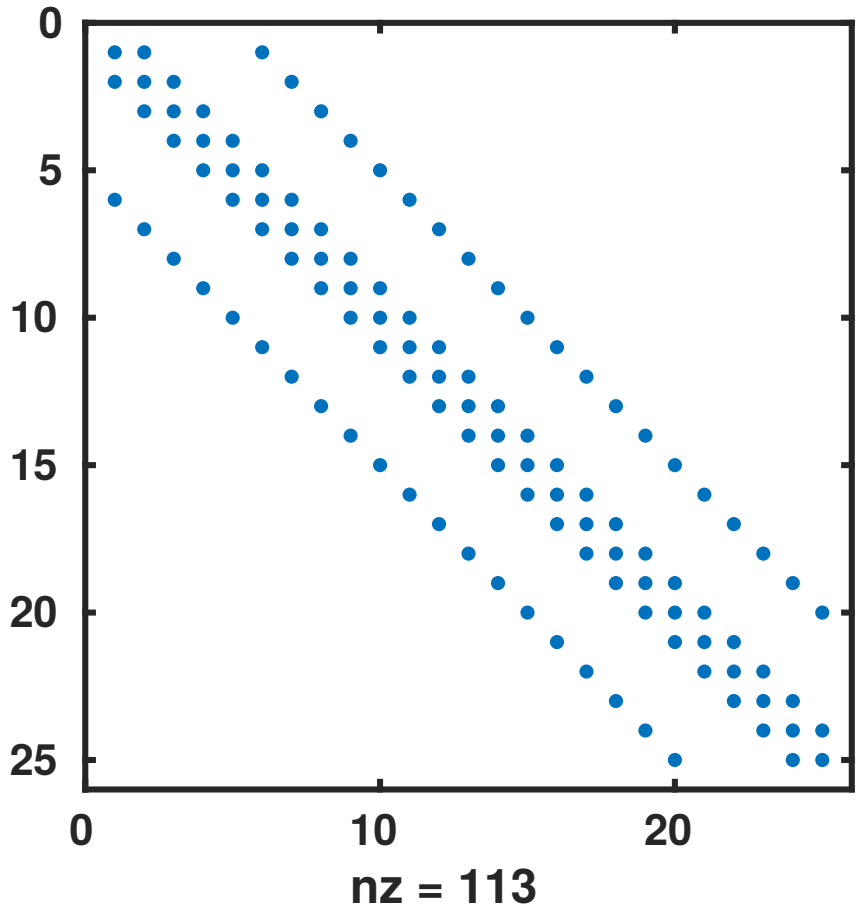
- The coefficients that have to be put on the diagonals arranged as columns in a matrix
- The position of the bands with respect to the main diagonal
- Size of the resulting matrix (in our case square $N_xN_y \times N_xN_y$)

Matrix sparsity

- Let's check the matrix layout:

```
>> spy(A)
```

- This command shows the non-zero values of a 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...
- Find the boundary node indices using $k = i + Nx(j-1)$
  - `i = 1, j = 1:Ny`
  - `i = Nx, j = 1:Ny`
  - `j = 1, i = 1:Nx`
  - `j = Ny, i = 1:Nx`
- Reset the row in A to zeros, set $A_{kk} = 1$
- Set value in rhs: $b_k = T_{k,\text{boundary}}$
- Boundary conditions are often more elaborate to implement! See `setBoundaryConditions.m`.

Partial implementation of the boundary conditions

See `setBoundaryConditions.m`.

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)

% Set boundary conditions over x-direction
for i=1:Nx
    j = 1;
    ind = i + Nx * (j-1);
    A(ind,:) = 0;    % Reset matrix for boudary cells
    A(ind,ind) = 1; % Add a 1 on the diagonal
    b(ind) = Tb(1);
    j = Ny;
    ind = i + Nx * (j-1);
    A(ind,:) = 0;    % Reset matrix for boudary cells
    A(ind,ind) = 1; % Add a 1 on the diagonal
    b(ind) = Tb(2);
end

%% Repeat for y-direction
```

How applying boundary conditions affects the linear system

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)
```

How applying boundary conditions affects the linear system

```
function [A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny)
```

- Make sure that matrix `A` and right hand side vector `b` are in your workspace, as well as `Nx` and `N_y`
- Create a vector that holds the temperature at each boundary:

```
>> T = [10 20 30 40];
```

- Call the function, store A and b in new variables:

```
>> [A2,b2] = setBoundaryConditions(A,b,T,Nx,Ny);
```

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

```
>> subplot(1,2,1); spy(A2);
>> subplot(1,2,2); spy(b2);
```

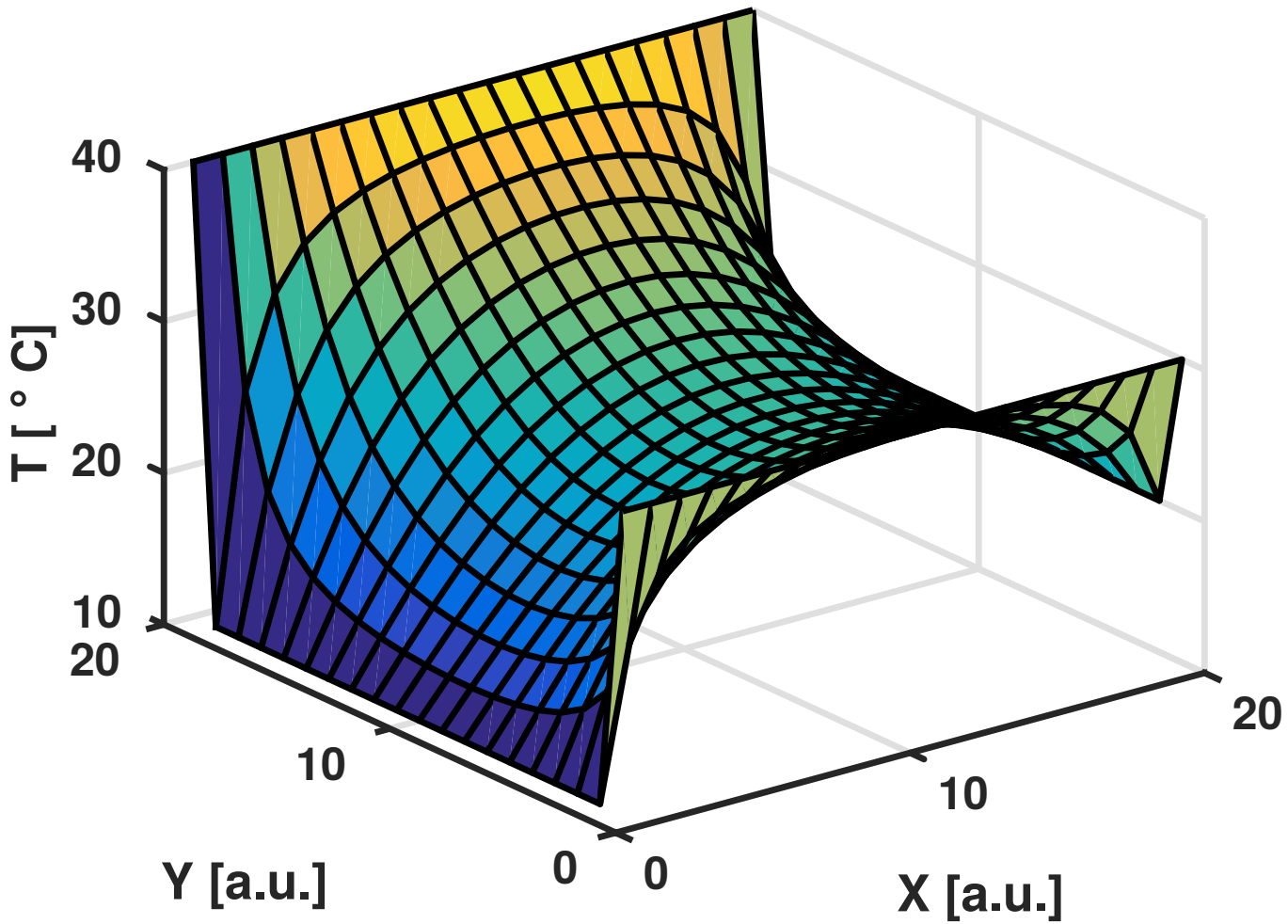
A full program, including solver

The program and auxiliary functions are on Canvas (`solveLaplaceEq.m`)

```
function [x,y,T,A] = solveLaplaceEq(Nx,Ny)
% Solves the steady-state Laplace equation

Tb = [10 20 30 40]; % Fixed boundary temperatures

% Fill sparse matrix with [1 1 -4 1 1]
e = ones(Nx*Ny,1);
A = spdiags([e,e,-4*e,e,e],[-Nx,-1,0,1,Nx],Nx*Ny,Nx*Ny);
b = zeros(Nx*Ny,1);

[A,b] = setBoundaryConditions(A,b,Tb,Nx,Ny);

T = A\b;  % Solve matrix
Tc = reshape(T,[Nx,Ny]); % Reshape x-vec to mat Nx,Ny
[xc yc] = meshgrid(1:Nx,1:Ny); % Get position arrays
surf(xc,yc,Tc); % Surface plot
```

Sample results

Solved for a 20×20 system with $T_b = [10\ 20\ 30\ 40]$.



LU decomposition of a sparse matrix

```
>> [L,U,P] = lu(A)
>> subplot(1,2,1)
>> spy(L)
>> subplot(1,2,2)
>> spy(U)
```

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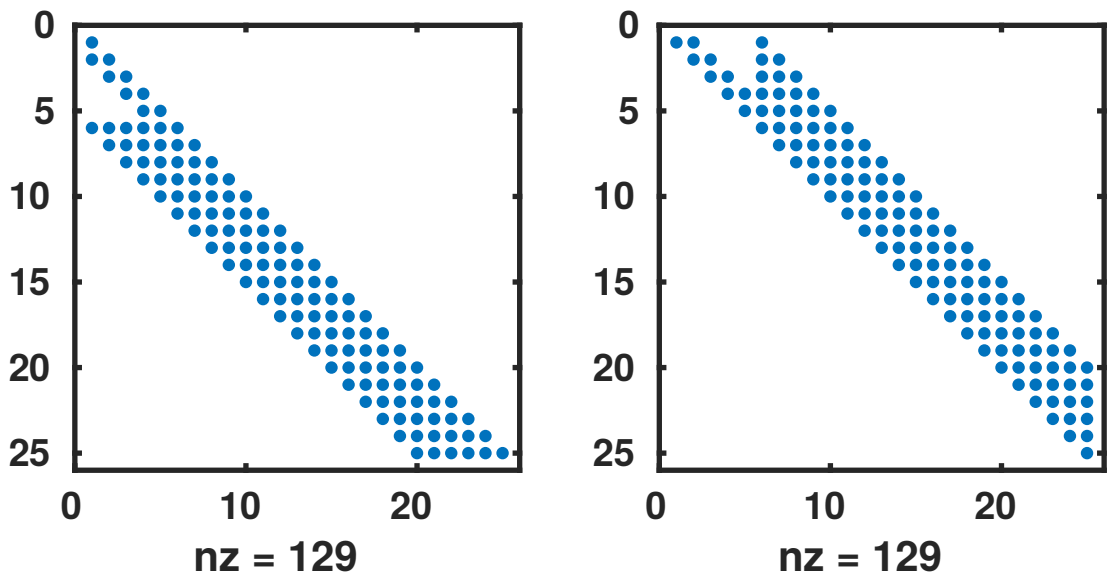
- With LU decomposition we produce matrices that are less sparse than the original matrix.
- Sparse storage often required, and also numerical techniques that fully utilizes this!



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 MATLAB
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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 PDEs of higher dimensions

Today's outline

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.m` (from Canvas)

```
% Grid size
nx = 40; ny = 40;
```

Jacobi method for Laplace's equation

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```
% Grid size
nx = 40; ny = 40;
% The temperature field + boundaries at old and new times
T = zeros(nx,ny);
T(1,:) = 40;  % Left
T(nx,:) = 60; % Right
T(:,1) = 20;  % Bottom
T(:,ny) = 30; % Top
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Tnew = T;
% For plotting
[x y] = meshgrid(1:nx, 1:ny);
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Tnew = T;
% For plotting
[x y] = meshgrid(1:nx, 1:ny);
for iter = 1:1000
  for i = 2:nx-1
    for j = 2:ny-1
      Tnew(i,j) = (T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))/4.0;
    end
  end
```

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[x y] = meshgrid(1:nx, 1:ny);
for iter = 1:1000
  for i = 2:nx-1
    for j = 2:ny-1
      Tnew(i,j) = (T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))/4.0;
    end
  end
  surf(x,y,Tnew);
  title(['Iteration: ' num2str(iter)]);
  drawnow
  T = Tnew; % Update T
end
```

About the straightforward implementation

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

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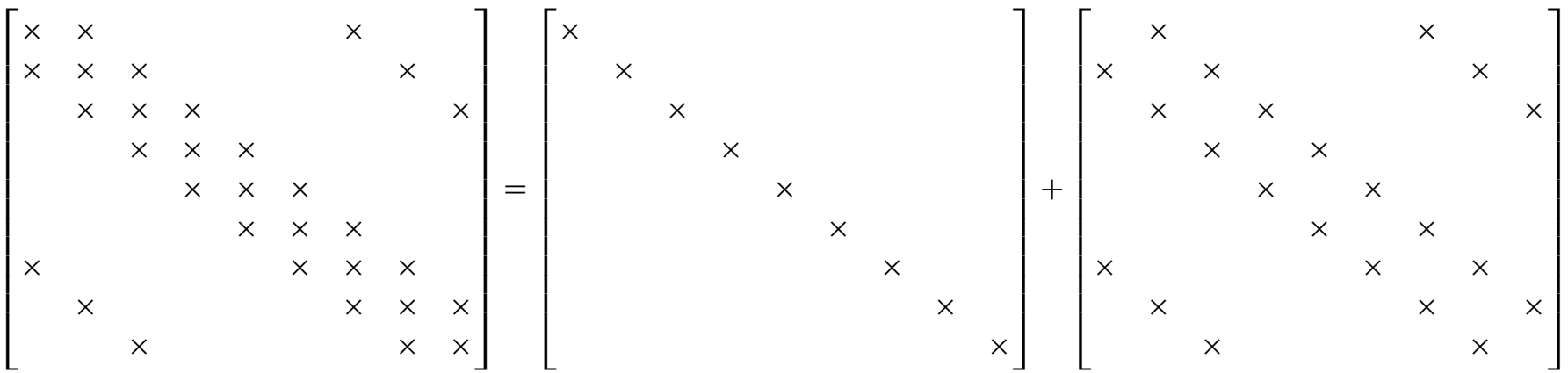
- For generic systems of linear equations, the implementation cannot be used.

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:

$$A = D + R$$



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:

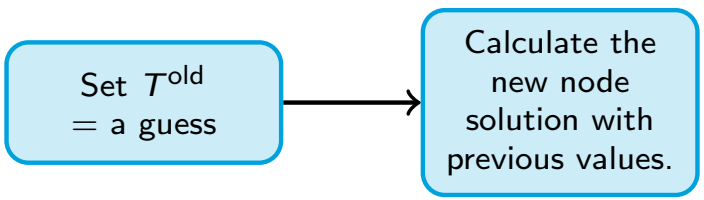
$$x^{n+1} = D^{-1}\left(b - Rx^{n}\right)$$

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

Diagram of the Jacobi method

Set T^{old}
= a guess

Diagram of the Jacobi method



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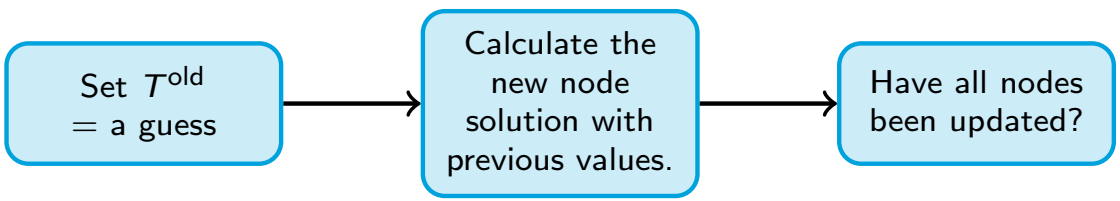

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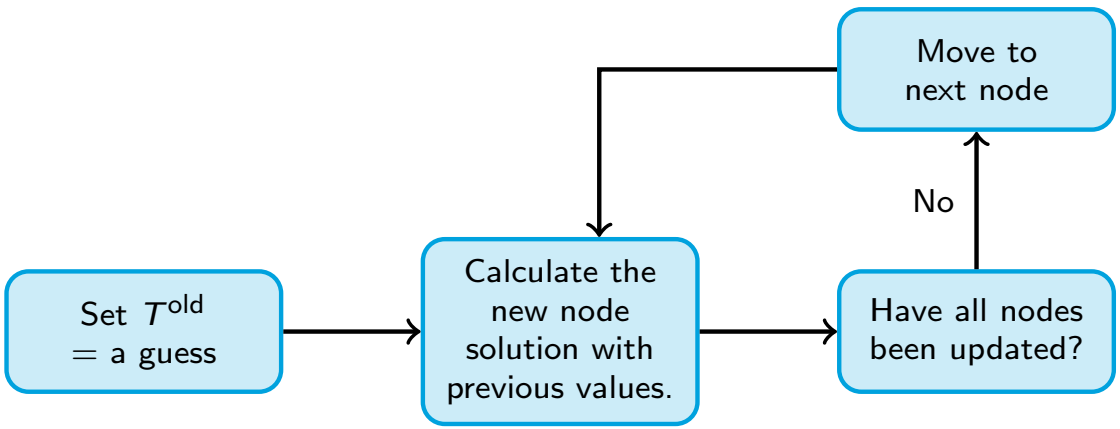

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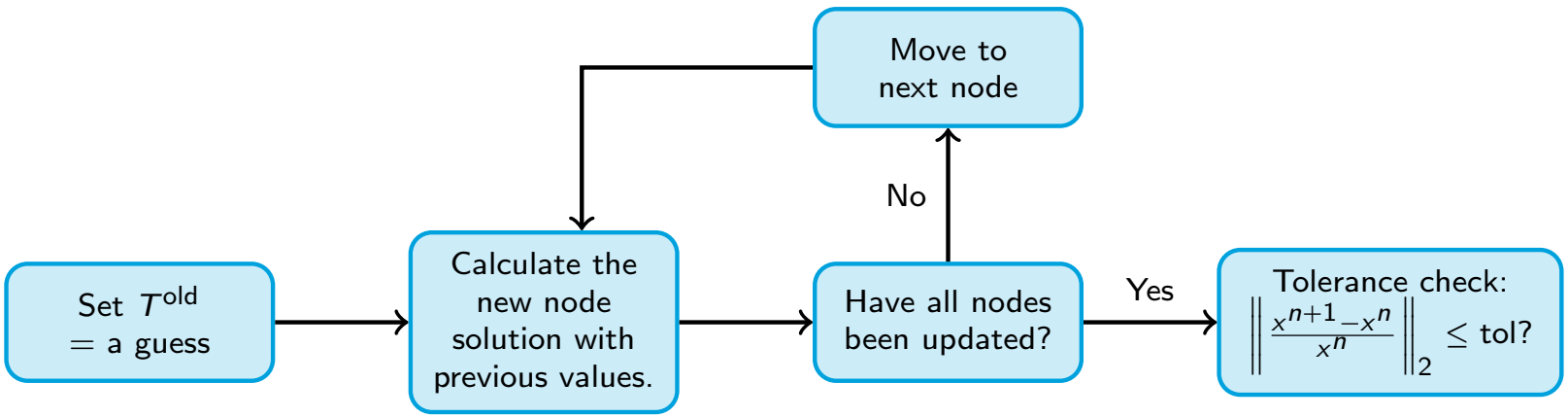

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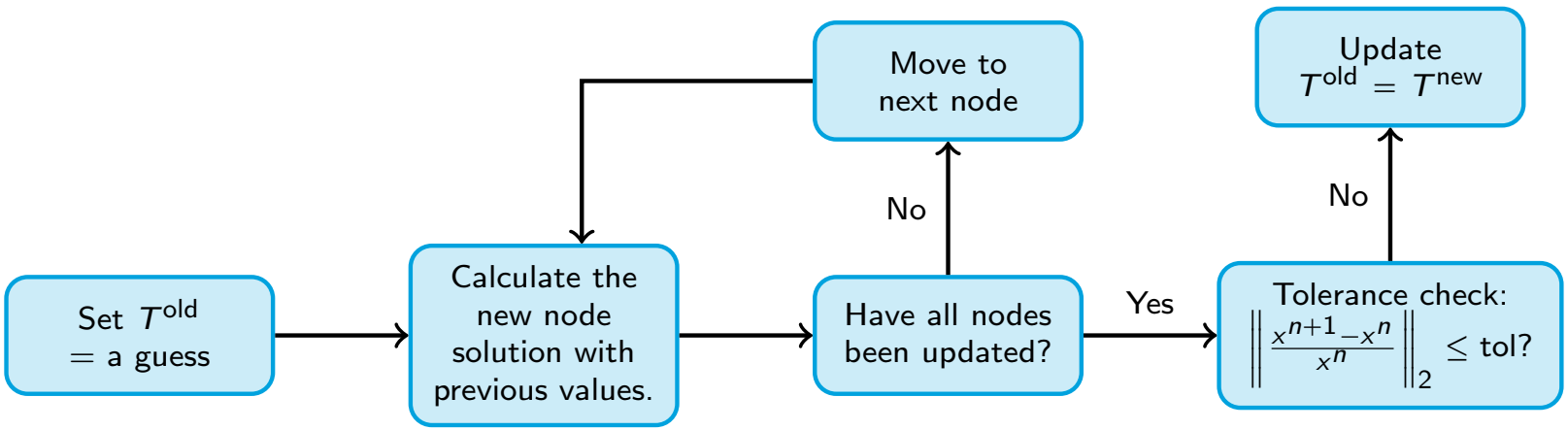

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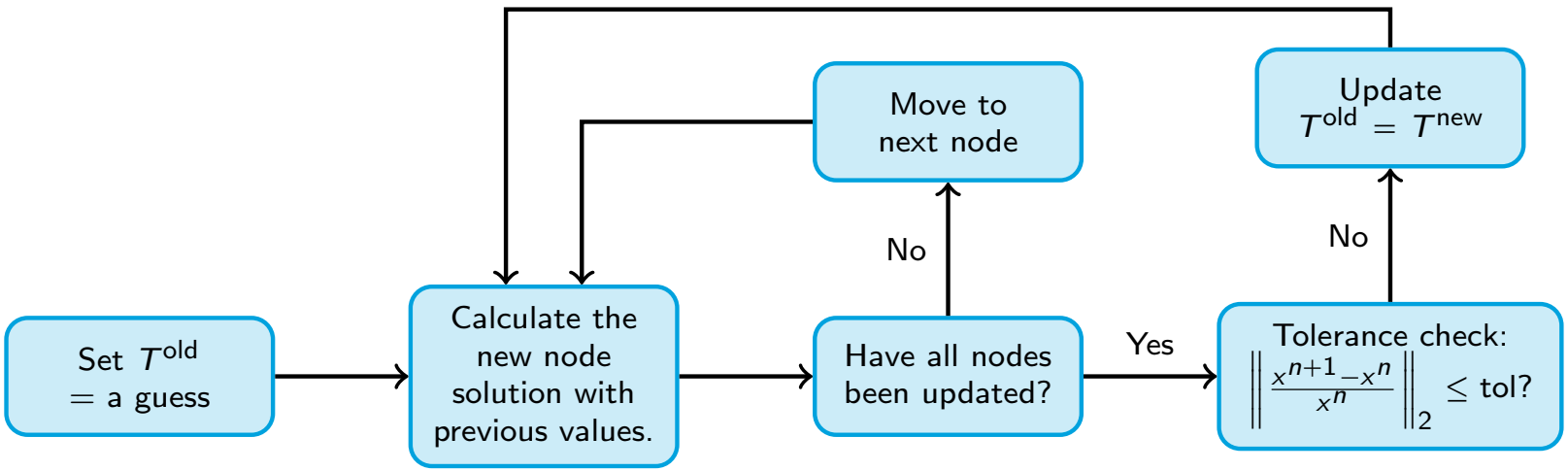

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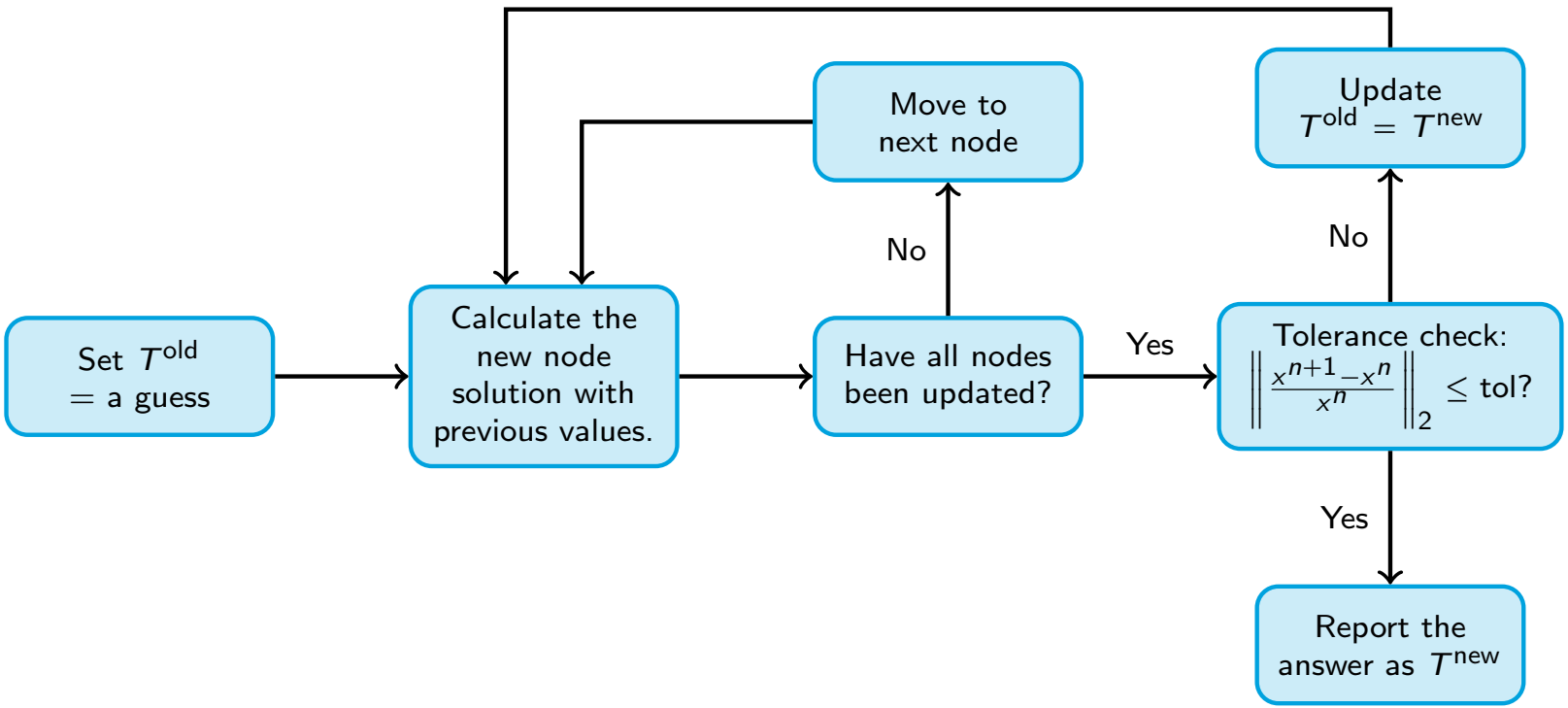

The core of the solver

The full file is on Canvas, `solveJacobi.m`.

```
  while ( xDiff > tol && it_jac < 1000 )
    x_old = x;
    for i=1:N
        s = 0;
        for j = 1:N
            if (j ~= i)
                s = s+A(i,j)*x_old(j);
            end
        end
        x(i) = (b(i)-s)/A(i,i);
    end
    it_jac = it_jac+1;
    xDiff = norm((x-x_old)./x,2);
end
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Try to call it from the `solveLaplaceEq.m` file, instead of using `\`.

A few details on this algorithm

- The while loop holds two aspects
  - A convergence criterion (`norm((x-x_old)./x,2)> tol`). Some considerations are:
    - L_1-norm (sum)
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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!

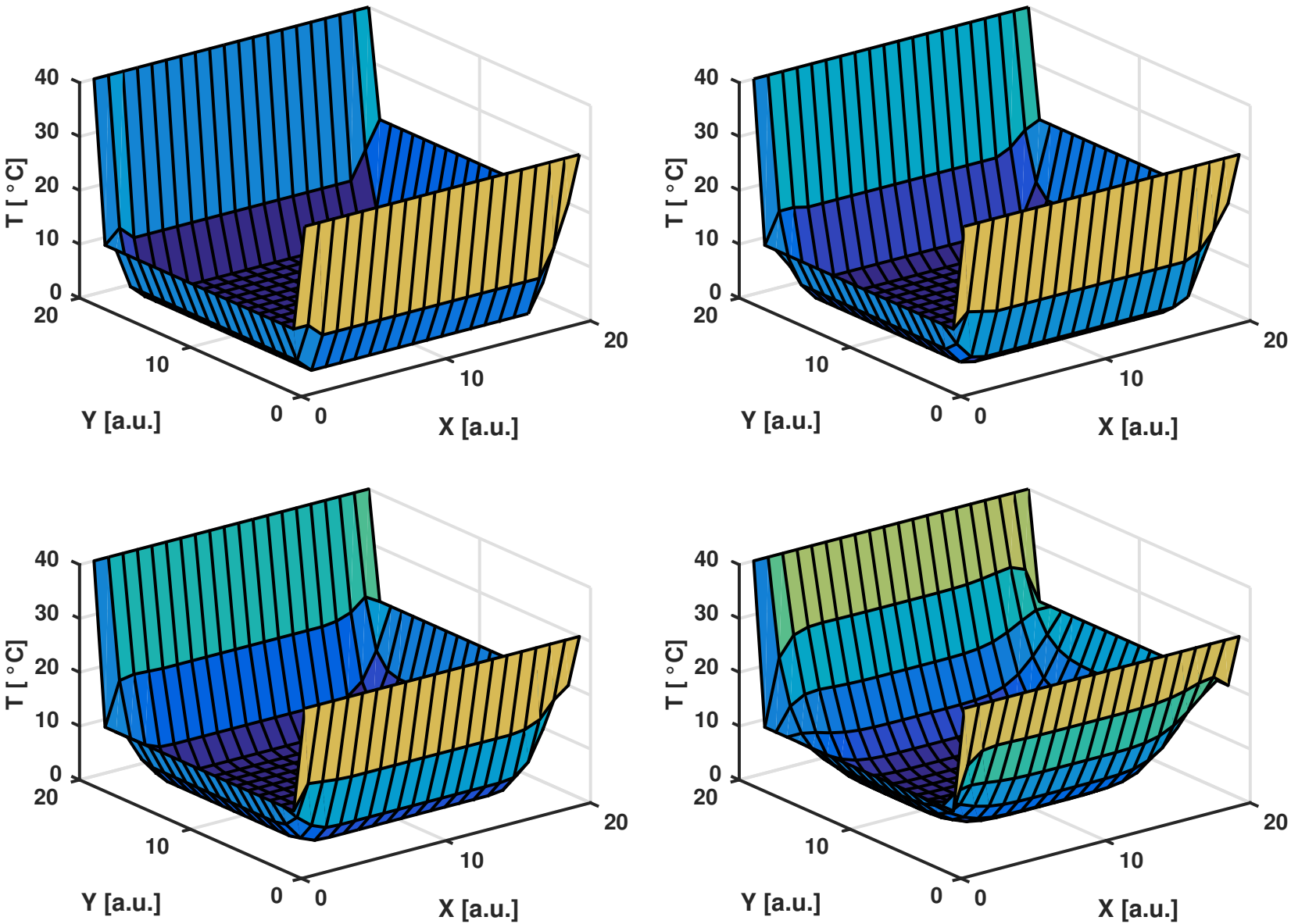
The solver using array indices

Make a copy of the Jacobian solver, and replace the for-loop by a vector-operation:

```
% While not converged or max_it not reached
while ( xDiff > tol && it_jac < 1000 )
  x_old = x;
  for i=1:N
    % Sum off-diagonal*x_old
    offDiagonalIndex = [1:(i-1) (i+1):N];
    Aij_Xj = A(i,offDiagonalIndex)*x_old(offDiagonalIndex);

    % Compute new x value
    x(i) = (b(i)-Aij_Xj)/A(i,i);
  end
  it_jac = it_jac+1;
  xDiff = norm((x-x_old)./x,2);
end
```

Iterations 1, 2, 3 and 10



Gauss-Seidel method

The Gauss-Seidel method is quite similar to Jacobi method

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  - Do not perform the update step `T=Tnew`
  - See `laplace_gaussseidel.m` 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:

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

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

Today's outline

Summary

- Partial differential equations can be written as sparse systems of linear equations
- Sparse systems can be handled with a direct method like Gaussian elimination
- 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 may be attractive.
- The Jacobi method was introduced. Many other methods are based on the Jacobi method (SOR method, for example)