Modeling Document

- **Governing Equations**

$$\begin{aligned} -k\nabla^2 T(x,y) &= q(x,y) \text{ in } \Omega \\ T(x,y) &= T_{masa}(x,y) \text{ on } \partial\Omega \end{aligned} \tag{1}$$

where,

Ω is a 2D bounded domain
$\partial\Omega$ is the boundary of the domain
T is the material's temperature field
q is the heat source term
k is the thermal conductivity

We have the Dirichlet boundary conditions.

- **Assumptions**
  - The thermal conductivity is assumed to be constant.
  - We assume a square domain $\Omega = \{ (x,y) : x \in [0,L], y \in [0,L] \}$ for the 2D case. For 1D, it will obviously be a line $\Omega = \{ (x,y) : x \in [0,L] \}$
  - Dirichlet boundary condition is assumed at the boundaries
  - For the fourth order scheme, we assume that the values at the points adjacent to the boundary points are known from the `MASA` solution. This is to reduce the cumbersome effort required to come up with different schemes at the boundary.
  - For the 2D case we assume symmetrical discretization i.e. the number of grid points in both directions are the same and $\Delta x = \Delta y = h$.

- **Nomenclature for discretization** Our numerical methods are all node based (as will be reiterated later).
  - 1D We have $(N+1)$ points $\{x_0, x_1, x_2, \dots x_N\}$ in the x-direction with $x_i = i\Delta x$, where $\Delta x = L/N$
  - 2D We have $(N+1)$ points $\{x_0, x_1, x_2, \dots x_N\}$ in the x-direction with $x_i = i\Delta x$, where $\Delta x = L/N = h$ and $(N+1)$ points $\{y_0, y_1, y_2, \dots y_N\}$ in the y-direction with $y_j = j\Delta y$, where $\Delta y = L/N = h$. Hence, we have a $(N+1) \times (N+1)$ grid.
  - i is always associated with the indexing in x-direction and j is always associated with the indexing in y-direction.

- $T(x_i, y_j)$ is given the shorthand notation $T(i, j)$ and $q(x_i, y_j)$ is given the shorthand notation $q(i, j)$
- The composite index for 2D grid is given by $k = i + (N + 1)j$.

- **Numerical Method**

  Our numerical methods are all node based (as will be reiterated later).

  - **2^{nd} order finite difference approximation**

    Definition

    $$\frac{\partial^2 T}{\partial x^2} \approx \frac{T(x + \Delta x) - 2T(x) + T(x - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

    Discretized heat equation

    1. 1D

    $$\begin{cases} -k\left(\frac{T(i+1)-2T(i)+T(i-1)}{\Delta x^2}\right) + \mathcal{O}(\Delta x^2) = q(i), \;\; i \in \{1, 2, 3, \ldots, N-1\} \\ T(0) = T_{masa}(0) \;\text{ and }\; T(N) = T_{masa}(L) \end{cases} \tag{2}$$

    2. 2D

    $$\begin{cases} -k\left(\frac{T(i+1,j)-2T(i,j)+T(i-1,j)}{h^2}\right) - k\left(\frac{T(i,j+1)-2T(i,j)+T(i,j-1)}{h^2}\right) \\ +\mathcal{O}(h^2) = q(i,j), \;\; i \in \{1, 2, 3, \ldots, N-1\} \;\; j \in \{1, 2, 3, \ldots, N-1\} \\ \\ T(i,j) = T_{masa}(x_i, y_j) \;\text{ for }\; i \in \{0, N\},\; j \in \{0, 1, 2, \ldots, N\} \\ T(i,j) = T_{masa}(x_i, y_j) \;\text{ for }\; i \in \{0, 1, 2, \ldots, N\},\; j \in \{0, N\} \end{cases} \tag{3}$$

  - **4^{th} order finite difference approximation**

    Definition

    $$\frac{\partial^2 T}{\partial x^2} \approx \frac{-T(x - 2\Delta x) + 16T(x - \Delta x) - 30T(x) + 16T(x + \Delta x) - T(x + 2\Delta x)}{12\Delta x^2} + \mathcal{O}(\Delta x^4)$$

    Discretized heat equation

    We have Dirichlet boundary conditions at both the boundary points and adjacent to boundary points.

    1. 1D

    $$\begin{cases} -k\left(\frac{-T(i-2)+16T(i-1)-30T(i)+16T(i+1)-T(i+2)}{12\Delta x^2}\right) + \mathcal{O}(\Delta x^4) = q(i), \;\; i \in \{2, 3, \ldots, N-2\} \\ T(i) = T_{masa}(x_i), \;\; i \in \{0, 1, N-1, N\} \end{cases} \tag{4}$$

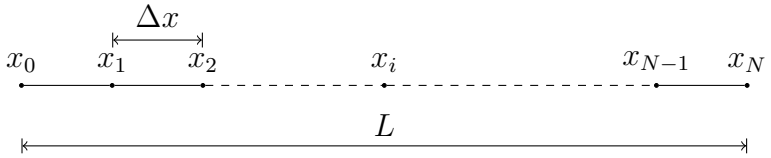
2. 2D

$$\begin{cases} -k\left(\frac{-T(i-2,j)+16T(i-1,j)-30T(i,j)+16T(i+1,j)-T(i+2,j)}{12h^2}\right) \\ -k\left(\frac{-T(i,j-2)+16T(i,j-1)-30T(i,j)+16T(i,j+1)-T(i,j+2)}{12h^2}\right) + \mathcal{O}(h^4) = q(i,j), \\ \quad i \in \{2,\ldots,N-2\}, j \in \{2,\ldots,N-2\} \\ \\ T(i,j) = T_{masa}(x_i,y_j) \text{ for } i \in \{0,1,N-1,N\},\ j \in \{0,1,2,\ldots,N\} \\ T(i,j) = T_{masa}(x_i,y_j) \text{ for } i \in \{0,1,2,\ldots,N\},\ j \in \{0,1,N-1,N\} \end{cases} \tag{5}$$

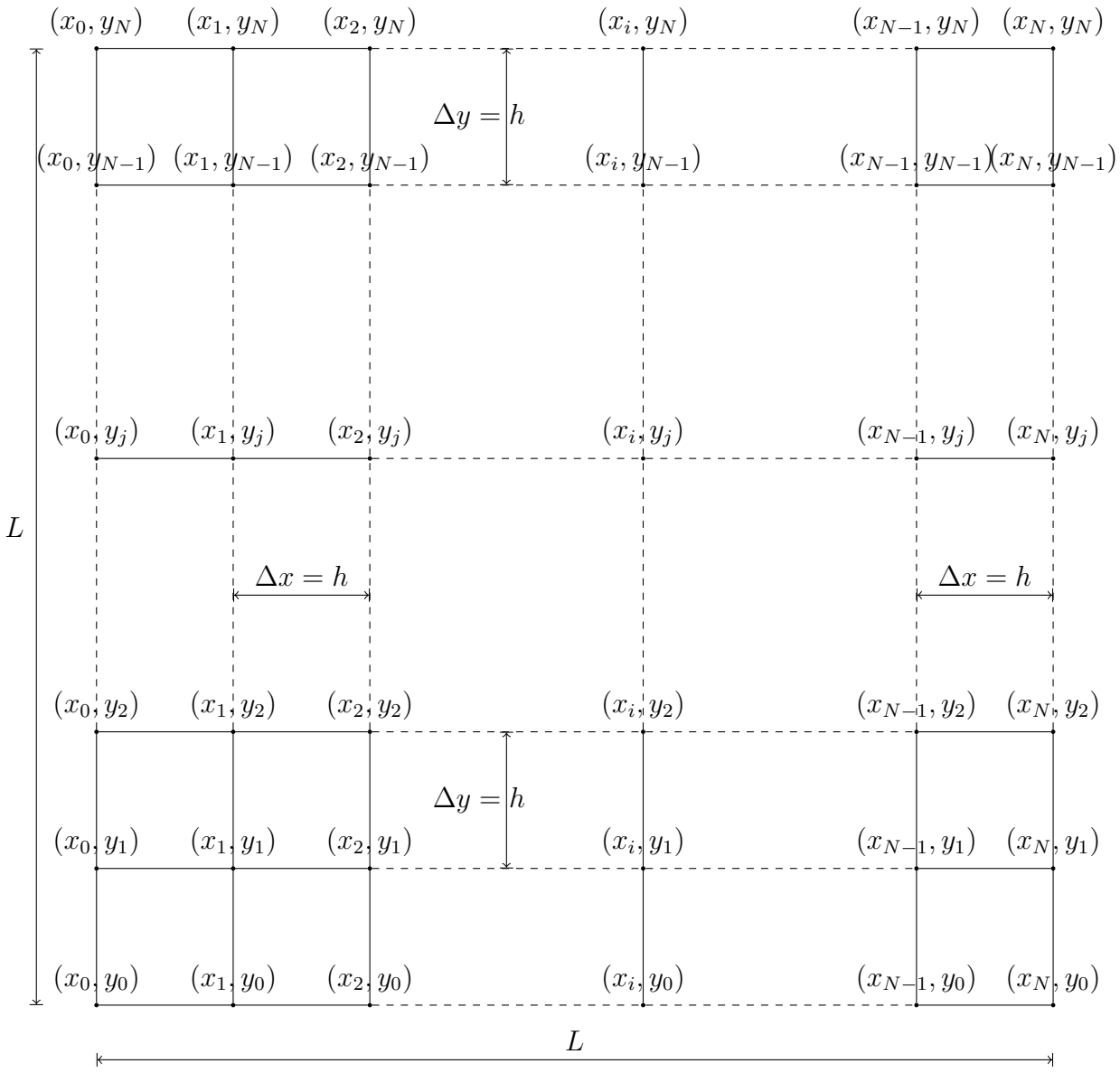
- **Mesh diagrams**

  Our schemes are node based.

  1. 1D



  2. 2D



- **Linear system of Equations**
  - **2nd order finite difference approximation**
    1. 1D
       We first define the following vectors

$$\mathbf{q} = \left[T_{masa}(0), \frac{\Delta x^2}{k} q(1), \ldots, \frac{\Delta x^2}{k} q(N-1), T_{masa}(L)\right]^T$$
$$\mathbf{T} = [T(0), \ldots, T(N)]^T$$

We now define a $(N+1) \times (N+1)$ tridiagonal matrix $\mathbf{A}$ such that,

$$\mathbf{A} = \begin{bmatrix} 1 & & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & & 1 \end{bmatrix}$$

Now (**??**) can be written as,

$$\mathbf{AT} = \mathbf{q}$$

The first and last rows are different because they account for boundary conditions. The sparsity pattern of A can be given by,

$$\mathbf{A} = \begin{bmatrix} \times & & & & & & \\ \times & \times & \times & & & & \\ & \times & \times & \times & & & \\ & & \times & \times & \times & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & \times & \times & \times \\ & & & & & \times & \times & \times \\ & & & & & & & \times \end{bmatrix}$$

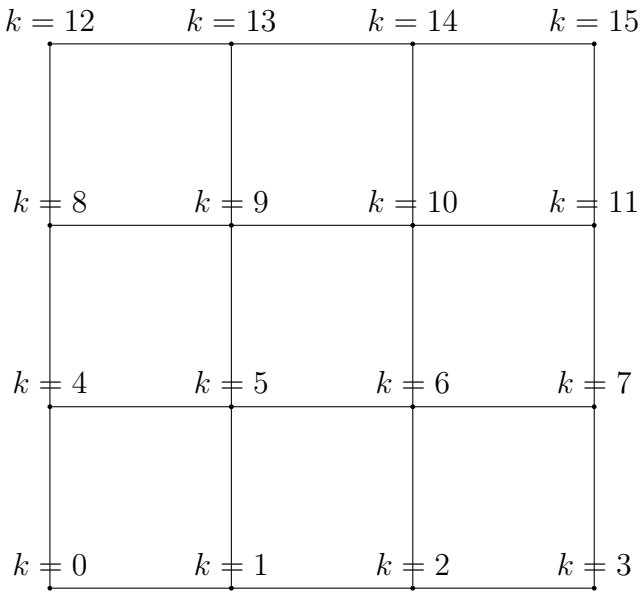
`Number of non-zero elements on an interior row of the matrix =` 3

2. 2D

The elements will be numbered in the following fashion

$$k = i + (N+1)j,\ i \in [0, \ldots, N],\ j \in [0, \ldots, N]$$

Here is an illustration for a 4×4 grid i.e. $N = 3$,



So we can imagine how the matrix is going to look: the terms of second derivative in x-direction will be adjacent to each other, but they terms of the second derivative in y-direction will be offset by N points. This will become clear in the visual representation below. We first define the following $(N+1)^2 \times 1$ vectors

$$\mathbf{q}(k) = \begin{cases} \frac{h^2}{k} q(i,j) \text{ if } i \in \{1,2,\ldots,N-1\},\ j \in \{1,2,\ldots,J-1\} \\ T_{masa}(x_i, y_j) \text{ otherwise i.e. at boundaries} \end{cases}$$

$$\mathbf{T} = [T(0), T(1), \ldots, T((N+1)^2)]^T$$

We now define $(N+1)^2 \times (N+1)^2$ matrices $\mathbf{A_x}$ (interior x-direction derivatives), $\mathbf{A_y}$ (interior y-direction derivatives) and $\mathbf{A_b}$ (dirichlet nodes) such that,

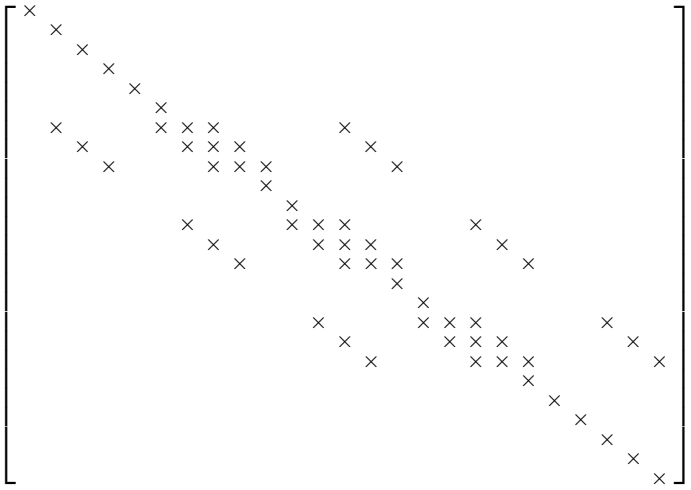
$$\mathbf{A_x} = \begin{cases} \mathbf{A_x}(i,i) = \begin{cases} 2 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i-1) = \begin{cases} -1 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i+1) = \begin{cases} -1 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

$$\mathbf{A_y} = \begin{cases} \mathbf{A_y}(j,j) = \begin{cases} 2 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j-N) = \begin{cases} -1 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j+N) = \begin{cases} -1 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

$$\mathbf{A_b} = \begin{cases} \mathbf{A_b}(i,i) = \begin{cases} 1 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

Now, the net matrix is $\mathbf{A} = \mathbf{A_x} + \mathbf{A_y} + \mathbf{A_b}$. The sparsity pattern of $\mathbf{A}$ is given by, (illustration for a 5×5 grid)

$\mathbf{A} =$



`Number of non-zero elements on an interior row of the matrix =` 5.

The repeating interior block of $\mathbf{A}$ is given by,

$$\mathbf{A} = \begin{bmatrix} & & & & 1 & & & & \\ -1 & \dots & -1 & 4 & -1 & \dots & -1 & & \\ & -1 & \dots & -1 & 4 & -1 & \dots & -1 & \\ & & -1 & \dots & -1 & 4 & -1 & \dots & -1 \\ & & & & & & 1 & & \end{bmatrix}$$

Now (**??**) can be written as,

$$\mathbf{AT} = \mathbf{q}$$

– **4^{th} order finite difference approximation**

1. 1D
   We first define the following vectors

$$\mathbf{q} = \left[T_{masa}(0), T_{masa}(x_1), \frac{12\Delta x^2}{k} q(3) \ldots, \frac{12\Delta x^2}{k} q(N-2), T_{masa}(x_{N-1}), T_{masa}(L)\right]^T$$

$$\mathbf{T} = [T(0), \ldots, T(N)]^T$$

   We now define a $(N+1) \times (N+1)$ pentadiagonal matrix $\mathbf{A}$ such that (blank elements are 0),

$$\mathbf{A} = \begin{bmatrix}
1 & & & & & & & & & \\
 & 1 & & & & & & & & \\
1 & -16 & 30 & -16 & 1 & & & & & \\
 & 1 & -16 & 30 & -16 & 1 & & & & \\
 & & 1 & -16 & 30 & -16 & 1 & & & \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & & 1 & -16 & 30 & -16 & 1 & \\
 & & & & & 1 & -16 & 30 & -16 & 1 \\
 & & & & & & & & 1 & \\
 & & & & & & & & & 1
\end{bmatrix}$$

   Now (**??**) can be written as,

$$\mathbf{AT} = \mathbf{q}$$

   Note that the first and last two rows in $\mathbf{A}$ looks different because we accounted for the Dirichlet conditions. The sparsity pattern of the matrix is given by,

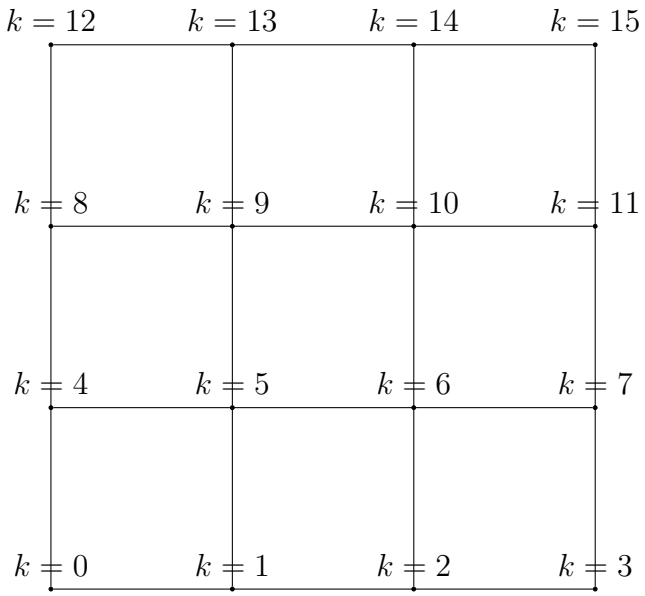
$$\mathbf{A} = \begin{bmatrix}
\times & & & & & & & & & \\
 & \times & & & & & & & & \\
\times & \times & \times & \times & \times & & & & & \\
 & \times & \times & \times & \times & \times & & & & \\
 & & \times & \times & \times & \times & \times & & & \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & & \times & \times & \times & \times & \times & \\
 & & & & & \times & \times & \times & \times & \times \\
 & & & & & & & & \times & \\
 & & & & & & & & & \times
\end{bmatrix}$$

   `Number of non-zero elements on an interior row of the matrix =` 5.

2. 2D The elements will be numbered in the following fashion

$$k = i + (N+1)j,\ i \in [0, \ldots, N],\ j \in [0, \ldots, N]$$

Here is an illustration for a 4×4 grid i.e. $N = 3$,



So we can imagine how the matrix is going to look: the terms of second derivative in x-direction will be adjacent to each other, but they terms of the second derivative in y-direction will be offset by N points. This will become clear in the visual representation below. We first define the following $(N+1)^2 \times 1$ vectors

$$\mathbf{q}(k) = \begin{cases} \frac{12h^2}{k} q(i,j) \text{ if } i \in \{1, 2, \ldots, N-1\},\ j \in \{1, 2, \ldots, N-1\} \\ T_{masa}(x_i, y_j) \text{ otherwise} \end{cases}$$

$$\mathbf{T} = [T(0), T(1), \ldots, T((N+1)^2)]^T$$

We now define $(N+1)^2 \times (N+1)^2$ matrices $\mathbf{A_x}$ (interior x-direction derivatives), $\mathbf{A_y}$ (interior y-direction derivatives) and $\mathbf{A_b}$ (boundary and close to boundary elements) such that,

$$\mathbf{A_x} = \begin{cases} \mathbf{A_x}(i,i) = \begin{cases} 30 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i-1) = \begin{cases} -16 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i+1) = \begin{cases} -16 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i+2) = \begin{cases} 1 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_x}(i,i-2) = \begin{cases} 1 & \text{if } i \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

$$\mathbf{A_y} = \begin{cases} \mathbf{A_y}(j,j) = \begin{cases} 30 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j-N) = \begin{cases} -16 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j+N) = \begin{cases} -16 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j+2N) = \begin{cases} 1 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \\ \mathbf{A_y}(j,j-2N) = \begin{cases} 1 & \text{if } j \text{ corresponds to an interior point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

$$\mathbf{A_b} = \begin{cases} \mathbf{A_b}(j,j) = \begin{cases} 1 & \text{if } j \text{ is a boundary point or an adjacent to boundary point} \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

Now, the net matrix is $\mathbf{A} = \mathbf{A_x} + \mathbf{A_y} + \mathbf{A_b}$. The sparsity pattern of $\mathbf{A}$ is given

by, (illustration for a 7×7 grid, which means the interior matrix is 3×3)

$$\mathbf{A} = \left[\begin{array}{ccccccccccccccccccccccccc}
 & & & & & & & \ddots & & & & & & & & & & & & & & & & & \\
 & & & & & & & \times & & & & & & & & & & & & & & & & & \\
 & & & & & & & & \times & & & & & & & & & & & & & & & & \\
 & & & & & & & & & \times & & & & & & & & & & & & & & & \\
 & & & & & & & & & & \times & & & & & & & & & & & & & & \\
\times & & & \times & & & & \times & \times & \times & \times & & & \times & & & & \times & & & & & & & \\
 & \times & & & \times & & & \times & \times & \times & \times & \times & & & \times & & & & \times & & & & & & \\
 & & \times & & & \times & & & \times & \times & \times & \times & \times & & & \times & & & & \times & & & & & \\
 & & & & & & & & & & \times & & & & & & & & & & & & & & \\
 & & & & & & & & & & & \times & & & & & & & & & & & & & \\
 & & & & & & & & & & & & \times & & & & & & & & & & & & \\
 & & & & & & & & & & & & \times & & & & & & & & & & & & \\
 & & & \times & & & & \times & & & \times & \times & \times & \times & & & & \times & & & & & \times & & \\
 & & \times & & & & \times & & & & \times & \times & \times & \times & \times & & & & \times & & & & & \times & & \\
 & & & \times & & & & \times & & & \times & \times & \times & \times & \times & & & & \times & & & & & & \times & \\
 & & & & & & & & & & & & & \times & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & \times & & & & & & & & & & \\
 & & & & & & & & & & & & & & & \times & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \times & & & & & & & & \\
 & & & & & & & \times & & & \times & & & \times & \times & \times & \times & \times & & & & \times & & \times & \\
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 & & & & & & & & & & & & & & & & & & & \times & & & & & \\
 & & & & & & & & & & & & & & & & & & & & \times & & & & \\
 & & & & & & & & & & & & & & & & & & & & & \ddots & & & \\
\end{array}\right]$$

`Number of non-zero elements on an interior row of the matrix =` 9.

The repeating interior block of $\mathbf{A}$ is given by,

$$\mathbf{A} = \left[\begin{array}{ccccccccccccccccccccc}
 & & & & & & 1 & & & & & & & & & & & & & & \\
 & & & & & & & & 1 & & & & & & & & & & & & \\
1 & \ldots & -16 & \ldots & 1 & -16 & 60 & -16 & 1 & \ldots & -16 & \ldots & 1 & & & & & & & & \\
 & 1 & \ldots & -16 & \ldots & 1 & -16 & 60 & -16 & 1 & \ldots & -16 & \ldots & 1 & & & & & & & \\
 & & 1 & \ldots & -16 & \ldots & 1 & -16 & 60 & -16 & 1 & \ldots & -16 & \ldots & 1 & & & & & & \\
 & & & & & & & & & & 1 & & & & & & & & & & \\
 & & & & & & & & & & & & 1 & & & & & & & & \\
\end{array}\right]$$

Now (**??**) can be written as,

$$\mathbf{AT} = \mathbf{q}$$

- **Iterative solvers**

  Here is the pseudo-code for dense matrix solvers (the actual implementation might be for sparse matrices or not, this is not decided yet).

  1. **Jacobi**

```
subroutine jacobi (A,q, TOL, max_iter)
!!! Find T = inv(A)*q using Jacobi iteration

K = size(q)
iters = 0 !!! Number of iterations
error = 0 !!! Compare to tolerance
T(1:K) = 0 !!! Initialize entire T array to zero

do while (iters <= max_iter)

    T_old(:) = T(:)

    do i = 1,...,K
```

```
                !!! We use only the old values and none of the ↩
                    updated values for the update.

                T(i) =  1/A(i,i) * (q(i)-Σ_{j≠i}^{K} A(i,j)T_old(j))
            end do

            error = ||T_old−T|| / ||T||

            iters = iters + 1

            if (error <= TOL)
                break
            end if


        end do

        return T
        end subroutine
```

2. **Gauss-Seidel**

```
        subroutine gauss_seidel (A,q, TOL, max_iter)
        !!! Find T = inv(A)*q using Gauss Seidel iteration

        K = size(q)
        iters = 0 !!! Number of iterations
        error = 0 !!! Compare to tolerance
        T(1:K) = 0 !!! Initialize entire T array to zero

        do while (iters <= max_iter)

            T_old(:) = T(:)

            do i = 1,...,K
                !!! T_old is not used at all, we use older values↩
                    for >i and new values for <i.

                T(i) =  1/A(i,i) * (q(i)-Σ_{j≠i}^{K} A(i,j)T(j))
            end do

            error = ||T_old−T|| / ||T||
            iters = iters + 1
            if (error <= TOL)
                break
            end if



        end do

        return T
        end subroutine
```

- **Estimate of memory requirements**

  We assume that our matrices are stored as normal, dense matrices (assuming that our iterative solvers have generic, dense implementations).

  - Second order approximation

    * 1D

Variable	Dimension	Memory
T	N+1	$8\times$(N+1)
q	N+1	$8\times$(N+1)
A	(N+1)$\times$(N+1)	$8\times$(N+1)^2
N	1	4
L	1	8
Δx	1	8
k	1	8
	Total	8(N+2)^2+20

    * 2D

Variable	Dimension	Memory
T	(N+1)(N+1)	$8\times$(N+1)^2
q	(N+1)(N+1)	$8\times$(N+1)^2
A	(N+1)(N+1)$\times$(N+1)(N+1)	$8\times$(N+1)^4
N	1	4
L	1	8
Δx	1	8
Δy	1	8
k	1	8
	Total	8(N+1)^4+16(N+1)^2+36

  - Fourth order approximation

    * 1D

Variable	Dimension	Memory
T	N+1	$8\times$(N+1)
q	N+1	$8\times$(N+1)
A	(N+1)$\times$(N+1)	$8\times(N+1)^2$
N	1	4
L	1	8
Δx	1	8
k	1	8
	Total	$8(N+2)^2+20$

$*$ 2D

Variable	Dimension	Memory
T	(N+1)(N+1)	$8\times(N+1)^2$
q	(N+1)(N+1)	$8\times(N+1)^2$
A	(N+1)(N+1)$\times$(N+1)(N+1)	$8\times(N+1)^4$
N	1	4
L	1	8
Δx	1	8
Δy	1	8
k	1	8
	Total	$8(N+1)^4+16(N+1)^2+36$