NUMERICAL MODELING OF STEADY TEMPERATURE FIELDS

Modern designs of energy machinery are characterised by the pursuit of high efficiency and high power density. Parts of these machines are often exposed to high temperatures and significant thermal stresses. Therefore, great attention is paid to methods for accurately calculating temperature fields in components with complex shapes, under given boundary conditions. Among the methods for solving heat conduction equations, numerical methods, including the finite difference method, are of decisive importance. Analytical methods fail when dealing with the complex shapes of modern machines and can only serve to verify the accuracy of solutions obtained by other methods.

1. Finite Difference Method (FDM)

The finite difference method involves approximating derivatives with difference quotients. To derive difference formulas for the derivatives $\frac{\partial T}{\partial x}$ and $\frac{\partial T}{\partial y}$, the function $T(x,y)$ is expanded in a Taylor series around the point $x_{i,j}$. From the expansion, it follows that for the derivative $\frac{\partial T}{\partial x}$, the series takes the form:

$$T_{i+1,j} = T_{i,j} + \left(\frac{\partial T}{\partial x}\right)_{i,j} \cdot \Delta x + \left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \cdot \frac{(\Delta x)^2}{2} + \left(\frac{\partial^3 T}{\partial x^3}\right)_{i,j} \cdot \frac{(\Delta x)^3}{6} + \cdots \tag{1}$$

After rearranging expression (1), the derivative $\frac{\partial T}{\partial x}$ can be represented as a difference quotient:

$$\left(\frac{\partial T}{\partial x}\right)_{i,j} = \frac{T_{i+1,j} - T_{i,j}}{\Delta x} - \left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \cdot \frac{(\Delta x)}{2} - \left(\frac{\partial^3 T}{\partial x^3}\right)_{i,j} \cdot \frac{(\Delta x)^2}{6} + \cdots \approx \frac{T_{i+1,j} - T_{i,j}}{\Delta x} \tag{2}$$

A similar approach applies for the derivative $\frac{\partial T}{\partial y}$:

$$\left(\frac{\partial T}{\partial y}\right)_{i,j} = \frac{T_{i,j+1} - T_{i,j}}{\Delta y} - \left(\frac{\partial^2 T}{\partial y^2}\right)_{i,j} \cdot \frac{(\Delta y)}{2} - \left(\frac{\partial^3 T}{\partial y^3}\right)_{i,j} \cdot \frac{(\Delta y)^2}{6} + \cdots \approx \frac{T_{i,j+1} - T_{i,j}}{\Delta y} \tag{3}$$

For the case of steady heat conduction in a body with a constant thermal conductivity coefficient and no internal heat sources, the heat conduction equation takes the form of Laplace's differential equation:

$$\nabla^2 T = \Delta T = 0 \tag{4}$$

which, for a two-dimensional case, becomes:

$$\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)_{i,j} = 0 \tag{5}$$

For the area shown in Fig. 1, the first derivatives for the point with indices (i,j) take the form (6):

$$\begin{cases} \left(\frac{\partial T}{\partial x}\right)_{i,j} \approx \frac{T_{i+1,j} - T_{i,j}}{\triangle x} \\ \left(\frac{\partial T}{\partial x}\right)_{i-1,j} \approx \frac{T_{i,j} - T_{i-1,j}}{\triangle x} \\ \left(\frac{\partial T}{\partial y}\right)_{i,j} \approx \frac{T_{i,j+1} - T_{i,j}}{\triangle y} \\ \left(\frac{\partial T}{\partial y}\right)_{i,j-1} \approx \frac{T_{i,j} - T_{i,j-1}}{\triangle y} \end{cases} \tag{6}$$

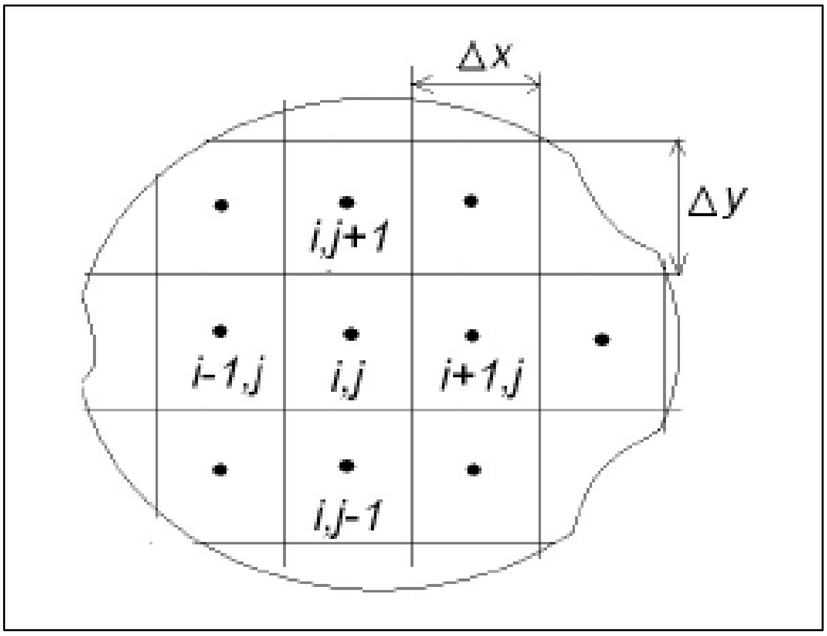


Fig. 1. Example of the discretization area using the finite difference method.

Based on the difference quotients of the first derivatives, the difference quotients of the second derivatives for the point with indices (i,j) were determined:

$$\begin{cases} \left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \approx \frac{\left(\frac{\partial T}{\partial x}\right)_{i,j} - \left(\frac{\partial T}{\partial x}\right)_{i-1,j}}{\Delta x} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} \\ \left(\frac{\partial^2 T}{\partial y^2}\right)_{i,j} \approx \frac{\left(\frac{\partial T}{\partial y}\right)_{i,j} - \left(\frac{\partial T}{\partial y}\right)_{i-1,j}}{\Delta y} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} \end{cases} \tag{7}$$

By substituting the difference quotients (7) into expression (5), the following relationships were obtained:

$$\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)_{i,j} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta x)^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta y)^2} = 0 \tag{8}$$

If $\Delta x = \Delta y$, then:

$$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0 \tag{9}$$

From expression (9), it follows that the temperature for the point $T_{i,j}$ is the arithmetic mean (10):

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4} \tag{10}$$

1.1. Example application of the Finite Difference Method (FDM)

Calculate the temperature distribution field in a square plate with a side length of π, heated from one side. The view of the plate is shown in Fig. 2a.

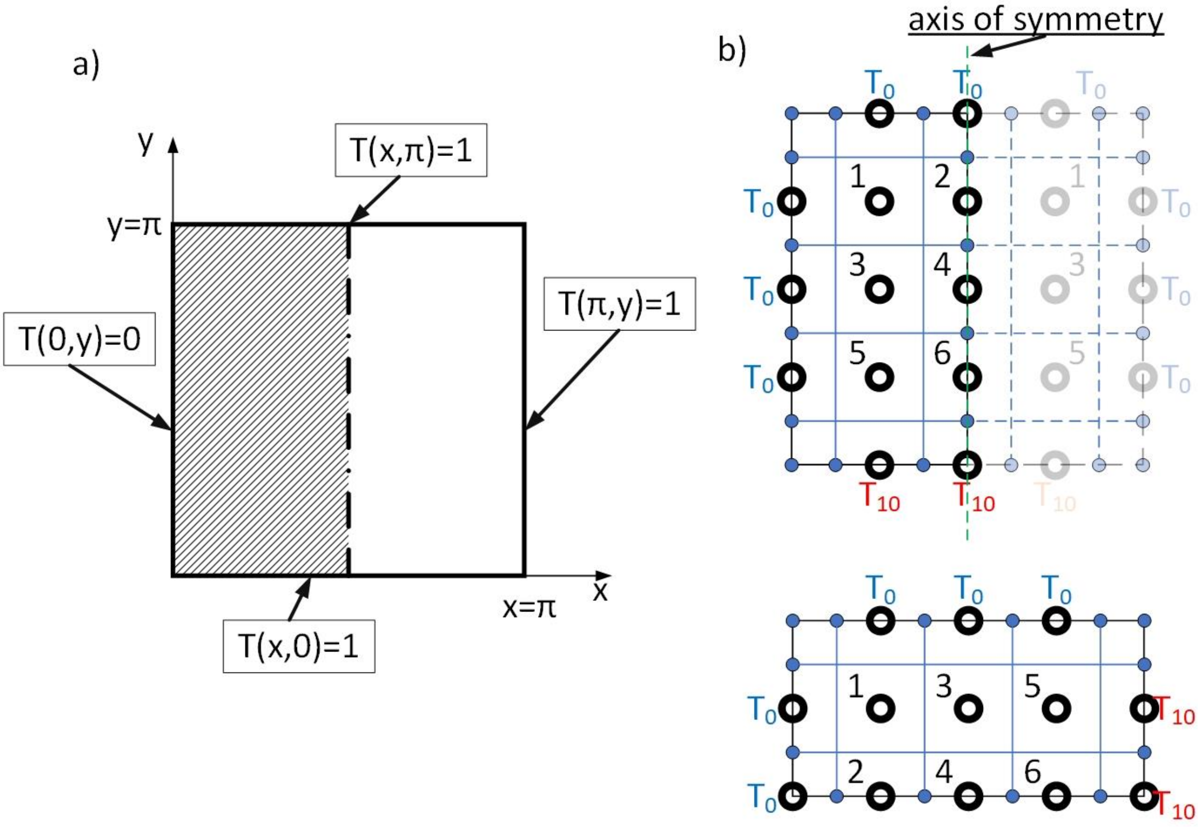


Fig. 2. a) Square plate heated along one side, b) discretization of half of the square area and node numbering with a discretization step of $\pi/4$

The following first-type boundary conditions (BC) on the plate's perimeter were assumed:

$$\begin{cases} T(0,y) = T(\pi,y) = 0 \; dla \; 0 < y < \pi \\ T(x,0) = 1 \; dla \; 0 < x < \pi \\ T(x,\pi) = 0 \; dla \; 0 < x < \pi \end{cases} \tag{11}$$

Figure 2b shows the discretised area for calculations. Due to the symmetric nature of the considered case, only half of the square plate's area is discretised. The symmetry axis of the plate passes through nodes 2, 4, and 6. The discretization was carried out so that some nodes are exactly on the boundary of the area. In nodes marked as T_0 and T_{10}, values consistent with the boundary conditions were assumed: $T_0 = 0$ and $T_{10} = 1$.

For node 1, according to the grid shown in Fig. 2b and equation (9), we have:

$$T_3 + T_0 + T_2 + T_0 - 4T_1 = 0 \tag{12}$$

where $T_{i+1,j} = T_3, T_{i-1,j} = T_0, T_{i,j+1} = T_2, T_{i,j-1} = T_0$

Thus, the temperature at node 1 will be:

$$T_1 = \frac{T_3 + T_0 + T_2 + T_0}{4} \tag{13}$$

By rearranging the terms in expression (12) and adding temperatures for nodes 4, 5, 6 with zero coefficients, the following equation is obtained:

$$-4T_1 + T_2 + T_3 + 0T_4 + 0T_5 + 0T_6 = -2T_0 \tag{14}$$

Repeating the above operations for the remaining nodes (from 2 to 6), a system of linear equations was obtained:

$$\begin{cases} -4T_1 + T_2 + T_3 + 0 + 0 + 0 = -2T_0 \\ 2T_1 - 4T_2 + 0 + T_4 + 0 + 0 = -T_0 \\ T_1 + 0 - 4T_3 + T_4 + T_5 + 0 = -T_0 \\ 0 + T_2 + 2T_3 - 4T_4 + 0 + T_6 = 0 \\ 0 + 0 + T_3 + 0 - 4T_5 + T_6 = -(T_0 + T_{10}) \\ 0 + 0 + 0 + T_4 + 2T_5 - 4T_6 = -T_{10} \end{cases} \tag{15}$$

This can be written using the following matrices:

$$A = \begin{bmatrix} -4 & 1 & 1 & 0 & 0 & 0 \\ 2 & -4 & 0 & 1 & 0 & 0 \\ 1 & 0 & -4 & 1 & 1 & 0 \\ 0 & 1 & 2 & -4 & 0 & 1 \\ 0 & 0 & 1 & 0 & -4 & 1 \\ 0 & 0 & 0 & 1 & 2 & -4 \end{bmatrix}, \quad T = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ -1 \end{bmatrix} \tag{16}$$

where: *A* is the coefficient matrix, *T* is the temperature vector, and *B* is the free-term vector.

The system of linear equations in matrix form is given by:

$$A \cdot T = B \tag{17}$$

The solution of the presented system of equations was carried out using the inverse matrix and iterative methods. Applying the inverse matrix to matrix *A* provides the relationship:

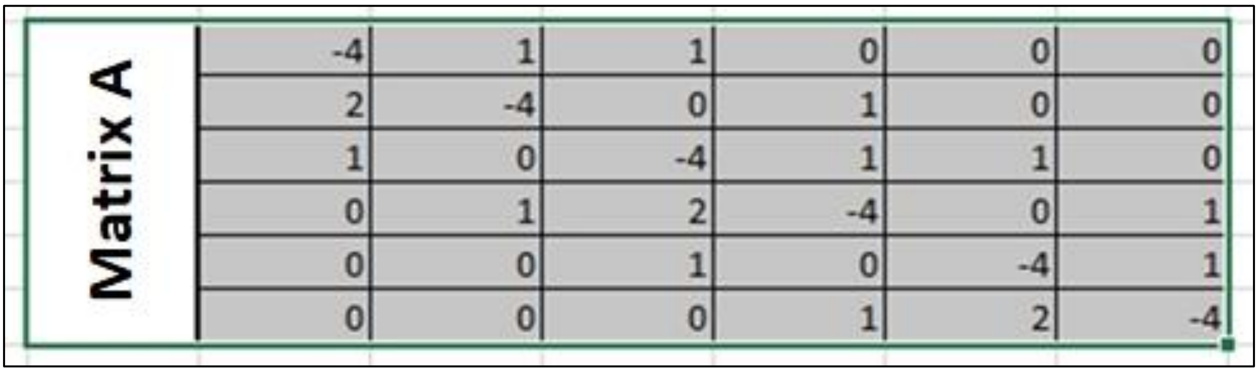
$$T = A^{-1} \cdot B \tag{18}$$

This system of equations can be solved using a spreadsheet such as Excel or a computational package such as Matlab. The following is a guide on how to perform the calculations using the inverse matrix in Excel.

1.2.1.2. Calculations of the system of Equations Using Excel.

NOTE!!!: The outlined procedure applies to Excel 2010. In newer versions, the commands for matrix operations may differ.

Step 1: Create matrix *A* containing the coefficients of the equations. Figure 3 shows an example of the coefficient matrix *A*.



Matrix A	-4	1	1	0	0	0
	2	-4	0	1	0	0
	1	0	-4	1	1	0
	0	1	2	-4	0	1
	0	0	1	0	-4	1
	0	0	0	1	2	-4

Fig. 3. Coefficient matrix *A* of the linear equations

Step 2: Create vector *B* containing the free terms. Figure 4 shows an example of the free-term vector *B*.

Matrix B	0
	0
	0
	0
	-1
	-1

Fig. 4. Vector *B* containing the free terms

Step 3: Select the area where the values of the inverse matrix A^{-1} will be displayed. Press the key combination Ctrl+Shift+F2, then, after the "=" sign, enter the formula `MINVERSE(array)`(MACIERZ.ODW(*tablica*) in Polish), using the cell range containing the values of matrix *A* as the argument. Confirm the formula by pressing Ctrl+Shift+Enter. Figure 5 shows an example of calculating the inverse matrix A^{-1}. Figure 6 shows the result of the calculation for the example inverse matrix A^{-1}.

Inverse Matrix A^{-1}	=MACIERZ.ODW(C6:H11)					

Fig. 5. Calculation of the inverse matrix A^{-1}

Inverse Matrix A^{-1}	-0,330357	-0,09821	-0,125	-0,0625	-0,04464	-0,02679
	-0,196429	-0,33036	-0,125	-0,125	-0,05357	-0,04464
	-0,125	-0,0625	-0,375	-0,125	-0,125	-0,0625
	-0,125	-0,125	-0,25	-0,375	-0,125	-0,125
	-0,044643	-0,02679	-0,125	-0,0625	-0,33036	-0,09821
	-0,053571	-0,04464	-0,125	-0,125	-0,19643	-0,33036

Fig. 6. Inverse matrix A^{-1}

Step 4: Select the area where the values of the temperature vector *T* will be displayed. Press the key combination Ctrl+Shift+F2, then, after the "=" sign, enter the formula `MMULT(array1, array2)`(MACIERZ.ILOCZYN(*tablica1*;*tablica2*) in Polish), substituting the cell range containing the values of the inverse matrix A^{-1} for `array1` and the cell range containing the values of vector *B* for `array2`. Confirm the formula by pressing Ctrl+Shift+Enter. Figure 7 shows an example of calculating the temperature vector *T*. Figure 8 shows the result of the calculation of the temperature vector *T*.

Matrix T	=MACIERZ.ILOCZYN(K6:P11;C14:C19)	
		T_2
		T_3
		T_4
		T_5
		T_6

Fig. 7. Calculation of the temperature vector *T*

Matrix T	0,0714286	T_1
	0,0982143	T_2
	0,1875	T_3
	0,25	T_4
	0,4285714	T_5
	0,5267857	T_6

Fig. 8. Temperature vector *T*

2. Methods of Successive Approximation, Successive Over-Relaxation

The methods of successive approximation use relationship (10) to calculate the temperature values at the nodes of the given case. The initial temperature distribution was assumed as shown in Fig. 9.

	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,6000	0,6000	0,6000	0
0	0,8000	0,8000	0,8000	0
	1	1	1	

Fig. 9. Assumed temperature distribution

Then the values in the individual nodes (cells) were calculated based on relationship (10), each time substituting the new value in the selected node. The order of the calculations in the first approximation is shown in Fig. 10.

a	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,6000	0,6000	0,6000	0
0	0,6000	0,8000	0,8000	0
	1	1	1	

b	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,6000	0,6000	0,6000	0
0	0,6000	0,7500	0,8000	0
	1	1	1	

c	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,6000	0,6000	0,6000	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

d	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,4000	0,6000	0,6000	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

e	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,4000	0,5375	0,6000	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

f	0	0	0	
0	0,4000	0,4000	0,4000	0
0	0,4000	0,5375	0,3813	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

g	0	0	0	
0	0,2000	0,4000	0,4000	0
0	0,4000	0,5375	0,3813	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

h	0	0	0	
0	0,2000	0,2844	0,4000	0
0	0,4000	0,5375	0,3813	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

i	0	0	0	
0	0,2000	0,2844	0,1664	0
0	0,4000	0,5375	0,3813	0
0	0,6000	0,7500	0,5875	0
	1	1	1	

Fig. 10. Order of the calculations in the first approximation

The figure above presents only the first approximation. To ensure that the results for the iterative method are close to those obtained using the inverse matrix, the calculations had to be repeated about 15 times. Figure 11 shows the calculation results.

	0	0	0	
0	0,0714	0,0982	0,0714	0
0	0,1875	0,2500	0,1875	0
0	0,4286	0,5268	0,4286	0
	1	1	1	

Fig. 11. Results of the calculations using the successive approximation for the considered case

To obtain a solution more quickly, the method of successive approximation is modified by introducing a relaxation factor. If the relaxation factor ω falls within the range $(1; 2)$, the method is then called successive over-relaxation. The relaxation factor is introduced into expression (10) as follows:

$$T_{i,j}^{(n+1)} = (1-\omega) \cdot T_{i,j}^{(n)} + \frac{\omega \cdot \left(T_{i+1,j}^{(n)} + T_{i-1,j}^{(n)} + T_{i,j+1}^{(n)} + T_{i,j-1}^{(n)}\right)}{4} \tag{20}$$

3. Primary Sources of Errors in Numerical Calculations and Concepts Related to Errors

Problems solved using numerical methods are generally subject to some errors. The following types of error can be distinguished:

- Method errors - These are associated with the formulation of the mathematical problem itself, which rarely describes real phenomena, but rather represents an idealized model.
- Truncation errors - These occur due to the necessity of terminating calculations at a certain term of a sequence or the sum of a series that is used in numerical computations.
- Rounding errors - These arise from rounding numbers, which involves discarding all digits starting from a certain place.
- Initial errors - These occur due to the presence of numerical parameters in mathematical formulas, whose values can only be determined approximately, such as physical constants.
- Arithmetic Operation Errors – These are related to performing arithmetic operations on approximate numbers. As a result of arithmetic operations on approximate numbers, initial data errors are carried over into the calculations.

The absolute error Δ of an approximate number a is defined as the absolute value of the difference between the exact number *A* and the approximate number a:

$$\Delta = |A - a| \tag{21}$$

The relative error δ of an approximate number *a* is defined as the ratio of the absolute error Δ of that number to the absolute value of the exact number *A* ($A \neq 0$):

$$\delta = \frac{\Delta}{|A|} \tag{22}$$

4. Exercise Procedure

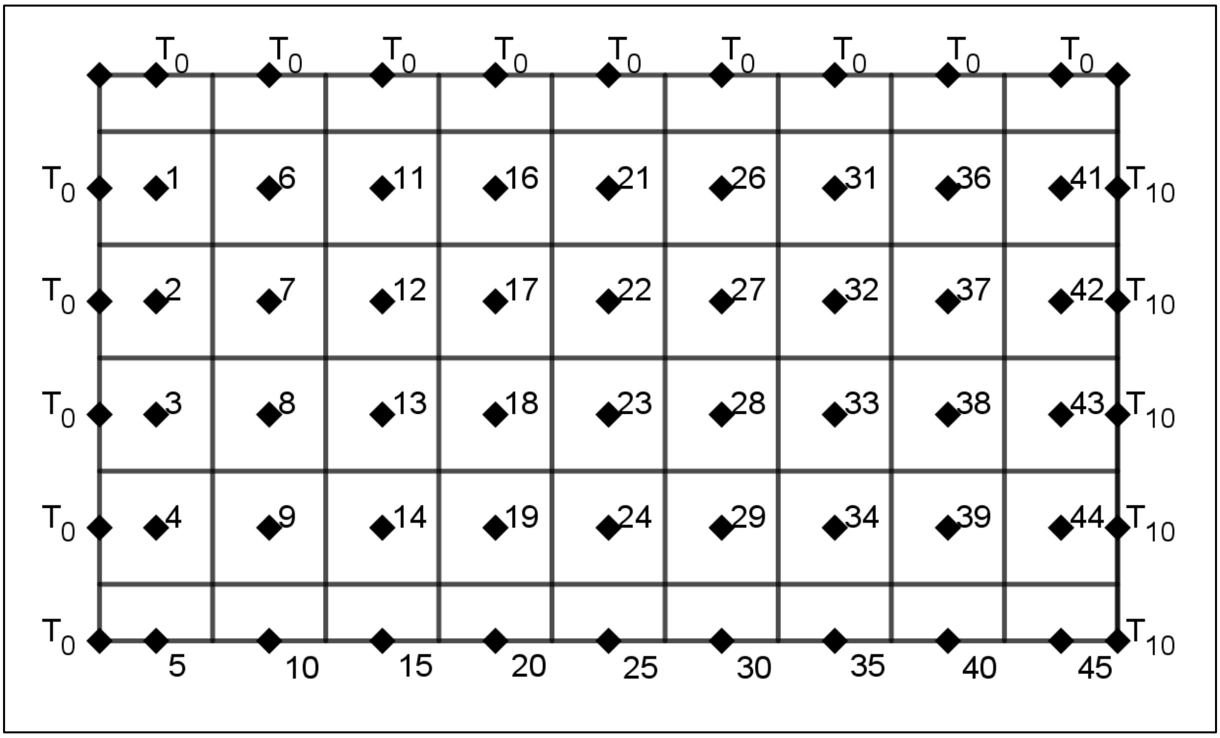


Fig. 9. Discretization of half of the square area and numbering with a discretization step of 0.1π

The analytical solution for the example shown in Fig. 9 is given by series (23):

$$T(x, y) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{sin[(2n-1)x]\, sinh[(2n-1)(\pi - y)]}{(2m-1)\, sinh[(2n-1)\pi]} \tag{23}$$

Assuming a series term count of *n* = 38, the solution obtained is presented in Table 1 below.

Table 1 Results of analytical calculations

y	x				
	0,1Π	0,2Π	0,3Π	0,4Π	0,5Π
0,9Π	0,0109	0,0208	0,0285	0,0334	0,0351
0,8Π	0,0230	0,0437	0,0599	0,0702	0,0737
0,7Π	0,0375	0,0711	0,0972	0,1138	0,1194
0,6Π	0,0562	0,1060	0,1444	0,1684	0,1765
0,5Π	0,0816	0,1528	0,2063	0,2391	0,2500
0,4Π	0,1180	0,2178	0,2895	0,3316	0,3454
0,3Π	0,1745	0,3122	0,4028	0,4523	0,4679
0,2Π	0,2740	0,4563	0,5569	0,6060	0,6208
0,1Π	0,4891	0,6823	0,7594	0,7923	0,8017

Steps:

1. Open the Excel sheet attached to the instructions.
2. Open the "Temperature Calculations" sheet.
3. Use matrix functions to calculate the inverse matrix A^{-1} of the determinant matrix *A*.
4. Use matrix functions to determine the values of the temperature vector *T* by calculating the product of the free term vector A^{-1} and the inverse matrix A^{-1}.
5. Enter the calculation results of the temperature values in vector *T* into Table 2 (Sheet: "Temp. Distribution and Error Calc.") to achieve a distribution consistent with Fig. 9.
6. Using expressions (19) and (20), calculate the absolute and relative errors concerning the results of analytical calculations listed in Table 1 (Sheet: "Temp. Distribution and Error Calc."). Place the results accordingly in Tables 2Δ and 2δ.
7. Using the "Methods of Successive Approximation" sheet, determine the number of iterations needed to calculate the given case.
8. Using the "Methods of Successive Approximation" sheet, determine the number of iterations for the successive over-relaxation method by varying the relaxation factor from 1.1 to 1.9 in 0.1 steps.
9. Calculate the absolute and relative errors for the methods of successive approximation and over-relaxation with the relaxation factor that achieves the fastest convergence. Place the distribution results and errors in Tables 3, 3Δ, 3δ, and 4, 4Δ, 4δ in the sheet "Temp. Distribution and error calc."

5. Questions

1. Write the differential form of Laplace's equation for the two-dimensional case.
2. What is the temperature T_{ij} at any point on the grid for the two-dimensional case of steady heat transfer in a body with a constant thermal conductivity coefficient and no internal heat sources?
3. For what type of heat conduction is Laplace's differential equation used?
4. Write the formulas for calculating absolute and relative errors and describe them.
5. List the types of errors that occur in numerical calculations.
6. Provide methods for solving linear equations used in numerical calculations.
7. What series are used when applying the finite difference method? Provide an example of the function $T(x, y)$ expanded into this series around the point with indices (i, j) with respect to one of the variables.
8. List the boundary conditions used in the heat transfer calculations and briefly describe them.
9. Describe the method of successive approximation.

6. Report requirements

- Include a description of the calculations performed, the calculation results in the form of a two-dimensional table with a colour scale, and the corresponding tables related to the calculation of absolute and relative errors.
- Include sample error calculations.
- Provide a bar chart comparing the number of iterations required to obtain results for the finite difference method and the successive over-relaxation method for different values of ω.
- In the conclusions, refer to the results obtained and the error values. Compare the methods used.