NUMERICAL SOLUTION OF HEAT DIFFUSION EQUATION USING THE GENERALIZED FDM

***Sylwia Lara-Dziembek*[1], *Edyta Pawlak*[2]**

Institute of Mathematics and Computer Science, Czestochowa University of Technology, Poland
email: [1] laras@imi.pcz.pl, [2] epawlak@imi.pcz.pl

Abstract. In the paper the numerical solution of boundary-initial problem described by the Fourier equation and adequate conditions is discussed. The algorithm bases on the concept of generalized finite difference method (GFDM). In the first part the mathematical formulation of the problem and a short description of GFDM algorithm are presented. In the second part the examples of numerical computations are shown. On the stage of computation the explicit version of GFDM is used.

1. Governing equations

The following linear Fourier equation describing the heat diffusion in 2D domain oriented in Cartesian co-ordinate system is consider

$$(x, y) \in \Omega: \qquad \frac{\partial T(x, y, t)}{\partial t} = a\left[\frac{\partial^2 T(x, y, t)}{\partial x^2} + \frac{\partial^2 T(x, y, t)}{\partial y^2}\right] \tag{1}$$

where a is a diffusion coefficient ($a = \lambda/c$, λ is a thermal conductivity, c is a volumetric specific heat), T, x, y, t denote temperature, spatial co-ordinates and time.

The typical conditions given on the external boundary of a system are the following

$$\begin{cases} (x, y) \in \Gamma_1: & T(x, y, t) = T_b \\ (x, y) \in \Gamma_2: & q(x, y, t) = -\lambda \dfrac{\partial T(x, y, t)}{\partial n} = q_b \\ (x, y) \in \Gamma_3: & q(x, y, t) = \alpha\left[T(x, y, t) - T_a\right] \end{cases} \tag{2}$$

where $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ is the boundary limiting the domain considered, T_b is a boundary temperature, q_b is a boundary heat flux, $\partial T/\partial n$ is a normal derivative, α is a heat transfer coefficient, T_a is an ambient temperature.

The initial condition

$$t = 0: \quad T(x, y, 0) = T_0(x, y) \tag{3}$$

is also known.

2. Generalized FDM

The geometrical mesh (in the variant of FDM here discussed) is defined in an optional way by the set of points (nodes) located in the interior of domain and its boundary (Fig. 1).

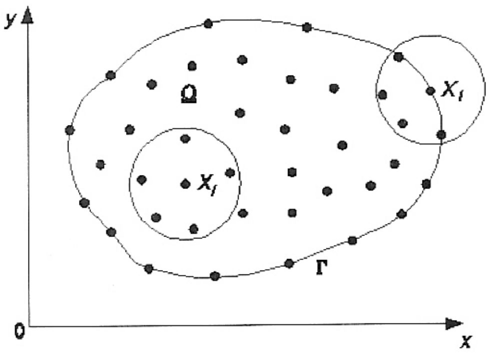

Fig. 1. Discretization

The internal and boundary stars are created by a central node and a certain number of nodes from its neighbourhood. In this place one can introduce the criterion determining the successive stars (e.g. constant number of nodes or variable number of nodes located inside a circle of given radius *r*).

Let us assume that position of the central node P_i corresponds to point (x_i, y_i), while the distance between P_i and node P_j equals $x_j - x_i = h_j$, $y_j - y_i = k_j$. Developing the function *T* into Taylor series one obtains

$$\begin{aligned} T\left(x,\, y,\, t^{f-1}\right) = {} & T\left(x_i, y_i,\, t^{f-1}\right) + \left(\frac{\partial T}{\partial x}\right)_i (x - x_i) + \left(\frac{\partial T}{\partial y}\right)_i (y - y_i) + \\ & + \left(\frac{\partial^2 T}{\partial x^2}\right)_i \frac{(x - x_i)^2}{2!} + \left(\frac{\partial^2 T}{\partial y^2}\right)_i \frac{(y - y_i)^2}{2!} + \left(\frac{\partial^2 T}{\partial x \partial y}\right)_i (x - x_i)(y - y_i) \end{aligned} \tag{4}$$

where $f - 1$ denotes a certain time level.

The last formula for node P_j can be written in the form

$$\begin{aligned} T_j^{f-1} &= T_i^{f-1} + \left(T_x\right)_i^{f-1} h_j + \left(T_y\right)_i^{f-1} k_j + \\ &+ 0.5\left(T_{xx}\right)_i^{f-1} h_j^2 + 0.5\left(T_{yy}\right)_i^{f-1} k_j^2 + \left(T_{xy}\right)_i^{f-1} h_j k_j \end{aligned} \tag{5}$$

The best approximation of the local values of the first and second derivatives appearing in equation (5) results from the least squares criterion in the form

$$\begin{aligned} F = \sum_{j=1}^{n} \Bigg\{ \Bigg[& T_i^{f-1} - T_j^{f-1} + \left(T_x\right)_i^{f-1} h_j + \left(T_y\right)_i^{f-1} k_j + 0.5\left(T_{xx}\right)_i^{f-1} h_j^2 + \\ & + 0.5\left(T_{yy}\right)_i^{f-1} k_j^2 + \left(T_{xy}\right)_i^{f-1} h_j k_j \Bigg] \frac{1}{\rho_j^m} \Bigg\}^2 = \min \end{aligned} \tag{6}$$

where

$$\rho_j = \sqrt{\left(x_j - x_i\right)^2 + \left(y_j - y_i\right)^2} \tag{7}$$

while m is a natural number (e.g. $m = 3$). The expression containing ρ plays a role of tapering function controlling the influence of distance between P_i and P_j on the final approximation of derivatives.

The necessary condition of functional F minimum is a nullity of derivatives $\partial F \big/ \partial \left(T_x\right)_i^{f-1}$, …, $\partial F \big/ \partial \left(T_{xy}\right)_i^{f-1}$ and then (the upper index $f - 1$ is here neglected)

$$\begin{aligned}
&\sum_{j=1}^{n} \left[T_i - T_j + \left(T_x\right)_i h_j + \left(T_y\right)_i k_j + 0.5\left(T_{xx}\right)_i h_j^2 + 0.5\left(T_{yy}\right)_i k_j^2 + \left(T_{xy}\right)_i h_j k_j \right] \frac{h_j}{\rho_j^{2m}} = 0 \\
&\sum_{j=1}^{n} \left[T_i - T_j + \left(T_x\right)_i h_j + \left(T_y\right)_i k_j + 0.5\left(T_{xx}\right)_i h_j^2 + 0.5\left(T_{yy}\right)_i k_j^2 + \left(T_{xy}\right)_i h_j k_j \right] \frac{k_j}{\rho_j^{2m}} = 0 \\
&\sum_{j=1}^{n} \left[T_i - T_j + \left(T_x\right)_i h_j + \left(T_y\right)_i k_j + 0.5\left(T_{xx}\right)_i h_j^2 + 0.5\left(T_{yy}\right)_i k_j^2 + \left(T_{xy}\right)_i h_j k_j \right] \frac{h_j^2}{2\rho_j^{2m}} = 0 \\
&\sum_{j=1}^{n} \left[T_i - T_j + \left(T_x\right)_i h_j + \left(T_y\right)_i k_j + 0.5\left(T_{xx}\right)_i h_j^2 + 0.5\left(T_{yy}\right)_i k_j^2 + \left(T_{xy}\right)_i h_j k_j \right] \frac{k_j^2}{2\rho_j^{2m}} = 0 \\
&\sum_{j=1}^{n} \left[T_i - T_j + \left(T_x\right)_i h_j + \left(T_y\right)_i k_j + 0.5\left(T_{xx}\right)_i h_j^2 + 0.5\left(T_{yy}\right)_i k_j^2 + \left(T_{xy}\right)_i h_j k_j \right] \frac{h_j k_j}{\rho_j^{2m}} = 0
\end{aligned} \tag{8}$$

Taking into account the form of functional F the condition (7) is simultaneously the sufficient one. The system (8) can be written in a matrix form

$$
\begin{bmatrix}
\sum\limits_{j=1}^{n}\frac{h_j^2}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^3}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j^2}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j}{\rho_j^{2m}} \\
\sum\limits_{j=1}^{n}\frac{h_jk_j}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{k_j^2}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{k_j^3}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j^2}{\rho_j^{2m}} \\
\sum\limits_{j=1}^{n}\frac{h_j^3}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^4}{4\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j^2}{4\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^3k_j}{2\rho_j^{2m}} \\
\sum\limits_{j=1}^{n}\frac{h_jk_j^2}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{k_j^3}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j^2}{4\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{k_j^4}{4\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j^3}{\rho_j^{2m}} \\
\sum\limits_{j=1}^{n}\frac{h_j^2k_j}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j^2}{\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^3k_j}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_jk_j^3}{2\rho_j^{2m}} & \sum\limits_{j=1}^{n}\frac{h_j^2k_j^2}{\rho_j^{2m}}
\end{bmatrix}
\cdot
\begin{bmatrix}
(T_x)_i \\ (T_y)_i \\ (T_{xx})_i \\ (T_{yy})_i \\ (T_{xy})_i
\end{bmatrix}
=
\begin{bmatrix}
\sum\limits_{j=1}^{n}\frac{h_j}{\rho_j^{2m}}\left(T_j-T_i\right) \\
\sum\limits_{j=1}^{n}\frac{k_j}{\rho_j^{2m}}\left(T_j-T_i\right) \\
\sum\limits_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j-T_i\right) \\
\sum\limits_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j-T_i\right) \\
\sum\limits_{j=1}^{n}\frac{h_jk_j}{\rho_j^{2m}}\left(T_j-T_i\right)
\end{bmatrix}
\tag{9}
$$

Denoting by **G** the inverse matrix resulting from the main matrix of system (9) one obtains (the index $f-1$ is again 'restored')

$$
\begin{bmatrix}
(T_x)_i^{f-1} \\ (T_y)_i^{f-1} \\ (T_{xx})_i^{f-1} \\ (T_{yy})_i^{f-1} \\ (T_{xy})_i^{f-1}
\end{bmatrix}
=
\begin{bmatrix}
g_{11} & g_{12} & g_{13} & g_{14} & g_{15} \\
g_{21} & g_{22} & g_{23} & g_{24} & g_{25} \\
g_{31} & g_{32} & g_{33} & g_{34} & g_{35} \\
g_{41} & g_{42} & g_{43} & g_{44} & g_{45} \\
g_{51} & g_{52} & g_{53} & g_{54} & g_{55}
\end{bmatrix}
\cdot
\begin{bmatrix}
\sum\limits_{j=1}^{n}\frac{h_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right) \\
\sum\limits_{j=1}^{n}\frac{k_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right) \\
\sum\limits_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right) \\
\sum\limits_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right) \\
\sum\limits_{j=1}^{n}\frac{h_jk_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)
\end{bmatrix}
\tag{10}
$$

This system of equations allows to determine the best approximation of the first and second derivatives at point P_i. A computer program realizing this part of algorithm and next creating a system of equations for transition from time t^{f-1} to time t^f is rather complex, but the details of numerical realization are not here discussed.

3. Explicit differential scheme

Let us consider the change of temperature field from time t^{f-1} to time t^f. The distance between these two levels will be denoted as Δt. According to the rules of explicit approach, the approximation of left hand side of diffusion equation should be written for time t^{f-1} corresponding to the beginning of time interval Δt.

So

$$\begin{aligned}(T_{xx})_i^{f-1} = {} & g_{31}\sum_{j=1}^{n}\frac{h_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+g_{32}\sum_{j=1}^{n}\frac{k_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+\\ & +g_{33}\sum_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+g_{34}\sum_{j=1}^{n}\frac{k_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+\\ & +g_{35}\sum_{j=1}^{n}\frac{h_j k_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)\end{aligned} \tag{11}$$

and

$$\begin{aligned}(T_{yy})_i^{f-1} = {} & g_{41}\sum_{j=1}^{n}\frac{h_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+g_{42}\sum_{j=1}^{n}\frac{k_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+\\ & +g_{43}\sum_{j=1}^{n}\frac{h_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+g_{44}\sum_{j=1}^{n}\frac{k_j^2}{2\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)+\\ & +g_{45}\sum_{j=1}^{n}\frac{h_j k_j}{\rho_j^{2m}}\left(T_j^{f-1}-T_i^{f-1}\right)\end{aligned} \tag{12}$$

Substituting the derivative $\partial T/\partial t$ by the right hand side differential quotient one has

$$\frac{T_i^f - T_i^{f-1}}{\Delta t} = a\left[(T_{xx})_i^{f-1} + (T_{yy})_i^{f-1}\right] \tag{13}$$

or

$$T_i^f = T_i^{f-1} + a\,\Delta t\left[\left(T_{xx}\right)_i^{f-1} + \left(T_{yy}\right)_i^{f-1}\right] \tag{14}$$

The discussion of stability condition of scheme presented can be found in [1], while the way of boundary conditions modelling in [2].

4. Testing computations

The first example has an analytic solution [3, 4] and it gives a possibility of numerical algorithm verification. The square of dimensions 1×1 made from material for which $a=1$ is considered. The initial temperature of domain (initial condition) equals $T(x,y,0)=T_0=100$, the external surfaces have a constant temperature $T_b=0$ (boundary conditions).
An analytical solution of the problem considered is of the form

$$T(x,y,t)=\frac{16T_0}{\pi^2}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{\sin(2i-1)\pi x\ \sin(2j-1)\pi y}{2i-1}\cdot \cdot\frac{\exp\left\{-\left[(2i-1)^2+(2j-1)^2\right]\pi^2 t\right\}}{2j-1} \tag{15}$$

and in the next figures a comparison between above solution and numerical one will be shown.

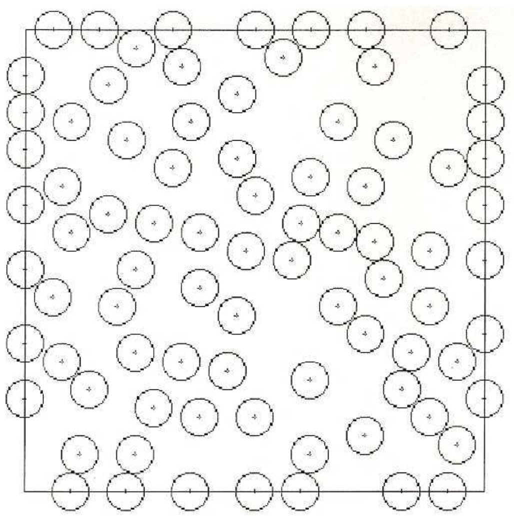

Fig. 2. Position of nodes

In Figure 2 the position of internal and boundary nodes is presented. The co-ordinate of points have been determined in a random way, but the distance between two adjacent nodes had to fulfill the condition $\left| P_i P_j \right| > 2R$ (R is a certain given radius - c.f. Figure 2).

In Figures 3, 4, 5 the numerical and exact solutions at the points marked in Figure 2 for times 0.025, 0.05, 0.1 are compared.

The next example concerns the comparison of the results obtained with the other numerical solution. The same bar ($a = 1$) with a square section is considered, the position of nodes is also the same. The boundary conditions are the following: for $x = 0$: $q_b = 0$, for $x = 1$: $\alpha = 50$, $T_a = 0$ (Robin condition), for $y = 0$: $T_b = 0$, for $y = 1$: $T_b = 1$, initial condition $T(x, y, 0) = 0$.

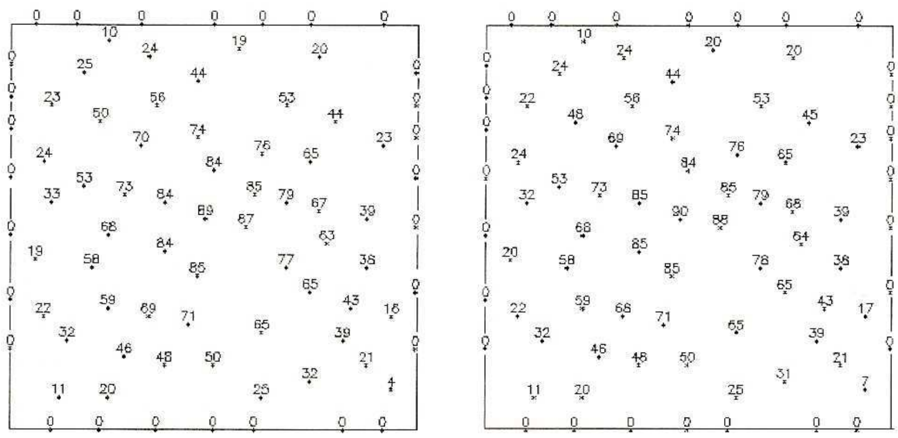

Fig. 3. Approximate and exact solutions for t = 0.025

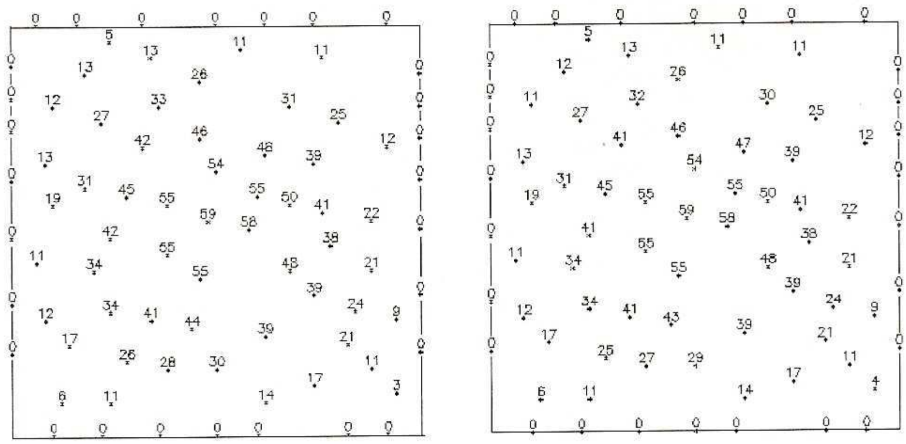

Fig. 4. Approximate and exact solutions for t = 0.05

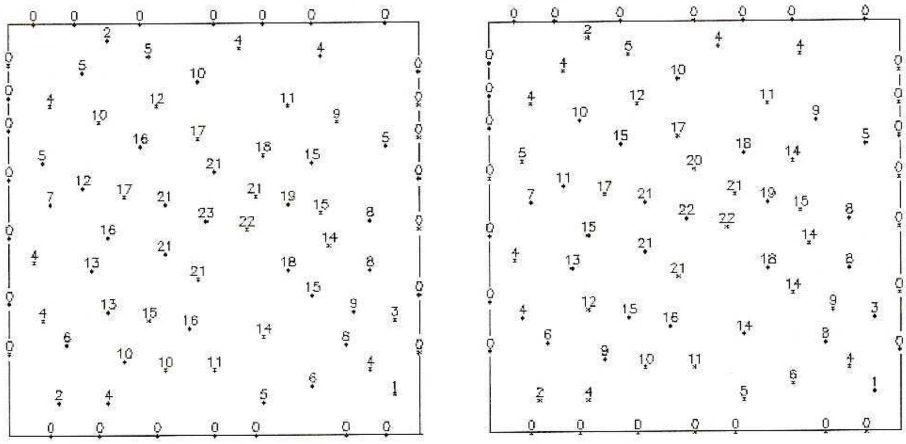

Fig. 5. Approximate and exact solutions for $t = 0.1$

So, in Figure 6 the comparison of solutions is presented ($t = 0.2$). The first solution has been obtained using the GFDM (9-points stars), while the second one has been found using the classical variant of FDM. The domain has been covered by the regular mesh containing 2500 nodes ($\Delta t = 0.00005$).

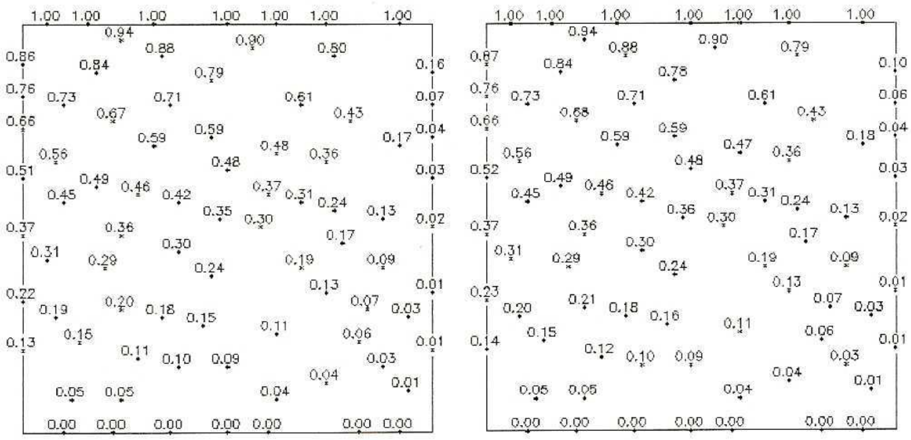

Fig. 6. Comparison of solutions for time $t = 0.2$

One can see, that the compatibility of results is very good. The visible differences can be noticed only at the right upper corner, in this fragment of domain the drastic change of boundary conditions takes place.
Summing up, the GFDM algorithm seems to be an effective tool for numerical simulation of heat diffusion process.

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