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Numerical Modeling Of Boundary Value Problems For Parabolic Differential Equations

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Abstract. *This article examines numerical methods for solving boundary value problems for parabolic differential equations, which are widely used in modeling physical processes such as the filtration of oil, gas, and water in porous media, as well as heat transfer processes. The primary focus is on the differential-difference method, which is characterized by its high accuracy and ease of programming. The theoretical aspects of the method are presented, including algorithmic implementation, the use of the differential sweep method, and an analysis of the stability of the computational process. Special attention is given to the advantages of the differential-difference approach, such as the ability to automatically fulfill internal conditions during phase transitions, ensure absolute computational stability, and simplify programming. The article also describes the solution algorithm, which includes a longitudinal-transverse scheme that enables efficient problem-solving using parallel computations. Additionally, numerical calculation results are provided, including comparisons with analytical solutions that demonstrate the method's high accuracy. It is shown that the developed algorithms can be easily adapted for solving other classes of problems, making them a universal tool for numerical modeling in computational mathematics. The conclusions are supported by graphical results and error analysis, confirming the reliability of the proposed approach.*

Keywords: *numerical modeling, differential equations, parabolic type, differential-difference method, differential sweep method, mathematical model, algorithms, computational stability, Runge-Kutta method, parallel computations.*

I. INTRODUCTION

The development of computer technology, the creation of new mathematical models, computational methods, efficient algorithms, and software tools designed to solve various classes of problems is one of the central directions in the advancement of fundamental and applied scientific research.

The numerical solution of boundary value problems for parabolic differential equations and their theoretical justification are actively developing areas in modern computational mathematics. The solution of various classes of problems in mathematical

physics that describe processes and phenomena involving parabolic differential equations is of particular interest.

It is known that mathematical models of many physical processes are formulated as parabolic differential equations, including problems of oil, gas, and water filtration in porous media, heat transfer problems, and so on. Finding analytical or approximate analytical solutions to such problems in generalized cases is a very challenging task. For this reason, their solution is impossible without resorting to numerical methods.

Currently, numerical methods are widely used for solving various boundary value problems of physical processes on computers, with the results presented visually in 3D graphics. Such a representation of calculation results is important for studying and analyzing processes. Presenting results in a computer-visualized format allows for the visualization and analysis of processes such as oil, gas, and water filtration in deep underground layers, as well as various physical processes occurring in unseen locations.

Numerous numerical models and methods for solving problems in mathematical physics were developed in the 20th century. Significant contributions to their development were made by N.N. Veregin, B.N. Nikolaevsky, I.I. Malchanov, and many other scientists. With the advancement of computers, the most efficient numerical and approximate methods, based on the ideas of finite-difference and differential-difference schemes, were applied to solve mathematical physics problems. In this field, the work of scientists such as A.A. Dorodnitsyn, A. Tikhonov, A.A. Samarsky, N.N. Yanenko, G.I. Marchuk, F.B. Abutaliev, and others made it possible to create a well-founded theory of numerical and approximate modeling for solving boundary value problems in mathematical physics [1, 2, 3, 9].

For certain classes of mathematical physics problems, it is appropriate to apply differential-difference schemes. Their main distinction from finite-difference schemes lies in the fact that not all derivatives in the differential problem are approximated by difference operators. Therefore, the original differential problem is transformed into an approximate one. The approximation error between the exact and approximate problems is associated with the corresponding differential-difference operators.

In many cases, when numerically modeling boundary value problems, the original differential problem is replaced by a differential-difference one, which is solved using the numerical method of differential sweep [5, 10, 11].

It is important to note that using the differential sweep method in numerical modeling has the following advantages:

- Automatic fulfillment of internal conditions when transitioning from one phase to another;
- High accuracy in solving the Cauchy problem for sweep coefficients by using the well-known Runge-Kutta or Kutta-Merson methods;
- No need for extensive programming when using the Runge-Kutta or Kutta-Merson methods, as suitable software packages are readily available;
- Numerical integration stability: The normalization procedure for control coefficients and Runge-Kutta coefficients during Cauchy problem integration ensures the computational process's stability. At each iteration, the normalized vector U_i is inserted into the right side of the system to

compute U_{i+1}, contributing to stable solutions for the Cauchy problem;

- Ensures absolute stability of the computational process;
- Convenient organization and implementation of parallel computations;
- Simpler programming compared to other numerical methods for solving boundary value problems of parabolic type.

II. MATHEMATICAL MODEL

Let the following two-dimensional boundary value problem of the parabolic type be solved using numerical methods. Consider the domain $G\{0 < x < 1, 0 < y < 1\}$ as a rectangle. Then the mathematical model of the boundary value problem can be written as:

$$\frac{1}{a}\frac{\delta P}{\delta t} = \frac{\delta^2 P}{\delta x^2} + \frac{\delta^2 P}{\delta y^2} + f(x,y) \quad (1)$$

In the general case, the initial and boundary conditions can be written as follows:

$$P(x,y,t) = \phi(x,y),\ t = 0; \quad (2)$$

$$\begin{cases} -\left.\dfrac{\partial P}{\partial x}\right|_{x=0} = \alpha(P_A - P),\ x=0; \quad \left.\dfrac{\partial P}{\partial x}\right|_{x=1} = \alpha(P_A - P), \quad x=1; \\ -\left.\dfrac{\partial P}{\partial y}\right|_{y=0} = \alpha(P_A - P),\ y=0; \quad \left.\dfrac{\partial P}{\partial y}\right|_{y=1} = \alpha(P_A - P), \quad y=1; \end{cases} \quad (3)$$

Here

P - the desired function whose value is being computed;

P_A - the limiting value of the function;

$f(x,y)$ - a certain source provided in the considered domain (a source of heat or the production volume obtained from an oil reservoir);

a - the coefficient of impermeability;

α — defined as:

$$\alpha = \begin{cases} 0, & if\ the\ boundary\ is\ closed; \\ 1, & if\ the\ boundary\ is\ open. \end{cases}$$

To verify the correctness of the results and the adequacy of the mathematical model, we will obtain the analytical solution of the boundary value problem as follows:

$$P(x,y,t) = \mathrm{e}^{-2xyt}.$$

The boundary and initial conditions can then be defined as follows:

$$\begin{cases} P(x,y,0) = 1, \\ P(0,y,t) = 1, \\ P(1,y,t) = e^{-2yt} \\ P(x,0,t) = 1, \\ P(x,1,t) = e^{-2xt}, \end{cases} \quad (4)$$

$$f(x,y,t) = -2(2t^2(x^2+y^2) + xy)e^{-2xyt} \quad (5)$$

III. NUMERICAL MODEL

We apply the algorithmic concept of the longitudinal-transverse scheme to transform the boundary value problem into a differential-difference form. This approach enables the use of the differential sweep method along each coordinate axis *x*. Specifically, for each direction of the first

variable *x* and the second variable *y*, computations are carried out over the time interval *l+0.5*. Subsequently, at *l+1*, the solution is determined on this time interval by employing the differential sweep method for each direction of the variable *x*, following the same algorithm. This procedure is implemented iteratively at subsequent time steps.

We replace the differential operators of the equation with the corresponding three-point finite-difference operators at the time layers *l+0.5* and *l+1*:

$$\begin{cases} \dfrac{\partial}{\partial x}\left(\dfrac{\partial P_j^{(l+0.5)}(x)}{\partial x}\right) - \dfrac{1}{a0.5\Delta\tau} P_j^{(l+0.5)}(x) = -\dfrac{P_j^{(l)}(x)}{a0.5\Delta\tau} - \Lambda\left[P_{ij}^{(l)}\right], \\ \dfrac{\partial}{\partial y}\left(\dfrac{\partial P_i^{(l+1)}(y)}{\partial y}\right) - \dfrac{R}{a0.5\Delta\tau} P_i^{(l+1)}(y) = -\dfrac{P_i^{(l+0.5)}(y)}{a0.5\Delta\tau} - \Lambda\left[P_{ij}^{(l+0.5)}\right]. \end{cases} \quad (6)$$

Here

$$\Lambda\left[P_{ij}^{(l)}\right] = \frac{P_{i-1,j}^{(l)} - 2P_{ij}^{(l)} + P_{i+1,j}^{(l)}}{\Delta x^2}, \quad \Lambda\left[P_{ij}^{(l+0.5)}\right] = \frac{P_{i,j-1}^{(l+0.5)} - 2P_{ij}^{(l+0.5)} + P_{i,j+1}^{(l+0.5)}}{\Delta y^2},$$

$$i = 2,3,...,n-1, \quad j = 2,3,...,n-1.$$

$P_{i,j}^{(l)}$ - The value of the function at the time layer *l*.

$P_{i,j}^{(l+0.5)}$ - The value of the function at the time layer *l+0.5*.

$P_{i,j}^{(l+1)}$ - The value of the function at the time layer *l+1*.

The given system of differential-difference equations (6) is solved for the time layer *l+0.5* using the differential sweep method in the direction of the variable x_i, and then similarly in the direction of y_j at the layer *l+1*. In this case, the solution obtained at the layer *l+0.5* is used as the initial condition.

$$P_j^{(l+0.5)}(x) = \frac{\gamma_j(x)u_j(x) - \alpha_j(x)w_j(x)}{\alpha_j(x)v_j(x) - \beta_j(x)u_j(x)};$$

$$\frac{dP_j^{(l+0.5)}}{dx} = \frac{\gamma_j(x)v_j(x) - \beta_j(x)w_j(x)}{\alpha_j(x)v_j(x) - \beta_j(x)u_j(x)}, \quad j = 0,...,n. \quad (7)$$

$$P_i^{(l+1)}(y) = \frac{\gamma_i(y)u_i(y) - \alpha_i(y)w_i(y)}{\alpha_i(y)v_i(y) - \beta_i(y)u_i(y)};$$

$$\frac{dP_i^{(l+1)}}{dy} = \frac{1}{k_i(y)} \cdot \frac{\gamma_i(y)v_i(y) - \beta_i(y)w_i(y)}{\alpha_i(y)v_i(y) - \beta_i(y)u_i(y)}, \quad i = 0,1,2,...,n. \quad (8)$$

Here, *u(x), v(x), w(x)* and *α(x), β(x), γ(x)* are the right and left coefficients in the direction of xxx using the differential sweep method, determined as solutions of the Cauchy problem. The Cauchy problem for the coefficients of the method is formulated as follows:

$$\begin{cases} k_j \dfrac{du_j}{dx} = v_j, \\ \dfrac{dv_j}{dx} = Q_{1j} u_j, \\ \dfrac{dw_j}{dx} = R_{1j} u_j. \end{cases}$$

$$j = 1, 2, ..., n.$$

$$\begin{cases} k_j \dfrac{d\alpha_j}{dx} = \beta_j, \\ \dfrac{d\beta_j}{dx} = Q_{1j} \alpha_j, \\ \dfrac{d\gamma_j}{dx} = R_{1j} \alpha_j. \end{cases} \qquad (9)$$

$$j = n-1, n-2, ..., 0.$$

$$u_0 = k_1,\ v_0 = \alpha,\ \ w_0 = \alpha P_A.$$

$$\alpha_n = k_n,\ \beta_n = \alpha,\ \ \gamma_n = \alpha P_A.$$

Similarly, *u(y),v(y),w(y)* and *α(y),β(y),γ(y)* are the right and left coefficients in the direction of y using the differential sweep method, determined as solutions of the Cauchy problem. The Cauchy problem for the coefficients of the method is formulated as follows:

$$\begin{cases} k_j \dfrac{du_j}{dy} = v_j, \\ \dfrac{dv_j}{dy} = Q_{1j} u_j, \\ \dfrac{dw_j}{dy} = R_{1j} u_j. \end{cases}$$

$$j = 1, 2, ..., n.$$

$$\begin{cases} \dfrac{d\alpha_j}{dy} = \beta_j, \\ \dfrac{d\beta_j}{dy} = Q_{1j} \alpha_j, \\ \dfrac{d\gamma_j}{dy} = R_{1j} \alpha_j. \end{cases} \qquad (10)$$

$$j = n-1, n-2, ..., 0.$$

$$u_0 = k_1,\ v_0 = \alpha,\ \ w_0 = \alpha P_A.$$

$$\alpha_n = k_n,\ \beta_n = \alpha,\ \ \gamma_n = \alpha P_A.$$

In the system of equations above, the coefficients Q_{1j}, Q_{2i}, R_{1j}, R_{2i} are calculated as follows:

$$Q_{1j} = -\frac{P_{i,j}^{(l)}(x)}{a0.5\Delta\tau} - \Lambda\left[P_{i,j}^{(l)}\right]; \qquad R_{1j} = \frac{1}{a0.5\Delta\tau};$$

$$Q_{2i} = -\frac{P_{i,j}^{(l+0.5)}(y)}{a0.5\Delta\tau} - \Lambda\left[P_{i,j}^{(l+0.5)}\right]; \quad R_{2i} = \frac{1}{a0.5\Delta\tau}.$$

IV. ALGORITHM FOR SOLVING THE PROBLEM

The obtained differential-difference problem can be solved in the following two-step sequence:

Step One:

- The initial conditions for the Cauchy problem are determined from the boundary conditions.
- The Cauchy problem is solved from left to right at points along all directions of the *x*-axis using the Runge-Kutta or Kutta-Merson procedure with the initial condition.
- The Cauchy problem is solved from right to left at points along all directions of the *x*-axis using the Runge-Kutta or Kutta-Merson procedure with the initial condition.
- The solution, according to formula (10), involves determining the values of the function *Pi(x)* and its first-order differential values at all points of the variable *y* across all directions of the unknown *x*, i.e., obtaining the function values at all points for a half-step in time.

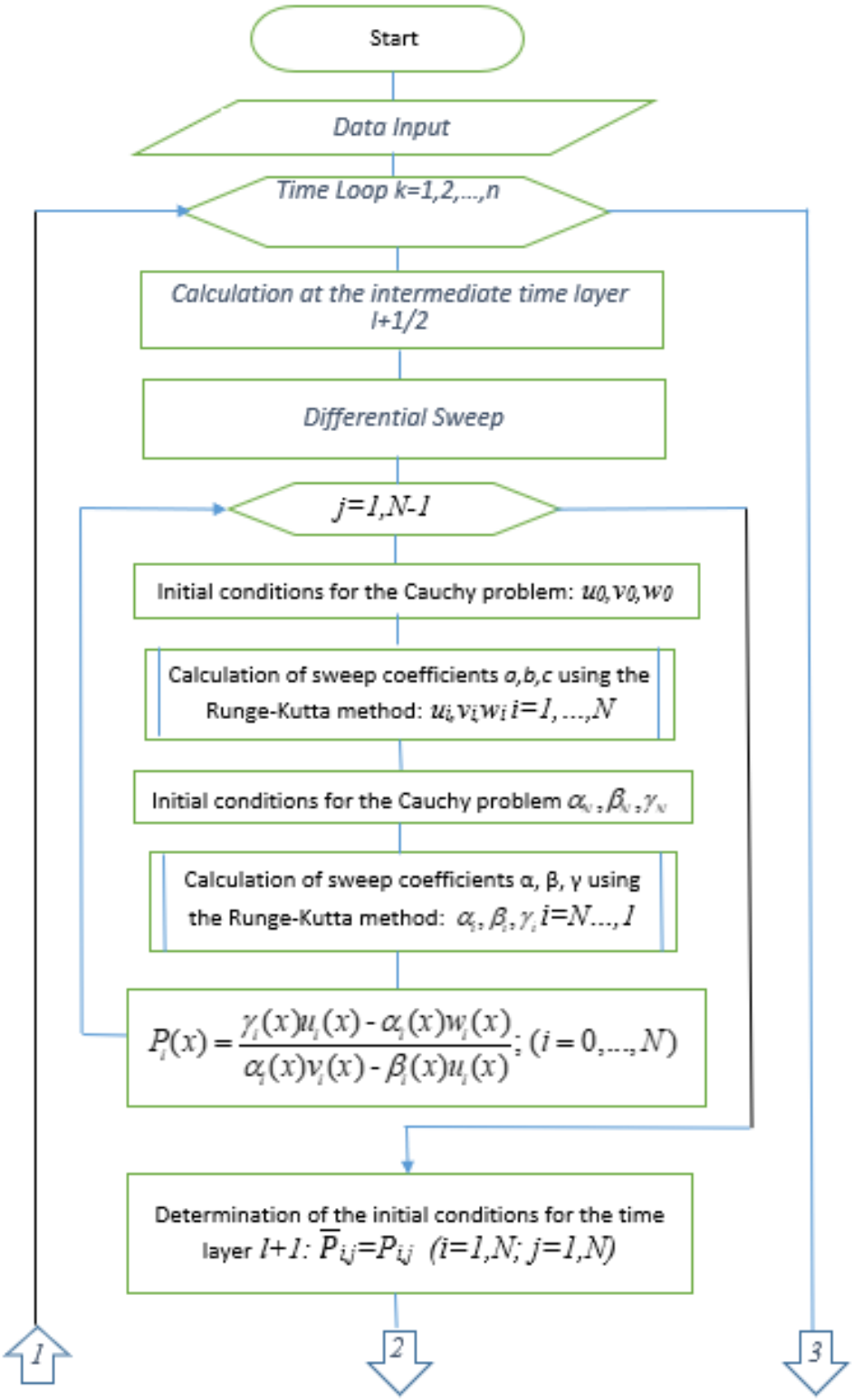
Step Two:

We move forward by a half-step in time and determine the values of the function *Pi(y)* for the next *l+1* step at all points. This step is performed in the same way as the first step. The process of solving the Cauchy problem using the Runge-Kutta method is carried out by applying the normalization procedure to the sweep coefficients and the coefficients of this method at each step. At each step, the normalized vector $\overline{U_i}$ $(U=(u,v,w))$ is replaced by the vector U_i on the right side when calculating the specified vector U_{i+1} in the Cauchy problem for the left side.

Similarly, when solving the Cauchy problem from left to right, during the computation of the vector A_{i-1}, the vector A_i on the right side is replaced by the normalized vector $\overline{A_i}$ $(A=(\alpha,\beta,\gamma))$. The normalization procedure is not used if the chosen method maintains stability.

Thus, when solving a boundary value problem for a two-dimensional parabolic differential equation using the alternating direction scheme, the differential problem is reduced to a differential-difference problem, which is solved using the differential sweep method.

The structural diagram of the algorithm for solving the boundary value problem for a second-order parabolic differential equation is presented in Figure 1.


Start
Data Input
Time Loop k=1,2,...,n
Calculation at the intermediate time layer l+1/2
Differential Sweep
j=1,N-1
Initial conditions for the Cauchy problem: u_0, v_0, w_0
Calculation of sweep coefficients a,b,c using the Runge-Kutta method: $u_i, v_i, w_i\ i=1,...,N$
Initial conditions for the Cauchy problem $\alpha_N, \beta_N, \gamma_N$
Calculation of sweep coefficients α, β, γ using the Runge-Kutta method: $\alpha_i, \beta_i, \gamma_i\ i=N...,1$
$P_i(x) = \frac{\gamma_i(x)u_i(x) - \alpha_i(x)w_i(x)}{\alpha_i(x)v_i(x) - \beta_i(x)u_i(x)};\ (i = 0,...,N)$
Determination of the initial conditions for the time layer l+1: $\overline{P}_{i,j}=P_{i,j}\ \ (i=1,N;\ j=1,N)$
1
2
3

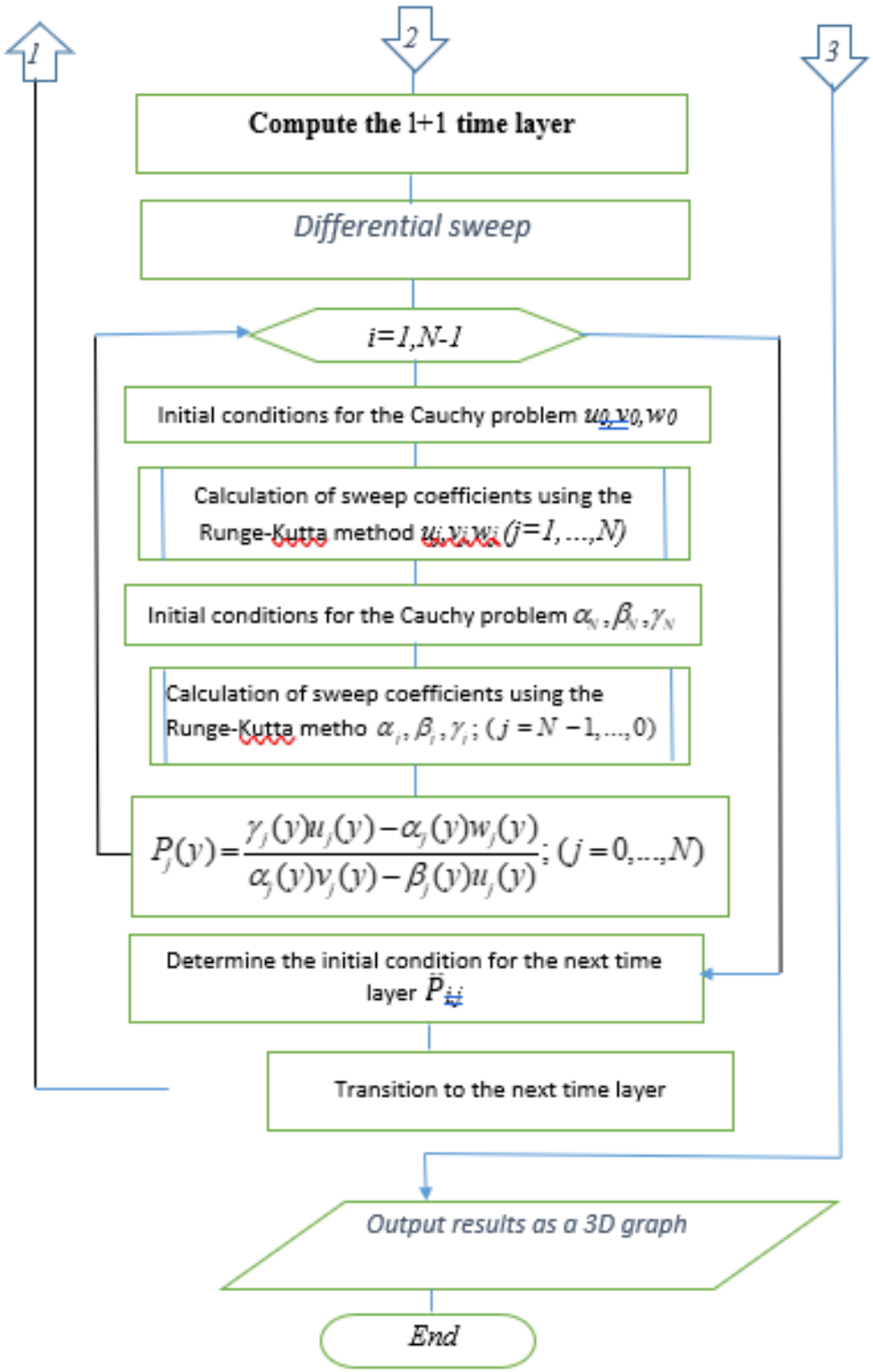


Figure 1. Structural diagram of the algorithm for solving the boundary value problem of a second-order parabolic differential equation

Parallel computation can also be organized when solving the developed numerically modeled differential-difference problem (6)-(10). To achieve this, the field in each direction is divided into two equal parts according to the alternating direction scheme, and calculations are performed along the *x*-axis in the time layer *1+0.5*. This calculation is carried out in parallel by solving the coefficients of the sweep method from left to right and from right to left (9) and (10) using the Runge-Kutta method. Similarly, this process is repeated for the *l+1* time layer.

5. Numerical Calculations for Problem Solving

To ensure the adequacy and reliability of the solution, let's consider problem (1) with its analytical solution and the initial and boundary conditions (4)-(5). In the numerical solution, the sweep coefficients are determined from the Cauchy problem (9) and (10) using the Runge-Kutta method. Here, the initial conditions are derived from the boundary conditions (4).

The results of solving problem (1)-(5) are presented in Fig. 2 and Table 1. The numerical results are compared with the analytical ones in the graph and the table.

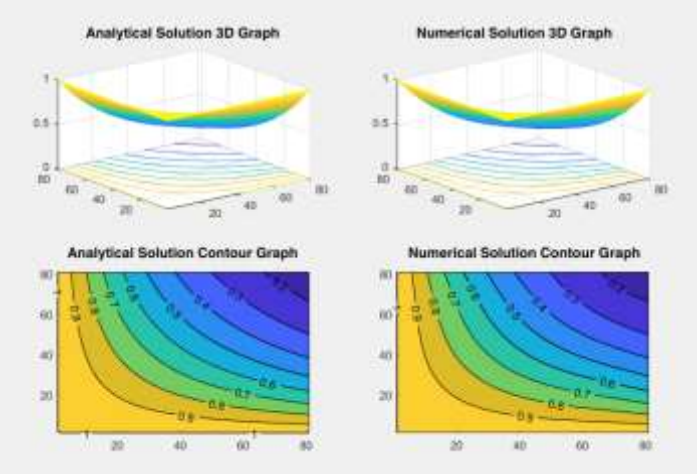


Figure 2. Graphical comparison of numerical results with exact ones

During the calculation, the spatial grid step was chosen as *h=1/180=0.0125* and the time step as τ=0.0125. Table 1 presents the absolute calculation error at the cross-section y=0.5 at 40 points along *x* {10, 20, 30, 40, 50, 60, 70, 80}.

$$u_0 = 0,\ v_0 = -1,\ \ w_0 = 1; \qquad \alpha_n = 0,\ \beta_n = -1,\ \gamma_n = \exp(-2 \cdot t \cdot y_n).$$

Table 1. Absolute Error of Calculation Results

x	10	20	30	40	50	60	70	80
Exact	0,8973	0,7956	0,7054	0,6254	0,5545	0,4916	0,4359	0,3864
Numerical	0,8968	0,7924	0,6994	0,6172	0,5461	0,4856	0,4334	0,3861
Error	0,0005	0,0032	0,0060	0,0082	0,0084	0,0060	0,0025	0,0003

From the presented graphs and table, it is evident that the computed numerical solution of the problem closely approximates the mathematical solution. This demonstrates that the use of the

differential-difference method for solving boundary problems of parabolic differential equations offers several advantages in programming and provides a sufficiently accurate numerical solution compared to other methods.

CONCLUSION

These results can be used in the creation of This study presented the development and application of numerical methods for solving boundary value problems for parabolic differential equations. The proposed differential-difference method demonstrated high computational accuracy and stability. By leveraging the Runge-Kutta method and differential sweep approach, the solution process effectively maintained stability while providing reliable results even for complex boundary conditions.

The structural algorithm employing longitudinal-transverse schemes facilitated efficient parallel computation, further optimizing computational resources and execution time. Comparative analysis between numerical and analytical solutions confirmed the accuracy of the proposed method, as demonstrated by graphical representations and error analysis.

The versatility of the developed algorithms enables their adaptation to other classes of boundary value problems, making them a valuable tool in computational mathematics for modeling various physical processes. This research underscores the efficiency of the differential-difference approach and its practical applications in solving complex mathematical physics problems.

GRATITUDE

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