APPROXIMATION OF THE EQUATION OF HEAT CONDUCTIVITY BY SPECTRAL-GRID METHODS

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ABSTRACT
For mathematical modeling of linear wave systems, numerical methods are increasingly being used. At the same time, their application to the solution of evolutionary problems with large gradients described by non-stationary partial differential equations run into serious difficulties. The spectral - grid method is applied for numerical modeling of initial - boundary value problems for heat conduction equations. The performed numerical calculations show a high computational efficiency of the spectral - grid method.
KEYWORDS: *numerical modeling, heat equation, spectral - grid method, evolutionary problems, Chebyshev polynomials of the first kind, algebraic system, interval of integration, grid approximation, approximate solution, efficiency.*

INTRODUCTION
The heat equation is a second-order partial differential equation that describes the temperature distribution in a given area of space and its change in time.

One of the most characteristic properties of wave movements is that they continue to exist even after the elimination of the causes that cause them [1-8]. Waves usually persist for a long time and can transmit disturbances over very long distances. In fact, waves acquire their most characteristic shape precisely after propagation to a "large" distance from the region in which they "originated". One of the important and difficult mathematical problems is related to the description of the behavior of low-amplitude waves that undergo weak dissipation over long time intervals.

Self-oscillating systems occupy a special place among linear systems [9-15]. Self-oscillating systems are clocks, lamp generators of electromagnetic oscillations, steam engines and internal combustion engines, in a word, all real systems that are capable of performing continuous oscillations in the absence of periodic external influences.

MAIN PART
One of the important and difficult mathematical problems is related to the description of the behavior of low-amplitude waves that experience weak dissipation over long time intervals [1]. These restrictions are not as special as they might seem at first glance. Since, as follows from observations, waves are indeed able to exist for a long time outside the sources, the limitations associated with the assumption of low dissipation and large time intervals are quite natural. In gas dynamics, there is weak dissipation, characterized by the dimensionless parameter Re^{-1}, where Re is the Reynolds number. In this case, the magnitude of the amplitude of wave ε is

small, but finite. In cases of greatest interest, the corresponding linear equation should be considered at time intervals of the order of ε^{-1}.

$$\frac{\partial u}{\partial t} = \upsilon \frac{\partial^2 u}{\partial \eta^2}, a < \eta < b, \qquad (1)$$

$$u(a,t) = 0,$$
$$u(b,t) = 0, \qquad (2)$$

$$u(\eta,0) = u_0(\eta). \qquad (3)$$

We divide the interval of integration $[a,b]$ into M different elements:

$$[\eta_0, \eta_1], [\eta_1, \eta_2], [\eta_2, \eta_3],..., [\eta_{i-1}, \eta_i],..., [\eta_{M-1}, \eta_M],$$

where $\eta_0 = a$, $\eta_M = b$. To represent the approximate solution in the form of series in Chebyshev polynomials, each element $[\eta_{i-1}, \eta_i]$ of integration interval $[a,b]$ is mapped to interval $[-1,1]$ using the following replacement of the independent variable

$$\eta_i = \frac{m_i}{2} + \frac{k_i}{2} y, \qquad (4)$$

here $m_i = \eta_i + \eta_{i-1}$, $k_i = \eta_i - \eta_{i-1}$ is the length of the i-th mesh element and $y \in [-1,1]$. After this transformation, problem (1) - (3) takes the form:

$$\frac{\partial u_i}{\partial t} = \upsilon \left(\frac{2}{k_i}\right)^2 \frac{\partial^2 u_i}{\partial y^2}, \quad i = 1,2,...,M \qquad (5)$$

$$u_i(1) = u_{i+1}(-1), \quad i = 1,2,...,M-1, \qquad (6)$$

$$\frac{1}{k_i} \frac{\partial u_i}{\partial y}(1) = \frac{1}{k_{i+1}} \frac{\partial u_{i+1}}{\partial y}, \quad i = 1,2,...,M-1, \qquad (7)$$

$$u_1(-1) = u_M(1) = 0, \qquad (8)$$

$$u_i(y,0) = u_0\left(\frac{m_i}{2} + \frac{k_i}{2} y, 0\right), \quad i = 1,2,...,M, \qquad (9)$$

where the equations (6) - (7) of the approximate solutions of continuity requirements and its first derivative in the internal nodes of the grid, equation (8) - form of the initial data (initial data for the future position of fundamental importance and have therefore not considered).

An approximate solution of equations (5) - (8) will be sought in the form of series in Chebyshev polynomials of the first kind $T_n(y)$ [8-15]:

For this, we introduce matrix notation as follows. Replace in (5) - (7) taking into account the derivatives by the expressions:

$$\frac{\partial v}{\partial y} = \hat{B}v, \qquad (10)$$

$$\frac{\partial^2 v}{\partial y^2} = \hat{A}v, \qquad (11)$$

where v is the vector of length $(N+1)M$ with components:

$$v \equiv \{u_1(y_0)...u_1(y_N), u_2(y_0)...u_2(y_N), u_3(y_0)...,u_M(y_0)...u_M(y_N),\} \qquad (12)$$

in $\hat{A}$ and $\hat{B}$ - square matrices of dimension $((N+1)M) \times ((N+1)M)$ with block-diagonal structure.

where $\hat{A}$ and $\hat{B}$ denote the following matrix products:

$$\hat{A} = TPT^*, \quad \hat{B} = TRT^*. \qquad (13)$$

where T is the matrix for Chebyshev polynomials of the first kind, $T*$ is the inverse matrix T, P and R are the matrices of the first and second spatial derivatives. T, $T*$, P and R are block-diagonal matrices of dimension $((N+1)M) \times ((N+1)M)$.

We also introduce matrices $\tilde{A}$ and $\tilde{B}$:

$$\tilde{A} = \upsilon K^2 \hat{A}, \ \tilde{B} = K\hat{B}, \qquad (14)$$

where K is a diagonal matrix.

Writing differential equations (5) only at the interior points of elements $(l = 1,..., N-1)$, conditions (6) and (7) at the boundary points of neighboring elements, and (8) at the boundary points of the interval, we arrive at the following system:

$$\frac{dS}{dt} = Av, \qquad (15)$$

$$Dv = 0. \qquad (16)$$

Here S is a vector of length $(N+1)M$:

$$S \equiv \{0, u_1(y_1)...u_1(y_{N-1}),0,0,u_2(y_1)...u_2(y_{N-1}),0,0, u_3(y_1)...,0,u_M(y_1)...u_M(y_{N-1}),0\}, \qquad (17)$$

matrix A of dimension $((N+1)M) \times ((N+1)M)$ and matrix D of dimension $2M \times ((N+1)M)$ are:

$$A = \begin{bmatrix}
0 & 0 & \cdots & 0 & 0 \\
a_{10}^1 & a_{11}^1 & \cdots & a_{1N-1}^1 & a_{1N}^1 \\
\vdots & \vdots & \cdots & \vdots & \vdots & & 0 & & 0 & & 0 \\
a_{N-10}^1 & a_{N-11}^1 & \cdots & a_{N-1N-1}^1 & a_{N-1N}^1 \\
0 & 0 & \cdots & 0 & 0 \\
& & & & & 0 & 0 & \cdots & 0 & 0 \\
& & & & & a_{10}^2 & a_{11}^2 & \cdots & a_{1N-1}^2 & a_{1N}^2 \\
& 0 & & & & \vdots & \vdots & \cdots & \vdots & \vdots & 0 & & 0 \\
& & & & & a_{N-10}^2 & a_{N-11}^2 & \cdots & a_{N-1N-1}^2 & a_{N-1N}^2 \\
& & & & & 0 & 0 & \cdots & 0 & 0 & & & 0 \\
& 0 & & & & & 0 & & & \ddots & 0 & 0 & \cdots & 0 & 0 \\
& & & & & & & & & & a_{10}^M & a_{11}^M & \cdots & a_{1N-1}^M & a_{1N}^M \\
& 0 & & & & & 0 & & & 0 & \vdots & \vdots & \cdots & \vdots & \vdots \\
& & & & & & & & & & a_{N-10}^M & a_{N-11}^M & \cdots & a_{N-1N-1}^M & a_{N-1N}^M \\
& & & & & & & & & & 0 & 0 & \cdots & 0 & 0
\end{bmatrix}$$

$$D = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & & & 0 \\
x & x & x & x & x & x & x & x & x & x \\
& & & & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
& & & & x & x & x & x & x & x & x & x & x & x \\
& & & & & & & & & \ddots \\
& & & & & & & & & & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
& 0 & & & & & & & & & x & x & x & x & x & x & x & x & x & x \\
& & & & & & & & & & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}$$

The coefficients of each shaded block matrix A coincide with the corresponding coefficients of matrix $\tilde{A}$. As for matrix D, its first and last rows contain the coefficients of conditions (8), the remaining even rows $(l = 2j, j = 2,..., M-1)$ contain the coefficients of equations (6), and odd $(l = 2j-1, j = 2,..., M)$ — the coefficients of equations (17) (corresponding rows of matrix 6).

System (15) - (16) is "differential-algebraic" - it contains $(N-1)M$ ordinary differential equations (14) and $2M$ linear algebraic conditions (16) with $(N+1)M$ unknowns. Let us show that it can be reduced to two

autonomous systems of equations: a differential system of a smaller order $(N-1)M$ only at the interior points of the interval and an algebraic system of the standard form $Ax = b$ for the remaining components of the solution (at the boundary points of the elements).

Let us denote by X, Y, V_j and W_j combinations of variables in conditions (15) and we will consider them as new dependent variables:

$$V_j \equiv u_j(y_N) - u_{j+1}(y_1) = 0, \qquad j = 1,...,M-1$$

$$W_j \equiv \frac{1}{K_j}\frac{\partial u_j}{\partial y}(y_N) - \frac{1}{K_{j+1}}\frac{\partial u_{j+1}}{\partial y}(y_1) = 0,$$

$$j = 1,...,M-1 \tag{18}$$

$$X \equiv u_1(y_0) = 0,$$

$$Y \equiv u_N(y_N) = 0,$$

then vector

$$w = \{X, u_1(y_1)...u_1(y_{N-1}), V_1, W_1, u_2(y_1)...u_2(y_{N-1}),$$
$$V_2, W_2,..., V_{M-1}, W_{M-1}, u_M(y_1)...u_M(y_{N-1}), Y\} \tag{19}$$

coincides with S from (18) and is related to v from (12) by the relation:

$$w = Gv. \tag{20}$$

Here G is a nondegenerate matrix of dimension $((N+1)M) \times ((N+1)M)$.

In which rows with numbers $j(N+1)$ $(j=1,...,M-1)$ are rows of matrix D with numbers $2j$ $(j=1,...,M-1)$, and rows $j(N+1)+1$ $(j=1,...,M-1)$ are its rows with numbers $2j+1$.

We also introduce the notation:

$$\hat{H} = AG^{-1}, \tag{21}$$

in which (14) takes the form:

$$\frac{dw}{dt} = \hat{H}w, \tag{22}$$

Thus, it can be seen from (22) that the system of ordinary differential equations (14) has been reduced to a system of lower dimension, and with a nondegenerate matrix H (all zero rows and all columns are excluded from matrix $\hat{H}$, whose elements are multiplied by the corresponding zero elements of vector w):

$$\frac{dr}{dt} = Hr, \tag{23}$$

Here the dimension is $H : (M(N-1)) \times (M(N-1))$, and

$$r = \{u_1(y_1)...u_1(y_{N-1}), u_2(y_1)...u_2(y_{N-1}),..., u_M(y_1)...u_M(y_{N-1})\},$$

are vectors of length $(M(N-1))$, moreover, the r vector differs from the vector v only by the absence of components numbered $(j-1)N+1$ and jN, where $j = 1,...,M$. The missing vector components are found by solving the linear algebraic system (20).

The system of equations (23) is evolutionary. For its numerical solution in this work, as already mentioned, the method [16,17] was used. Namely, for the transition to the next time layer, an explicit scheme of the form was used:

$$r(t+\tau) = r(t) + RQr(t),$$

$$R\varphi(t) = \frac{\tau}{12}[23\varphi(t) - 16\varphi(t-\tau) + 5\varphi(t-2\tau)], \tag{24}$$

$$Q = \frac{12}{\tau}\frac{(e^{H\tau} - E)}{(23E - 16e^{-H\tau} + 5e^{-2H\tau})},$$

where matrix Q is obtained using special transformations of system (23) - see [16], R is the operator of the third-order Adams-Bashfort scheme, E is the unit matrix, τ is the integration step. The use of scheme (24) in comparison with the usual Adams-Bashfort scheme makes it possible to significantly weaken the restrictions on τ associated with the requirements for its stability.

Thus, the sequence of calculations is as follows:

1) The region of integration is divided into a certain number of elements M ;

2) A one-step algorithm (for example, the Runge-Kutta method) finds a solution on the first two time layers: $t = \tau, t = 2\tau$;

3) A number of non-degenerate transformations of matrix H are carried out in order to weaken the stability condition;

4) According to the formula (24), the transition to a new time layer $t = \tau$ is carried out;

5) The components of the vector v at the boundary points of the elements are found from the solution of the algebraic system (20).

RESULTS AND DISCUSSION

The constructed algorithm was applied to calculations of one-dimensional initial-boundary value problems for heat conduction equations.

In the case of the heat equation:

$$\frac{\partial u}{\partial t} = \upsilon \frac{\partial^2 u}{\partial \eta^2} , \qquad (25)$$

a comparison was made with the analytical solution for error rates:

absolute:

$$\Delta = \max_j \left| u_r\left(\eta_j, t_\phi\right) - u_\tau\left(\eta_j, t_\phi\right) \right|, \qquad (26)$$

and relative:

$$\varepsilon = \frac{\Delta}{\max_j \left| u_r\left(\eta_j, t_\phi\right) \right|} , \qquad (27)$$

where $u_r\left(\eta, t_\phi\right)$ and $u_\tau\left(\eta, t_\phi\right)$ are, respectively, a numerical and analytical solution at a fixed moment t_ϕ.

The initial conditions at time $t = 0$ were chosen in the form of a Gaussian distribution normalized to 1. The exact analytical solution in this case has the form:

$$u_r(\eta, t) = \sqrt{\frac{t_0}{t + t_0}} \cdot \exp\left[-\frac{\eta^2}{4R(t + t_0)} \right], \qquad (28)$$

$$R = \upsilon, \ \eta \in \left]-\infty, \infty\right[.$$

Constant t_0 determines the half-width of the initial distribution:

the less t_0, the narrower it is. Everywhere in the calculations: $t_0 = 0.15$, $\upsilon = 10^{-2}/\pi, n = 32, \tau = 0.01$. Integration interval is selected $\left[-1,1\right]$. For a given half-width of the initial distribution, function (28) at the boundary points is equal to zero with an accuracy of 10^{-12}. Therefore, equation (28) was solved under the following boundary conditions:
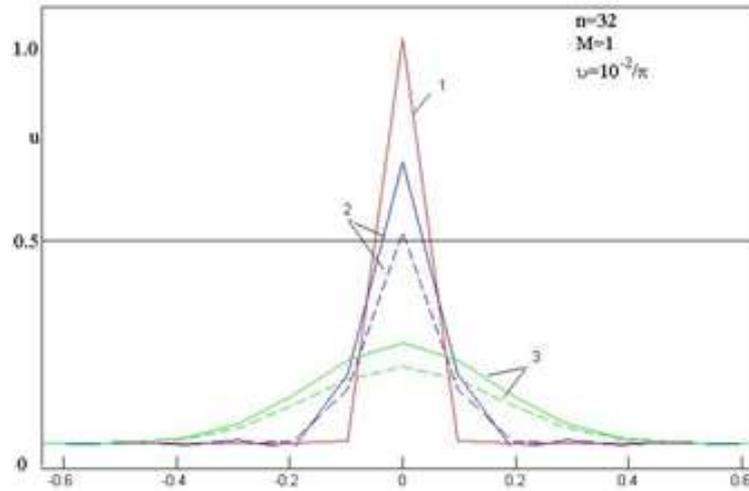
$$u(\pm 1, t) = 0, \qquad (29)$$

Fig.1

Figure 1 shows the evolution of the numerical solution of problem (25), (29), found using the constructed method in the case when the region of integration was not divided into elements $(M = 1)$. Solid curves 1, 2, 3 correspond to the numerical solution at times $t = 0, 40\tau, 400\tau$. Dotted curves 2, 3 correspond to the exact solution (28) at the same time instants. It can be seen that when using Chebyshev polynomials, the nodes on the interval are not rationally located - they thicken towards the edges of the interval, while only 14% of the nodes are in the region of rapid solution change. As a result, the solution accuracy turns out to be low: ε and Δ are of order 10^{-1} (see Table 1).
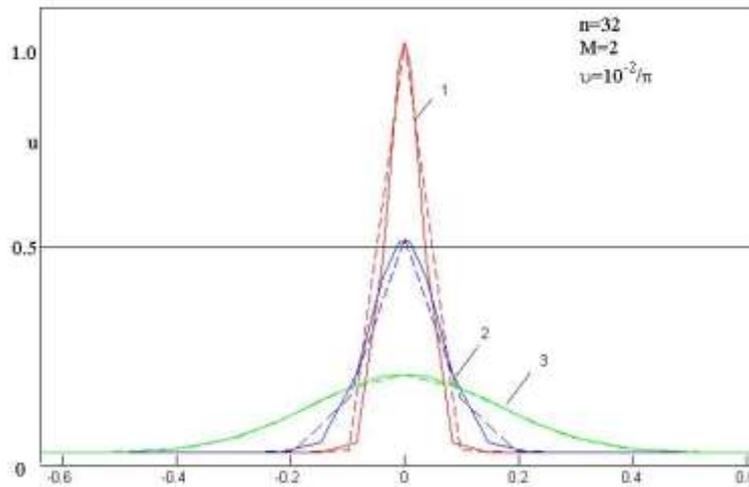
Fig.2

Figure: 2 shows the evolution of the numerical solution of the same problem for the case when the region of integration was divided into 2 elements: $[-1,0], [0,1]$. This division is more successful - about 30% of the grid nodes fall into the inhomogeneity region. The accuracy in this case is 2 orders of magnitude higher (see Table 2); therefore, the solid curves (numerical solution) and dashed curves (exact solution) in Fig. practically indistinguishable.

Table 1.
Calculation results

t	**0.01**	**0.1**	**0.4**	**2.0**	**4.2**
Δ	$2\cdot10^{-2}$	10^{-1}	$2\cdot10^{-1}$	$9\cdot10^{-2}$	$6\cdot10^{-2}$
ε	$2\cdot10^{-2}$	10^{-1}	$3\cdot10^{-1}$	$3\cdot10^{-1}$	$2\cdot10^{-1}$

Table 2.
Calculation results

t	0.01	0.1	0.4	2.0	4.2
Δ	$2{\cdot}10^{-2}$	$5{\cdot}10^{-3}$	$2{\cdot}10^{-3}$	$7{\cdot}10^{-4}$	$5{\cdot}10^{-4}$
ε	$2{\cdot}10^{-2}$	$6{\cdot}10^{-3}$	$4{\cdot}10^{-3}$	$3{\cdot}10^{-3}$	$2{\cdot}10^{-3}$

CONCLUSIONS
1. A spectral-grid explicit method for solving evolutionary problems with large gradients is constructed. Depending on the location of the regions of inhomogeneity, the integration interval is divided into a finite number of elements. On each of the elements, spectral approximation by finite series in basis functions is used.
2. Concrete calculations for the heat conduction equation have been performed, and a comparison has been made with the single-element pseudospectral method.
3. It is shown that the use of the spectral-grid approximation makes it possible to significantly increase the accuracy of calculations without increasing the total number of basis functions.

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