Numerical solution of mathematical physics problems by the collocation method

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Abstract. A modified collocation method for the numerical solving boundary value problems of mathematical physics is proposed. The irregular arrangement of collocation nodes in the problem solving domain can sharply increase the accuracy of the numerical solution by improving the quality of the linear algebraic equations system, to which the solved boundary value problem leads. Various basis functions systems are considered. The proposed method allows one to obtain an approximate solution of boundary value problems for a wide range of linear and nonlinear elliptic, parabolic and wave equations in an analytical form. This numerical method makes it possible to significantly expand the application field of traditional numerical methods when solving applied problems for modelling fields of various physical natures, described by linear and nonlinear equations of mathematical physics. The developed method is used to solve a quantum-mechanical problem for a hydrogen molecule ion. The results obtained in this work show the high potentialities of the complete collocation method, which are based on the universality of the method and high accuracy of numerical solutions. The energy of the ion ground state calculated with the minimum number of collocation nodes differs from the experimentally obtained value by 13%.

1. Introduction
Numerical modelling of different physical nature fields is one of the urgent physics problems. Currently the finite element method (FEM) and the finite difference method (FDM) [1-2] are the most frequently used to solve these problems. However, the using these methods in solving specific problems of mathematical physics, is not always justified.

High requirements for the numerical solution accuracy, the need to take into account the boundary conditions containing the normal derivative of the desired function on surfaces with a complex configuration, the difficulties in solving nonlinear problems force us to investigate and develop alternative numerical methods for solving boundary value problems.

The point-sources method (PSM) is a promising numerical method for solving problems of mathematical physics. PSM can be considered as one of the collocation method (CM) variants [3-8]. By PSM, an approximate solution is represented as a linear combination of basis functions that exactly satisfy the basic equation. However, in the collocation method, it is allowed to use other basic functions, which significantly expands the capabilities of the numerical method [9-10]. In this work, one of the collocation method variants is developed. It can be used to solve a fairly wide range of boundary value problems in mathematical physics, including nonlinear problems.

2. Method of complete collocations
Consider a domain Ω of a two-dimensional or three-dimensional space with a boundary ∂Ω, in which a boundary value problem for the equation
\[ L(r)U(r) = f(r), \quad r \in \Omega \]

is solved with conditions on the boundary \( \partial \Omega \)

\[ \Lambda(r)U(r) = g(r), \quad r \in \partial \Omega, \]

where \( L(r) \) and \( \Lambda(r) \) are linear operators in the domain \( \Omega \) and on the boundary \( \partial \Omega \); \( f(r) \) and \( g(r) \) are given functions in the domain \( \Omega \) and on the boundary \( \partial \Omega \). Let a system of linearly independent functions \( \{\phi_i(r)\} \) be given that have the completeness property in the domain \( \Omega \).

We represent the solution of problem (1), (2) in the form of a series

\[ U(r) = \sum_{i=0}^{\infty} C_i \phi_i(r). \]

Since finding an infinite number of expansion coefficients is practically impossible, we will seek an approximate solution to problem (1), (2) in the form of a finite sum

\[ U_N(r) = \sum_{i=0}^{N-1} c_i \phi_i(r). \]

To determine the unknown expansion coefficients in (3), we proceed as follows. We place nodal points \( N_v \) and \( N_G \), collocation points in the domain \( \Omega \) and on the boundary \( \partial \Omega \), respectively. The total number of collocation points \( N = N_v + N_G \) should correspond to the number of coefficients \( N \) in the expansion (3). The coordinates of the nodes, collocation points, in the domain \( \Omega \) we denote as \( r_k \), \( k = 1 \div N_v \), and on the boundary \( \partial \Omega \) \( r_k \), \( k = (N_v + 1) \div N \). To find the expansion coefficients \( c_i \), we substitute (3) in equation (1) and in boundary condition (2) and require their exact fulfillment at the collocation points. The result is a system of linear algebraic equations

\[ \sum_{i=0}^{N-1} c_i L(r_k) \phi_i(r_k) = f(r_k), \quad k = 1 \div N_v, \]

\[ \sum_{i=0}^{N-1} c_i \Lambda(r_k) \phi_i(r_k) = g(r_k), \quad k = (N_v + 1) \div N. \]

We obtain the desired numerical solution in the form of a finite sum (3) after solving the system of linear algebraic equations (4) - (5). It should be noted that relation (3) gives an approximate analytical expression for the desired function \( U(r) \). This means that the resulting solution \( U(r) \) can be treated like any other analytical expression. It can be differentiated, other actions can be performed, and at the same time there is no additional numerical error.

The described here collocation method variant, which leads to a system of linear algebraic equations in the form of relations (4) - (5), will be called the complete collocations method (CCM), and system (4) - (5) will be called the CCM system. The word “complete” in the name of the CCM indicates that the collocation conditions must be satisfied not only at all internal nodal points of the solution domain \( \Omega \), but also at its boundary \( \partial \Omega \).

The main problem that arises in finding an approximate solution to (3) is associated with the possibility of ill-conditioned system (4) - (5). For example, it was shown in [11] that when a function of two variables is interpolated by polynomials of degree \( n \), the determinant of the system vanishes if the collocation nodes lie on the same curve of order \( n \). A similar result takes place for functions of three variables. Therefore, with a regular, for example, with a uniform arrangement of collocation points, it is usually impossible to avoid bad conditioning. However, if you make adjustments in the location of the
collocation points, randomly making a small displacement of them, then the problem associated with the poor conditioning of the CCM system (4) - (5) can be eliminated.

Various variants of collocation methods differ from each other primarily in the system of used basis functions \( \{ \phi_i(\mathbf{r}) \} \). For example, solving two-dimensional problems, you can use functions of the form

\[
\phi_i(\mathbf{r}) = x^{i_x} y^{i_y},
\]

and solving three-dimensional boundary value problems, can use functions of the form

\[
\phi_i(\mathbf{r}) = x^{i_x} y^{i_y} z^{i_z}.
\]

Each the number value \( i \) in (6), (7) must correspond to a certain set of numbers \( i_x, i_y, i_z \). In addition, the basis functions must be ordered thus, that with an increase in the ordinal number of the basis function \( i \), the total degree of the basis function \( n = i_x + i_y + i_z \) does not decrease, moreover \( \phi_i(\mathbf{r}) = 1 \).

An approximate solution can also be searched in the form of a trigonometric sum (truncated Fourier series). Basic functions have certain attractiveness that taking a maximum, for example, a single value at the point of location of the corresponding collocation node and decrease with distance from this node. These can be, for example, functions of the following types:

\[
\phi_i(x, y) = \exp \left[ -k \left( x - x_i \right)^2 + \left( y - y_i \right)^2 \right],
\]

\[
\phi_i(x, y) = \left[ 1 + k \left( x - x_i \right)^2 + \left( y - y_i \right)^2 \right]^{-1}.
\]

Here, the constants \( k \) are selected in such a way as to provide the smallest error in the numerical solution. The possibility of using other basic functions to obtain a solution to boundary value problems using the CCM is not excluded.

The CCM can be successfully used to solve various problems of mathematical physics, both linear and nonlinear [12-14]. The CCM is most naturally used to solve boundary value problems for linear equations of mathematical physics. However, it is possible to successfully apply the method under consideration when solving boundary value problems for an equation of parabolic type [12-14]. Below, as an example, we solve a quantum mechanical problem for a hydrogen molecule ion.

3. Hydrogen molecule ion model

The hydrogen molecule ion \( \ce{H_2^+} \) consists of two hydrogen nuclei and one electron. Let us denote the distance between two hydrogen nuclei (nucleus A and nucleus B) through \( a \). We will assume that the value of \( a \) changes adiabatically and when solving the Schrödinger equation, it can be taken constant. This means that vibrations of nuclei around the equilibrium position, as well as rotation of nuclei around the center of gravity, will not be taken into account.

Let us consider the motion of an electron in a polar coordinate system \( (\rho, \varphi, z) \), placing nucleus A and nucleus B on the z axis at an equal distance from the origin. The potential energy of an electron in the Coulomb field of the nuclei of a molecule is determined by the expression

\[
U(\rho, z) = -e^2/(4\pi\varepsilon_0)^{1/2} \left( \frac{\rho^2 + (z - a/2)^2}{\rho^2 + (z + a/2)^2} \right)^{1/2}.
\]

The Schrödinger equation for an electron with zero orbital angular momentum has the form

\[
-h^2/(2m)^{1/2} \Delta \Psi = -e^2/(4\pi\varepsilon_0)^{1/2} \left( \frac{\rho^2 + (z - a/2)^2}{\rho^2 + (z + a/2)^2} \right)^{1/2} \Psi = E \Psi,
\]

where \( E \) is the electron energy.

We will seek ax symmetric solutions for which \( \Psi(\rho, z, \varphi) = \psi(\rho, z) \). Obviously, this solution corresponds, in particular, to the ground state of the ion.
Let's move on to atomic units of length $4\pi\varepsilon_0 h^2 (me^2)^{-1}$ and energy $me^4 (4\pi\varepsilon_0 h)^2$. In these units, the Schrödinger equation has the form

$$\Delta \psi + 2\rho \left[ E + \left( \rho^2 + (z-a/2)^2 \right)^{1/2} + \left( \rho^2 + (z+a/2)^2 \right)^{1/2} \right] \psi = 0.$$  

(10)

4. Results and discussion

Solving the problem numerically, it was first assumed that $a = 2.1$ au, which corresponds to the known equilibrium distance between the nuclei of the hydrogen molecule ion [15]. The solution domain $\Omega$ was specified as a square with side $L=8a$. It was assumed that the wave function vanishes at the boundaries of the domain $\Omega$. The correctness of this assumption was confirmed during subsequent testing of the problem.

The CCM system (4) - (5) for the problem being solved is homogeneous and its solution is reduced to finding such energy values $E$ for which the wave function $\psi(\rho, z)$ has a nontrivial solution that vanishes at the boundaries of the domain $\Omega$. To obtain a nontrivial solution, a certain point $M$ is set inside the domain $\Omega$, for example, between the hydrogen nuclei, in which the value of the wave function is certainly not zero. At this point, the value of the wave function is assumed to be equal to unity: $\psi(M) = 1$. This condition can be regarded as a condition for normalizing the wave function. After obtaining the solution, the wave function can be easily renormalized.

As shown above, the numerical solution of boundary value problems using the CCM assumes to use of a certain system of basis functions. When solving the Schrödinger equation (10), the impossibility of using power functions (6) was found due to the instability of the numerical solution. Satisfactory results can be obtained using exponential (8) or hyperbolic (9) basis functions.

The problem is solved in accordance with the following algorithm. The initial value of the electron energy $E_0$ and the step of energy variation $\delta E$ are set. It is desirable that this step be much less than the distance $\Delta E$ between the nearest energy eigenvalues, $\delta E \ll \Delta E$. For each energy value $E = E_0 + k\delta E$, therefore, at $k = 0, 1, 2, \ldots$, the CCM system (4) - (5) is solved. The parameter is calculated as a criterion for the problem on the energy eigenvalues

$$K = \left[ \sum_{k=1}^{N_s} \left| \text{abs}(\psi(r_k)) \right| \right]^{-1}.$$  

(11)

Here, the summation is performed over all points (not necessarily collocation nodes) located at random on the boundary of the domain $\Omega$. The number of these points is equal to $N_s$. We will call parameter (11) the boundary criterion.

On the graph of the dependence of the criterion $K$ on the energy $E$, the maxima should correspond to the eigenvalues of the electron energy. Figure 1 shows such a graph. The calculations were carried out with the total number of nodes $N = 426$, $N_8 = 100$; the constants $k$ in (8), (9) were set equal to $k = 7$. The electron energy varied from -40 eV to 0. The graph clearly shows three maxima corresponding to energies of -29.4 eV, -17.1 eV and -9.4 eV. Energy $E_0 = -29.4$ eV corresponds to the ground state of an electron in a hydrogen ion. The total energy of the ion is the sum of the energy of the electron and the energy of the Coulomb interaction of nuclei, equal (at 2.1 au) $U_0 = 13.0$ eV, which adds up to the energy of the ground state $W_0 = -16.4$ eV. The deviation from the experimental value of the energy equal to -18.8 eV [15] is about 13%. For the simplest numerical model presented here, this accuracy is quite acceptable.

Then, the dependence of the ground state energy of the ion $W_0$ on the intern clear distance $a$ was calculated. The distance $a$ was varied from 0.5 au to 5.0 au. Using a numerical model based on the CCM, the energy of the ground state of the electron in the ion was found for each value of $a$, and then the energy of the ion $W_0$. Figure 2 shows a graph of the dependence $W_0 = W_0(a)$. This dependence has a
minimum at 1.8 au. The deviation from the experimental value \( a = 2.1 \) au is 14\%, which also seems to be a quite acceptable error.

![Figure 1](image1.png)  
![Figure 2](image2.png)

**Figure 1.** Dependence of the boundary criterion \( K \) on the electron energy  
**Figure 2.** Dependence of the hydrogen ion ground state energy on the distance between the nuclei

5. Conclusion
The numerical solution of boundary value problems for elliptic and parabolic equations can become a difficult problem to solve, even if the sought solution is sufficiently smooth. Certain difficulties can arise if the original equation does not belong to the standard type of mathematical physics equations, or if the boundary conditions contain derivatives along the normal. In this case, the numerical solution of the boundary value problem using the finite element method (FEM) or the finite difference method (FDM) may have too slow convergence and not provide the required accuracy of the result. In these cases, as the results of the data presented here show, one can try to solve the boundary value problem using the CCM.

In these cases it is possible to solve the boundary value problem using the CCM. The results obtained confirm the possibility of using this method in solving not only two-dimensional, but also three-dimensional boundary value problems, including nonlinear ones. As in PSM, the solution using the CCM is obtained in an analytical form. Therefore, the obtained solution can be differentiated without loss of accuracy, and other mathematical operations can be performed with it.

Thus the presented methods compare favorably with FEM and FDM. It should also be noted the high accuracy of the results obtained using the CCM. All this makes the CCM a promising numerical method for modeling fields of various physical natures, using it in solving various physical problems, for example, quantum mechanical problems, an energy eigenvalues problems. Taking into account the extreme simplicity of the computer implementation of the CCM, further studies of this method possibilities should be considered promising.

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