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RESEARCH ARTICLE

Methods and effective algorithms for solving multidimensional integral equations

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Abstract

Objectives. Integral equations have long been used in mathematical physics to demonstrate existence and uniqueness theorems for solving boundary value problems for differential equations. However, despite integral equations have a number of advantages in comparison with corresponding boundary value problems where boundary conditions are present in the kernels of equations, they are rarely used for obtaining numerical solutions of problems due to the presence of equations with dense matrices that arise that when discretizing integral equations, as opposed to sparse matrices in the case of differential equations. Recently, due to the development of computer technology and methods of computational mathematics, integral equations have been used for the numerical solution of specific problems. In the present work, two methods for numerical solution of two-dimensional and three-dimensional integral equations are proposed for describing several significant classes of problems in mathematical physics.

Methods. The method of collocation on non-uniform and uniform grids is used to discretize integral equations. To obtain a numerical solution of the resulting systems of linear algebraic equations (SLAEs), iterative methods are used. In the case of a uniform grid, an efficient method for multiplying the SLAE matrix by vector is created.

Results. Corresponding SLAEs describing the considered classes of problems are set up. Efficient solution algorithms using fast Fourier transforms are proposed for solving systems of equations obtained using a uniform grid.

Conclusions. While SLAEs using a non-uniform grid can be used to describe complex domain configurations, there are significant constraints on the dimensionality of described systems. When using a uniform grid, the dimensionality of SLAEs can be several orders of magnitude higher; however, in this case, it may be difficult to describe the complex configuration of the domain. Selection of the particular method depends on the specific problem and available computational resources. Thus, SLAEs on a non-uniform grid may be preferable for many two-dimensional problems, while systems on a uniform grid may be preferable for three-dimensional problems.

Keywords: integral equations, collocation method, fast Fourier transform

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НАУЧНАЯ СТАТЬЯ

Методы и эффективные алгоритмы решения многомерных интегральных уравнений

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Резюме

Цели. Интегральные уравнения давно и широко используются в математической физике для доказательства теорем существования и единственности решения краевых задач для дифференциальных уравнений. Однако, несмотря на то что интегральные уравнения имеют ряд преимуществ по сравнению с соответствующими краевыми задачами – все краевые условия присутствуют в ядрах уравнений, они практически не использовались для численного решения задач. Это связано с тем, что при дискретизации интегральных уравнений возникают системы уравнений с плотными матрицами, в отличие от разреженных матриц в случае дифференциальных уравнений. В последнее время, в связи с развитием вычислительной техники и методов вычислительной математики, интегральные уравнения начали использоваться при численном решении конкретных задач. В работе предложены два метода численного решения двухмерных и трехмерных интегральных уравнений, описывающих многие важные классы задач математической физики.

Методы. Для дискретизации интегральных уравнений использовался метод коллокации на неравномерной и равномерной сетках. Для численного решения получившихся систем линейных алгебраических уравнений (СЛАУ) используются итерационные методы. Для случая равномерной сетки построен эффективный метод умножения матрицы СЛАУ на вектор.

Результаты. Построены соответствующие СЛАУ, описывающие рассматриваемые классы задач. Для решения систем уравнений, полученных с использованием равномерной сетки, предложены эффективные алгоритмы решения, использующие быстрое дискретное преобразование Фурье.

Выводы. СЛАУ с использованием неравномерной сетки имеют преимущество, связанное с хорошим описанием областей сложной конфигурации, но при этом есть существенные ограничения на размерность СЛАУ. При использовании равномерной сетки размерность СЛАУ может быть на несколько порядков больше, однако в этом случае могут возникать трудности с описанием сложной конфигурации области. Выбор того или иного метода зависит от конкретной задачи и имеющихся вычислительных ресурсов. Для многих двухмерных задач может быть предпочтительнее СЛАУ на неравномерной сетке, а для трехмерных задач – предпочтительнее СЛАУ на равномерной сетке.

Ключевые слова: интегральные уравнения, метод коллокации, быстрое преобразование Фурье

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INTRODUCTION

Let the bounded domain Q be given in Euclidean space E_n, where $n = 2, 3$. This means that Q is a figure on a plane ($n = 2$) or in space ($n = 3$). We shall consider the following integral equation in domain Q:

$$(1+\alpha\eta(x))u(x)+\int_Q \frac{K(x-y)}{R^m}\eta(y)u(y)dy = \\ = u^0(x),\ x\in Q,\ m\le n. \quad (1)$$

Here, $R = |x - y|$; $x = (x_1, \ldots, x_n)$; $y = (y_1, \ldots, y_n)$; α, η, K, u^0 are known functions with $K(x - y)$ being a differentiable coordinate function; u is the unknown function.

Equation (1) describes many practically significant classes of problems. Below are some problems in mathematical physics that may be reduced to equation (1):

- acoustic wave scattering on the inhomogeneous transparent obstacle [1]. In this case, $m < n$, $\alpha = 0$ while other functions included in equation (1) are scalar. Then the equation is the classical Fredholm integral equation of the 2nd kind;
- scattering of electromagnetic waves on the inhomogeneous, anisotropic in general, dielectric body [2, 3]. In this case, $m = n$, and therefore the integral operator in (1) is singular; u and u^0 are vector functions; and η and K are tensor functions. Value α determines the non-integral term of the singular operator and depends on the shape of the singularity and its center. For example, if the singularity is a sphere ($n = 3$) or a circle ($n = 2$), then $\alpha = 1/n$ [4, 5].

Other classes of problems in math physics may also be described using integral equations [6–8].

It is assumed that equation (1) has the only solution in the corresponding function space. It is possible to use only numerical methods for solution (1) when describing real problems. Then equation (1) is approximated by the system of linear algebraic equations (SLAE) with dense matrix using the Galerkin method or collocation method. In this case, the dimensionality N of resulting systems is usually very high ($N >> 1000$) due to the multidimensionality of the equation.

The main efficiency criteria of the numerical algorithm are the number of arithmetic operations T required for obtaining the original problem solution and the amount of computer memory M required for implementing the algorithm. When using the direct Gaussian method for solving SLAE, it is necessary to perform $T \sim N^3$ arithmetic operations and store about $M \sim N^2$ numbers in computer memory. It is clear that the solution for the considered problems requires significant computational resources. For iterative methods, the specified characteristics of algorithms are estimated by the following equations [9]:

$$T \sim LT_A,\ M \sim M_A, \quad (2)$$

where T_A is the number of arithmetic operations required to multiply the SLAE matrix by vector; L is the number of iterations required to obtain the solution with a given accuracy; M_A is the number of different matrix elements.

COLLOCATION METHOD

The collocation method is used for approximating integral equation (1) [3, 10, and 11]. Here, a significant difference between multidimensional problems and one-dimensional problems considered on interval $[a, b]$ should be noted. For such one-dimensional problems, the numerical solution does not cause problems related to describing the domain boundary. For two-dimensional and three-dimensional problems, certain difficulties arise in the discretization of integral equations defined in domains of complex shape.

The domain Q is presented as a union of N_Q cells $\Omega(i)$, $i = 1, \ldots, N_Q$. Nodal points in these cells are selected in their centers defined by the following equations [12]:

$$x_l^c = \frac{\int_\Omega x_l dx}{mes\,\Omega},\ l = 1,\ldots,n, \quad (3)$$

where $dx = dx_1dx_2$ for two-dimensional problems, $dx = dx_1dx_2dx_3$ for three-dimensional problems, and $x^c = (x_1^c,\ldots,x_n^c)$ is the center of the cell Ω with $mes\ \Omega$ being its volume ($n = 3$) or area ($n = 2$).

If the differentiable function of its arguments $f(x)$ is defined in domain Ω, then the following approximation is true:

$$\int_\Omega f(x)dx \approx f(x^c)mes\,\Omega. \quad (4)$$

Here, if $f(x)$ is a linear function of arguments, then expression (4) is exact equality.

If tetrahedrons ($n = 3$) or arbitrary triangles ($n = 2$) are considered as cells, then many complex configurations of domain Q may be described quite accurately. The center of corresponding cells is defined by the following simple equation:

$$x_l^c = \frac{\sum_{k=1}^{n+1} x_l^{(k)}}{n+1},\ l = 1,\ldots,n, \quad (5)$$

where $(x_1^{(k)},\ldots,x_n^{(k)})$ is Cartesian coordinates of the kth vertex of the cell.

We shall approximate integral equation (1) by SLAE of dimension $\sim N_Q$ with respect to the values of the unknown function at node points of domain Q located in centers x^{ci} of cells $\Omega(i)$, $i = 1, ..., N_Q$. The dimensions of cells are selected to provide the desired function weakly changing within a cell. Then corresponding SLAE may be written in the following form [3, 13]:

$$\gamma(i)u(i) + \sum_{j=1}^{N_Q} A(i,j)\eta(j)u(j) = u^0(i),$$
$$i = 1,..,N_Q,\ \gamma(i) = 1 + \alpha(i)\eta(i),$$

$$A(i,j) = \int\limits_{\Omega(j)} \frac{K(x^{ci} - y)}{\left|x^{ci} - y\right|^m} dy,\ i \neq j,\quad A(i,i) = 0,$$

$$u(i) = u(x^{ci}),\ u^0(i) = u^0(x^{ci}),\ \eta(i) = \eta(x^{ci}). \qquad (6)$$

For vector problems, tensor $\alpha(i)$ is determined by the shape of cell $\Omega(i)$ and its center.

Approximation (5) or more accurate numerical integration algorithms may be used for calculating integrals in (6). It should be noted that since nodal points are located in the center of cells, the approximation accuracy of integral operators is $\sim h^2$, where h is the maximum cell diameter (cell diameter is considered as the maximum distance between border points). For relatively small values $N_Q \leq 10\,000$, the system of equations (6) may be solved by direct or iterative methods. Efficient algorithms for solving the system of equations (6) using iterative methods are discussed below.

COLLOCATION METHOD ON UNIFORM GRID

In the kernel of integral equation (1), the term depending on the difference between the Cartesian coordinates of points x and y presents itself. However, this is not used in setting up SLAE (6). Below, we shall create the efficient numerical method for solving equation (1) using uniform grid and discrete Fourier transform (DFT).

We shall write some auxiliary equations using DFT first. Consider complex function $f(n)$ of discrete argument $n = 0, \pm1, \pm2, ...$ Here, it is assumed that $f(n)$ is a periodic function having period N, i.e., $f(n \pm N) = f(n)$ for any n.

The DTF of function $f(n)$ is defined by the following well-known equation:

$$F[f] = f^F(k) = \sum_{n=0}^{N-1} \exp\left(i\frac{2\pi}{N}kn\right) f(n),\ k = \overline{0, N-1}, \qquad (7)$$

where, obviously, the Fourier transform $f^F(k)$ is also a periodic function with period N.

If the Fourier transform $f^F(k)$ is known, then the initial function $f(n)$ may be restored using inverse DFT (IDFT), as follows:

$$F^{-1}[f^F] = f(n) =$$
$$= \frac{1}{N}\sum_{k=0}^{N-1} \exp\left(-i\frac{2\pi}{N}kn\right) f^F(k),\ n = \overline{0, N-1}. \qquad (8)$$

Generally, the number of arithmetic operations $T_F(N)$ required for calculating DFT without calculating functions of the form $\exp\left(i\frac{2\pi}{N}kn\right)$ additionally can be estimated by the following equation:

$$T_F(N) \sim N^2. \qquad (9)$$

When using fast Fourier transform (FFT) algorithms, the number of required arithmetic operations is estimated by the following equation [3]:

$$T_{FF}(N) \sim N\,\mathrm{LOG}(N), \qquad (10)$$

where LOG(N) is integer logarithm, i.e., the sum of all prime divisors of N. If N is a power of two, then $T_{FF}(N) \sim N \log2(N)$.

Let $A(l)$ be a periodic function of a discrete argument with period N. Consider sums of the following forms:

$$v(n) = \sum_{m=0}^{N-1} A(n-m)u(m),\quad n = \overline{0, N-1}. \qquad (11)$$

Sums (11) arise from multiplying circular matrices by vector. We shall apply DFT with period N to both parts of (11). It is easy to show that

$$v^F(k) = A^F(k)u^F(k),\quad k = \overline{0, N-1}. \qquad (12)$$

Using (12) and FFT algorithms, circular matrices may be efficiently multiplied by vector. However, circular matrices rarely appear in real problems. Although many problems, particularly those discussed below, require the calculation of sums of form (11) where the function $A(l)$, $-(N-1) \leq l \leq (N-1)$, is arbitrary within the specified range. Such sums arise from multiplying Toeplitz matrices by vector [14, 15]. The specified function $A(l)$ is defined at integer point $(2N-1)$. We shall predefine the function $A(l)$ by zero at point $l = N$ and extend it to all integer values with period $2N$. The function of discrete argument $u(m)$, $m = 0, ..., N-1$, is defined zero at points $m = N, ..., 2N-1$. We shall consider the sums of the following form:

$$v(n)=\sum_{m=0}^{2N-1}A(n-m)u(m),\quad n=\overline{0,2N-1}. \qquad (13)$$

It follows from the above that function $v(n)$ from (13) coincides with values $v(n)$ from (11) at $n = 0, ..., N - 1$. The following equation may be used for quickly calculating sums (13):

$$v^{\mathrm{F}}(k)=A^{\mathrm{F}}(k)u^{\mathrm{F}}(k),\quad k=\overline{0,2N-1}. \qquad (14)$$

In IDFT, components $v(n)$, $n=\overline{0,N-1}$, are of significance only. Thus, it follows from (10) that the number of arithmetic operations for calculating (11) may be estimated by the following equation:

$$T_{\mathrm{A}}\sim 2N\,\mathrm{LOG}(2N). \qquad (15)$$

In this case, the array with the number of the following elements should be stored in computer memory:

$$M_{\mathrm{A}}\sim 2N. \qquad (16)$$

Therefore, we shall discretize integral equation (1). First, three-dimensional problems are considered. Let us define parallelepiped P with domain Q being inside in the Cartesian rectangular coordinate system. The edges of the parallelepiped are parallel to the coordinate axes, while the edge lengths are equal to $N_l h_l$, l, = 1, 2, 3, where h_l are the grid steps in Cartesian coordinates. Then parallelepiped P can be represented as the union of cells (elementary parallelepipeds) P(p), $p = (p_1, p_2, p_3)$, $p_l = 0, \ldots, N_l - 1$. We shall define domain $\tilde{\mathrm{Q}}$ as the union of N_{Q} cells which centers are located inside domain Q. The nodal points at which function values are determined can be defined in the centers of cells and denoted as $x(p)$, while the function values at these points are denoted as $f(p)$.

Integral equation (1) is approximated, similarly to (6), using SLAE of the following form [5]:

$$\gamma(p)u(p)+\sum_{y(q)\in\mathrm{Q}}A(p-q)\eta(q)u(q)=u^0(p),\ x(p)\in\mathrm{Q},$$

$$A(p-q)=\int_{\Pi(q)}\frac{K(x(p)-y)}{|x(p)-y|^m}dy,\ p\neq q,\quad A(0)=0,$$

$$\gamma(p)=1+\alpha(p)\eta(p). \qquad (17)$$

Since the nodal points are located in the center of cells, the approximation accuracy of the integral operator is $\sim h^2$, $h=\sqrt{h_1^2+h_2^2+h_3^2}$.

It follows from (17) that the main computational costs when multiplying the SLAE matrix by vector (performing one iteration) are associated with calculating sums of the following form:

$$W(p)=\sum_{y(q)\in\mathrm{Q}}A(p-q)V(q),\quad x(p)\in\mathrm{Q}. \qquad (18)$$

For calculating $W(p)$ at nodal points $x(p) \in$ Q, it is necessary to perform $\sim N_{\mathrm{Q}}^2$ arithmetic operations, where N_{Q} is the number of nodal points in domain Q. However, the number of arithmetical operations may be reduced through using fast multiplication technique of Toeplitz matrices by vector discussed above.

We shall complete the definition of function $V(q)$ by zero at points $x(q)$ of parallelepiped P, which do not belong to Q. The following sums are considered:

$$W(p_1,p_2,p_3)=$$
$$=\sum_{q_1=0}^{N_1-1}\sum_{q_2=0}^{N_2-1}\sum_{q_3=0}^{N_3-1}A(p_1-q_1,p_2-q_2,p_3-q_3)V(q_1,q_2,q_3). \qquad (19)$$

Obviously, values $W(p)$ from (18) and (19) coincide at $x(p) \in$ Q. In (19), the matrix function of discrete argument $A(p)$ is defined for values $-(N_1 - 1) \le p_1 \le (N_1 - 1)$, $-(N_2 - 1) \le p_2 \le (N_2 - 1)$, $-(N_3 - 1) \le p_3 \le (N_3 - 1)$.

Let us denote the parallelepiped with sides $2N_1h_1$, $2N_2h_2$, and $2N_3h_3$ by P_2. We extend the matrix function of discrete argument $A(p_1, p_2, p_3)$ to all integer values p_1, p_2, and p_3 assuming it to be periodic for each variable with periods $2N_1$, $2N_2$, and $2N_3$, respectively. Here, we shall complete the definition of function $A(p_1, p_2, p_3)$ by zero at points where it is undefined. Let us further define the function of discrete argument $V(p_1, p_2, p_3)$ as zero at all nodal points P_2 not belonging to P and extend it to all integer values p_1, p_2, and p_3 assuming it to be periodic for each variable with periods $2N_1, 2N_2$, and $2N_3$, respectively.

We shall consider the following equation:

$$W(p_1,p_2,p_3)=$$
$$=\sum_{q_1=0}^{2N_1-1}\sum_{q_2=0}^{2N_2-1}\sum_{q_3=0}^{2N_3-1}A(p_1-q_1,p_2-q_2,p_3-q_3)V(q_1,q_2,q_3). \qquad (20)$$

Given the above, it is clear that function $W(p_1, p_2, p_3)$ from (20) coincides with values $W(p_1, p_2, p_3)$ from (18) at $x(p) \in$ Q. Integer parallelepipeds with the number of discrete arguments on each axis N_1, N_2, and N_3 and $2N_1$, $2N_2$, and $2N_3$ are denoted by P and P_2, respectively. Performing FDT on each variable from both parts of (20), the following equation may be written:

$$W^{\mathrm{F}}(k_1,k_2,k_3)=A^{\mathrm{F}}\left(k_1,k_2,k_3\right)V^{\mathrm{F}}(k_1,k_2,k_3),\ k\in\mathrm{P}_2. \qquad (21)$$

Thus, since transformation of function $A(p_1, p_2, p_3)$ is performed once before the iteration procedure, performing one iteration in solving SLAE (17) requires direct Fourier transformation of function $V(p_1, p_2, p_3)$ on each variable and an inverse transformation of function $W^F(k_1, k_2, k_3)$. The number of arithmetic operations and the amount of memory required for performing one iteration is estimated by the following equations:

$$T_A \sim 10N \,\mathrm{LOG}(N),\ M_A \sim 10N,\ N = N_1N_2N_3. \quad (22)$$

For solving two-dimensional problems in a Cartesian coordinate system, domain Q is located inside a defined rectangle. Further reasoning and calculations with obvious modifications repeat the considered case. The values M_A and T_A are evaluated by equations (22) where $N_3 = 1$.

When choosing grid steps and values N_1, N_2, and N_3 (three-dimensional problems) or N_1, N_2 (two-dimensional problems), it is necessary to be guided by the following criteria: first, the desired function varies little within the cells; second, domain $\tilde{Q}$, consisting of cells whose centers are inside Q, is sufficient for describing Q.

When using FFT algorithms, values N comprising multiples of a power of two are generally selected. However, when discretizing integral equations, this often results in significant additional computational costs due to the rather high duty cycle of numbers of a power of two. This may be examplified by the following.

Let $N_1 = N_2 = N_3 = N_0$, i.e., P is a cube. It is assumed that it would be sufficient to take value $N_0 = 150$ for approximating the solution with the required accuracy. The closest powers of two are numbers 128 and 256. Since the value 128 does not satisfy the requirement of approximating the solution, value $N_0 = 256$ should be taken for using conventional FFT. Let $T(N_0)$ be the number of arithmetic operations required to multiply the SLAE matrix by vector depending on values of N_0. Then the following maybe derived from (22):

$$\frac{T(256)}{T(150)} \approx \frac{256^3 \log_2(256)}{150^3\, LOG(150)} \approx 2.5.$$

The amount of memory for storing the SLAE matrix at $N_0 = 256$ is also several times larger than at $N_0 = 150$. Thus, using FFT for $N_0 = 150$ is much more efficient than using FFT with a power of two.

It should be noted that, for solving SLAE (17) using the considered algorithm, only iterative methods can be used. This is due to iterative algorithms being based on multiplying the SLAE matrix by vector. The number of arithmetic operations and the amount of memory required for solving SLAE (17) are estimated by equations (2) and (22). At the same time, the number of iterations required for obtaining a solution is typically much smaller than the SLAE dimensionality. Thus, it may be possible to numerically solve integral equation (1), which is reduced to high dimension SLAE $N_Q > 10^6$.

CONCLUSIONS

The paper deals with two methods for obtaining a numerical solution of two- and three-dimensional integral equations describing many significant classes of problems in mathematical physics. Here, the collocation method on non-uniform and uniform grids is used for discretizing equations. The corresponding SLAEs are set up. SLAEs using non-uniform grid may have the advantage of describing complex configuration domains well. However, there are significant constraints on the SLAE dimensionality. While the SLAE dimensionality may be several orders of magnitude higher when using a uniform grid, difficulties may arise when describing the domain complex configuration. The selection of one or another method depends on the specific problem and available computational resources. In the author's opinion, SLAE on a non-uniform grid may be preferable for many two-dimensional problems, while SLAE on a uniform grid may be preferable for three-dimensional problems.

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