Numerical Method of Integration on the Basis of Multidimensional Differential-Taylor Transformations

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***Abstract* — The paper presents a new numerical method integration for ordinary differential equations based on multidimensional differential-Taylor transformations. The method is designed to integrate differential equations whose right-hand side includes terms that are gradients of a potential function. A distinctive feature of the developed numerical-analytical method for integrating ordinary differential equations is that the calculation of accelerations in a differential equation is based on differential-Taylor transformations of various dimensions, while the calculation of the elements, used further in calculations based on one-dimensional differential-Taylor transformations, is made on the basis of multi-dimensional differential-Taylor transformations. The typical algorithm of a program for an explicit numerical scheme of integration by the developed method is proposed. The use of multidimensional differential-Taylor transformations reduces the methodological complexity of prescribing the initial data for developing a computerized integration procedure.**

Keywords — integration procedure, numerical method; multidimensional differential-Taylor transformations

I. INTRODUCTION

Nowadays, computer simulations are practiced in all human intellectual activities on a wide scale. Accordingly, there is a wide array of websites containing scientific and technical products, allowing visitors (clients) to carry out direct computer simulations in a remote access mode. The offered approach is a component of cloud computing technologies, which provides computer resources and capacities to a user as Internet services. In this scenario, users should only formulate their own computational problems, then enter the necessary numerical data, and start performing computations. Solutions to problems are provided to users on completion of the calculations [1].

II. STATE OF ART

The described use of Internet cloud computing services can be divided into two stages: the first one involves formulating (stating) a task and entering initial data by a user, the second one involves performing calculations and giving results. The distinguished stages often have a clear interconnection in the methodological and computational aspects. Therefore, developers, in the first instance, try to minimize (simplify) the methodological complexity of the implementation of the first stage. We can often achieve this through a compelled increase in computational complexity at the second stage. It can be affirmed that the described objective setting, aimed at reducing user methodical complexity, is not only expedient for Internet services, but also normal, regardless of the possible increase in computer computational complexity.

One of the possible problems of computer simulations is the computational solution of ordinary differential equations (ODE). In practice, tasks with right-hand side including a gradient (or partial derivatives) of a potential (or prescribed) function, and which are represented by ordinary differential equations, occur widely. For such tasks, at the above-described first stage of using a cloud computing service, a user needs to carry out analytical calculations to determine the right-hand side of a differential equation. It is quite logical that such analytical calculations increase the methodological complexity of this stage.

To avoid the described increase in methodological complexity, we can apply the mathematical apparatus of multidimensional differential-Taylor transformations (DTT). However, in all known methods, multidimensional DTT are used only to expand a previously solved problem of integrating ODE with one-dimensional DTT [2-6].

In view of the foregoing, it is important to develop a method of numerical integration of ordinary differential equations whose right-hand side includes terms that are gradients of potential functions, and which can be determined numerically and analytically for differential spectra without analytic calculations, on the basis of multidimensional differential-Taylor transformations.

III. PROBLEM SOLVING

Without loss of generality, we shall deal with the problem of numerical integration in which an ODE defines the motion of a material point in 3-dimensional space under the conservative forces defined by potential U and non-conservative forces (without potential) R [7]:

$$\frac{d^2x}{dt^2}=-\frac{\partial U}{\partial x}+R\text{, with } x_0=x(t_0),\ \dot{x}_0=\dot{x}_0(t_0), \quad (1)$$

where $x=(x_j)$, $j=\overline{1\ldots3}$, $\dot{x}$ is position and velocity vectors of the material point; t is physical time; x_0, $\dot{x}_0$, t_0 are initial values of the coordinates, velocity and time; $U=U(x)$, $\partial U/\partial x$ is potential and its gradient; $R=R(t,x,\dot{x})$ are non-conservative forces.

In practice, the problem type given in (1), where the potential U has a rather lengthy form, is often encountered. Moreover, defining the accelerations from the potential $U=U(x)$, defining the gradient $\partial U/\partial x$, is a separate problem, which can be solved by special methods. At the same time, the final formulas for defining (calculating) the accelerations in (1) from the potential are described by expressions that have a more lengthy form (include more constraints) and, accordingly, are more methodologically difficult to use in comparison with the expression for the initial potential.

In general, it can be stated that removing (or, at least, weakening) the effect of the above-described additional increase in methodological complexity, by reducing the necessary analytical calculations, is desirable for practical implementation in numerical integration of ODE (1).

Two-dimensional differential-Taylor transformations are called functional transformations [2-6]:

$$Q(k,k_w)=\frac{h^k h_w^{k_w}}{k!k_w!}\frac{\partial^{k+k_w}q(t_*,w_*)}{\partial t^k\partial w^{k_w}},$$

$$q(t,w)=\sum_{k_w=0}^{\infty}\sum_{k=0}^{\infty}\left(\frac{(t-t_*)^k}{h^k}\frac{(w-w_*)^{k_w}}{h_w^{k_w}}Q(k,k_w)\right), \quad (2)$$

where $q(t,w)$ is a scalar function having derivatives of the required order with respect to t and w; t, w are scalar arguments; t_*, w_* are values of the arguments at which the transformation is carried out; h, h_w are argument segments, on which $q(t,w)$ is represented by a Taylor's series with respect to t and w; k, k_w are integer arguments $0, 1,\ldots$; $Q(k,k_w)$ is discrete function with respect to the arguments k, k_w.

In (2), the first expression specifies the direct DTT, and the second is the inverse one. The DTT image $Q(k,k_w)$ is called T-spectrum, and its values are called T-discretes [2, 3, 6].

The potential gradient in (1) is as follows

$$\frac{\partial U(x)}{\partial x}=\left(\frac{\partial U(x)}{\partial x_j}\right)=\left(\frac{\partial U(x_1,x_2,x_3)}{\partial x_j}\right), \text{ with } j=\overline{1\ldots3}. \quad (3)$$

Taking into account the order of taking partial derivatives, the gradient (3) can be written as follows

$$\frac{\partial U(x)}{\partial x}=\left(\sum_{j_w=1}^{3}\frac{\partial U(x_1,x_2,x_3)}{\partial x_{j_w}}\frac{\partial x_{j_w}}{\partial x_j}\right),\ j=\overline{1..3}\Rightarrow$$

$$\Rightarrow\frac{\partial U(x)}{\partial x}=E_{3\times3}\left(\frac{\partial U(x)}{\partial x_1}\quad\frac{\partial U(x)}{\partial x_2}\quad\frac{\partial U(x)}{\partial x_3}\right)^T, \quad (4)$$

where $E_{3\times3}$ is the identity matrix.

We define the T-spectra of the vector elements x in accordance with (4). Then the application of DTT to $U(x)$ gives the T-spectrum in the following form:

$U(k_w)=U(X(k_w))$, with $X(k_w=0)=x_*$, $X(k_w=1)=h_wE_{3\times3}$, or, with the expansion of vector-matrix designations

$$\left(\begin{array}{l}U(X_1(k_w),X_2(k_w),X_3(k_w)):\{X_1(1)=h_w,X_2(1)=0,X_3(1)=0\}\\ U(X_1(k_w),X_2(k_w),X_3(k_w)):\{X_1(1)=0,X_2(1)=h_w,X_3(1)=0\}\\ U(X_1(k_w),X_2(k_w),X_3(k_w)):\{X_1(1)=0,X_2(1)=0,X_3(1)=h_w\}\end{array}\right):$$

$$\{X_1(0)=x_{1*},X_2(0)=x_{2*},X_3(0)=x_{3*}\}, \quad (5)$$

where $U(k_w)$, $X(k_w)$, $X_j(k_w)$, $j=\overline{1\ldots3}$ are the T-spectra of the potential, the vector x and its elements; x_{j_*}, $j=\overline{1,3}$ is values of the vector x and its elements, for which the T-spectrum is calculated; h_w is segment by vector elements x.

We consider the T-discrete in (5) with $k_w=1$ as follows:

$$U(k_w=1)=h_w\frac{\partial U(x_*)}{\partial x}. \quad (6)$$

From a comparison of (4) and (6) it can be seen that (6) is the sought-for gradient, up to a factor h_w. To obtain the gradient, it is necessary to perform the differentiation (6) with respect to k_w, in accordance with the properties of DTT [2-6]:

$$\frac{\partial U(x_*)}{\partial x}=D_{k_w}\{U(k_w=1)\}=\frac{1}{h_w}U(1). \quad (7)$$

Due to the fact that the segment of the argument h_w introduced in (5), is shortened in (7), it is advisable to prescribe it when defining the gradient

$$h_w=1. \quad (8)$$

Taking into account the properties of DTT, we obtain the method of integrating ODE (1) based on multidimensional DT-transformations, with reference to which we can write an explicit computational DTT scheme (1), where the T-spectrum of the gradient is determined by two-dimensional DTT in the form (5), (8):

$$\left\{\begin{array}{l}t_{i+1}=t_i+h_i,\ T(k)=t_i\delta_T(k)+h_i\delta_T(k-1),\quad X(0,0)=x(t_i),\\ X(1,0)=h_i\dot{x}(t_i),\quad X(k,1)=E_{3\times3}\delta_T(k,k_w-1),\\ U(k,k_w=1)=U(X(k,k_w)):\quad\{k_w=\overline{0\ldots1}\},\\ R(k)=R(T(k),X(k,0),\dfrac{k+1}{h_i}X(k+1,0)),\\ X(k+2,0)=\dfrac{h_i^{\,2}}{(k+2)(k+1)}(-U(k,1)+R(k)):\\ \qquad\qquad\{k=\overline{0\ldots(k_{\max}-2)}\},\end{array}\right.$$

$$x(t_{i+1}) = \sum_{k=0}^{k_{\max}} X(k,0),\ \dot{x}(t_{i+1}) = \sum_{k=0}^{k_{\max}} \frac{k+1}{h_i} X(k+1,0), \quad (9)$$

where $x(t_{i+1})$, $\dot{x}(t_{i+1})$ are the predicted position and speed; h_i, i is integration step and computational grid node; $X(k,k_w)$, $U(k,k_w)$ are two-dimensional spectra of the vector x and the potential U; $(k+1)/h_i\ X(k+1,0)$ is T-spectrum of the velocity; $R(k)$ is one-dimensional T-spectrum of non-conservative forces; $\delta_T(k)$, $\delta_T(k,k_w)$ are one and two-dimensional "tedas" [2]; $k_{\max}$ is the order of integration accuracy; $T(k)$ is T-spectrum of ODE independent variable t.

The algorithm of the ODE integration program for a uniform computational grid based on (9) is shown in Figure 1, with explanations in Table 1, where arrays are shown by square brackets, and round ones show functional dependencies. The use of arrays whose elements are arrays (including multidimensional ones), makes it possible to efficiently organize the computational process using an approach where the operations for determining DT images are implemented by a library of standard procedures.

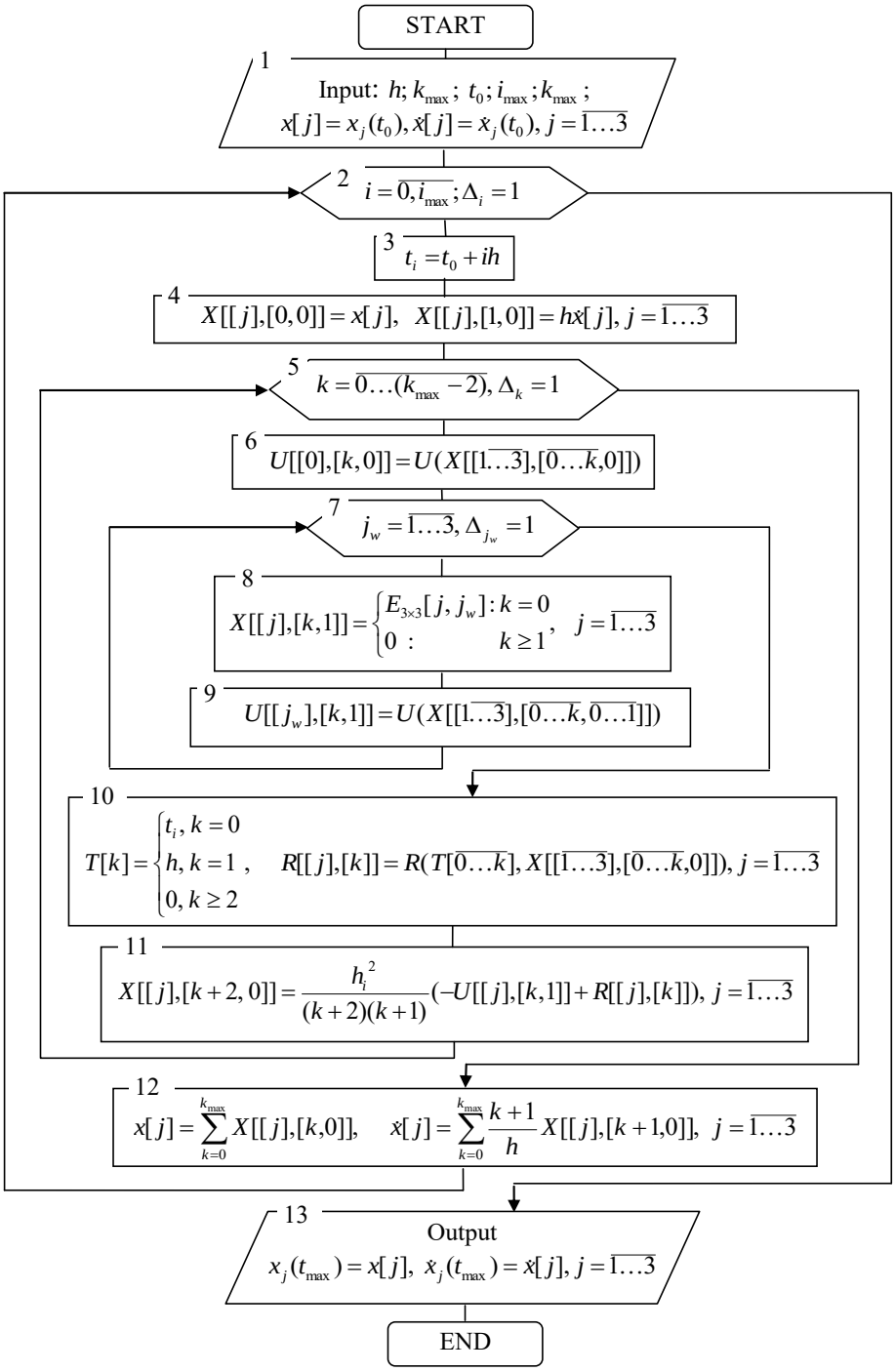

Fig. 1 Algorithm for implementing an explicit DT-scheme (9), (10) of integration (1)

Obtaining T-images of the right-hand side of the original differential equation (potential $U(k,k_w)$ and non-conservative forces $R(k)$) in the direct DTT is carried out (methodically simple) in the following order [2, 3, 6]: the

original functions $U = U(x)$, $R = R(t, x, \dot{x})$ are divided into "basic" mathematical operations (sum, subtraction, multiplication , division, exponentiation, trigonometric functions, etc.) that define the originals, then each operation (separately) together with the original is replaced with the corresponding T-image taken from the standard list.

TABLE 1. DESCRIPTION OF THE ALGORITHM BLOCKS IN FIG. 1

#	Operation and Arrays
1	Input of initial values: h, $k_{\max}$, t_0, $i_{\max}$, $x(t_0)$, $\dot{x}(t_0)$ are a step and an order of accuracy of integration, an initial value of time, a number of steps and element-wise initial values of coordinates and speed; $x[j], \dot{x}[j], j = \overline{1\ldots3}$ are arrays with size 3 of the elements of the vectors x and $\dot{x}$.
2	Integration step cycle.
3	Step with respect to the independent variable of ODE.
4	$X[[j],[k,k_w]]$, $j = \overline{1\ldots3}, k = \overline{1\ldots k_{\max}}, k_w = \overline{0\ldots1}$, is one-dimensional array (with respect to j), each element of which is a two-dimensional array (with respect to k, k_w) for storing the T-spectrum of the vector x.
5	Cycle for the recurrent calculation of the T-spectrum of the vector x.
6	Calculation of a T-discrete of the potential. $U[[j],[k,k_w]]$, $j = \overline{0\ldots3}, k = \overline{1, k_{\max}}, k_w = \overline{1, 2}$, is one-dimensional array (with respect to j), each element of which is a two-dimensional array (with respect to k, k_w) for storing the T-spectrum of the potential with $j = 0$ and the elements of the potential gradient vector with $j = \overline{1\ldots3}$.
7	Cycle for element-wise calculation of the T-spectrum of the gradient.
8	Filling of the vector $X[[j],[0,k_w = 1]]$, $j = \overline{1\ldots3}$ with a column of matrix $E_{3\times3}$.
9	Calculation of a T-discrete of the gradient element.
10	Calculation of a T-discrete of the nonconservative forces.
11	Recurrent calculation of a T-discrete of the vector x.
12	Calculation of the prediction results for the integration step vectors x and $\dot{x}$.

IV. EXPERIMENT AND RESULTS

The main property of the developed method (9) is the fact that it defines the accelerations from the potential, the definition of the gradient $\partial U/\partial x$ is carried out in a numerical-analytical form in the range of T-spectra, which reduces the methodological complexity of its realization in comparison with the traditional approach (analytical definition of the gradient) [7].

A distinctive feature of the developed method is that it is carried out in comparison with the traditional one (analytical definition of the gradient) for the problem of predicting the Earth's artificial satellite motion In such a task, the Earth's potential can include up to 320×320 terms, each of which is given by the product of 5-6 functions [7]. The results are shown in Table 2, where the decrease in methodological complexity is estimated in reducing the number of operators for calculating accelerations from the Earth potential, and the increase of computational complexity is estimated in increasing the number of elementary arithmetic operations (multiplications and divisions).

TABLE 2. COMPARATIVE CHARACTERISTICS OF THE DEVELOPED METHOD

Methodical complexity	Computational complexity
reduction up to 40%	increase from 2 to 4 times

V. CONCLUSION

The main property of DTT is the realization of a recurrent numerical and analytical definition of the terms of the Taylor series of any order in the absence of methodological errors, which can be formulated as follows: to define (calculate) the T-spectrum of a complex function, it is incumbent to specify the T-spectra of all its arguments according to its internal structure In this case, the dimensionality of the T-spectra of the arguments must coincide with the necessary dimensionality of the determined T-spectrum.

A distinctive feature of the developed numerical-analytical method for integrating ODE is that the calculation of accelerations in a differential equation is based on DTT of various dimensions, while the calculation of the elements, used further in calculations based on one-dimensional DTT, is made on the basis of multi-dimensional DTT.

Despite the fact that all the calculations are given for the ODE recorded for the three-dimensional space (1), the developed method is applicable to other ODEs whose right-hand side includes conservative forces, or partial derivatives of a prescribed function.

Therefore, the developed method can be effectively used for the numerical integration of ordinary differential equations of the type discussed above in systems, which provide Internet cloud computing services for solving such problems.

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