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METHOD OF APPROXIMATING SERIES FOR NUMERICAL INTEGRATION OF SYSTEMS OF DIFFERENTIAL EQUATIONS

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A method of numerical integration of systems of differential equations is proposed that can be used for equations that describe processes occurring in every field of physics, namely, fluid mechanics, nuclear physics, solid-state physics, etc. The APPROX program package, which implements the method of approximating series, makes it possible to write programs for computations in no more than 2-3 hours and reduces the calculation time by 1-2 orders in comparison with finite-difference methods.

Introduction. As investigations of the distribution of the processor time among problems solved on computers demonstrate, more than half of the time is spent on problems in which systems of differential equations are integrated. Most of all, this concerns problems of aerohydrodynamics and heat and mass transfer.

Despite the recent sharp increase in computer perfomance, overhead is a threshold parameter for the majority of problems that are of interest to researchers. In addition, a great number of problems have not yet been solved or are solved in an abbreviated physical formulation because of the prohibitively large overhead of processor time. Therefore, the problem of creating numerical methods that reduce the time for integrating systems of differential equations remains urgent.

1. Description of the Proposed Method. The sense of the method is that all the sought functions of differential equations are approximated by series (that is, are expanded in independent variables: space, time, and others). We then seek the coefficients of the expansion of the unknown functions. After that, we substitute the series into differential equations that are written for interior points of the calculation domain in a quantity sufficient to determine all the coefficients of the series (the number of points is to be equal in the total number of coefficients in the approximations of the sought functions). The location of the points within the domain is arbitrary and depends on the accuracy of the description of the physical process. The system of equations obtained is a system of nonlinear equations in the expansion coefficients in the general case and is solved by a method of solution for systems of nonlinear equations. After obtaining the coefficients of the series, the functions approximated by them can be found at the requisite points of the calculation domain.

By dividing the calculation domain into connected parts, describing differently the physical processes in parts of the calculation domain, changing variables, or transforming nonlinear terms, etc., it is possible to achieve a significant reduction in the number of sought coefficients and to reduce the calculation time.

Although the idea of approximate series of unknown functions lacks novelty (the following methods of integration of linear differential equations are well-known: integration by expanding the solution in a series, Krylov and Bogolyubov's approximate method [1], methods that use F-series to find a solution of Poisson's equation [21]), the method proposed has not been used for numerical integration of systems of differential equations and nonlinear differential equations. An explanation might be that creating a program for calculation according to the method proposed is at first sight a tedious activity since already when the number of coefficients is of the order of 20-30, writing down approximate series, differentiating them, substituting them into a system of differential equations, and writing the program itself will require at least as much time as creating a program using finite-difference methods. This seems especially true for the number of coefficients approaching 1000. However, this impression is

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false, since it is possible to develop mathematical expressions on modern computers. This is how the APPROX program package was made; it begins with the statement of the physical problem and the selection of approximating series and boundary and initial conditions and ends in a program in the high-level language FORTRAN or Ada with minimum expenses of the time and effort of an investigator.

2. Statement of the Problem. In the present work the method proposed is demonstrated for the case of a stationary flow of a viscous incompressible liquid in a two-dimensional channel of constant width.

The initial system

$$U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right), \tag{1}$$

$$U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y} = -\frac{1}{\rho}\frac{\partial P}{\partial y} + \nu\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right), \tag{2}$$

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \tag{3}$$

contains momentum equations (1), (2) and equation of continuity (3).

Eliminating P from Eqs. (1) and (2), we obtain a simpler system of differential equations. For this purpose we differentiate Eq. (1) with respect to y and (2) with respect to x and substract (2) from (1). Removing from the equation obtained the terms that satisfy the equation of continuity and the highest derivatives of it, we have

$$V\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right) - U\left(\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right) + \nu\left(\frac{\partial^3 V}{\partial x^3} - \frac{\partial^3 U}{\partial y^3} - 2\frac{\partial^3 U}{\partial y^2 \partial x}\right) = 0. \tag{4}$$

Equations (4) and (3) form a new system for determining the functions U and V. The system of equations is elliptical, so to integrate it it is necessary to state outlet conditions for U and V. If we state outlet conditions in the form of boundary conditions of the second kind (Neumann boundary conditions), a system is obtained that consists of four differential equations (equation (4) is nonlinear).

After finding the velocities it is possible to obtain the pressure P from Poisson's equation

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + 2\left[\left(\frac{\partial U}{\partial x}\right)^2 + \frac{\partial U}{\partial x}\frac{\partial V}{\partial y}\right] = 0. \tag{5}$$

Poisson's equation is written for the interior points and the boundaries of the calculation domain. Here, a system of linear equations in the coefficients of the expansion for P, which is solved more quickly than the system of nonlinear equations, is obtained.

3. Implementation of the Method. Several approximations for U and V, which differ in the degree of the polynomial in the x direction ($m_1 = 2$, $m_2 = 3$, $m_3 = 5$) were considered:

$$U = \sum_{n=1}^{5} \sin(n\pi y/l)\left(\sum_{j=1}^{m_i} Z_k x^j + A_n\right), \quad V = \sum_{n=1}^{5} \sin(n\pi y/l)\left(\sum_{n=1}^{m_j} D_k x^j + B_n\right), \tag{6}$$

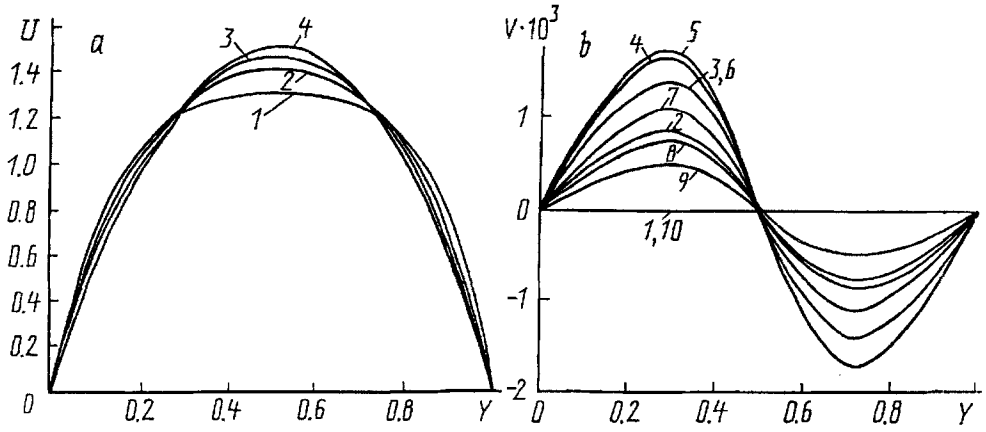

Fig. 1. Change in the velocity profile U along the channel length: 1) $x = 0$; 2) 6; 3) 12; 4) 18 (a) and change in the velocity profile V along the channel length: 1) $x = 0$; 2) 2; 3) 4; 4) 6; 5) 8; 6) 10; 7) 12; 8) 14; 9) 16; 10) 18 (b) U, V, dimensionless.

where $k = (n-1) \cdot m_i + j$; Z_k and D_k are the coefficients of the expansion for U and V; A_n and B_n are the coefficients of the initial expansion for U and V (at the channel entrance). The number of unknown coefficients of the system is $N_{m1} = 20$, $N_{m2} = 30$, $N_{m3} = 50$.

For the given problem it is possible to improve the accuracy of the initial expansion of the sought functions U and V. Then, however, the accuracy of the description of the functions at the entrance boundary will not conform with the accuracy of the description of the functions within the calculation domain.

As is seen from (6) the condition of "adherence" to walls is satisfied for the functions U and V, i.e., when $y = 0$ and $y = l$, $U = 0$ and $V = 0$. The channel length x is reckoned in channel widths l.

Satisfaction of the boundary conditions by the approximating series is unnecessary, but is desirable, since this eliminates the direct specification of boundary conditions and reduces the number of coefficients necessary for the description of the process.

For the solution of systems of nonlinear equations Newton's method [3], the gradient descent method, and the method of minimization of maximum discrepancies were used. The best results concerning rate of convergence towards the solution of the system of nonlinear equations were produced by Newton's method, which was also slightly modified for use in the calculation. According to Newton's method z^{n+1} is determined by iterations from the equation

$$z^{n+1} = z^n - W^{-1}(z^n) f(z^n), \tag{7}$$

where n is the step number, z^{n+1} is the column-vector of sought coefficients of the expansion; $W^{-1}(z^n)$ is inverse Jacobian of the functions $f(z^n)$ which are obtained by substitution of the approximating series into the differential equations of the system and are written for the interior points of the domain. The modification of Newton's method consists in that z^{n+1} is determined from the solution of the system of linear equations, written in the following form:

$$W(z^n) z^{n+1} = b^n, \tag{8}$$

where $b^n = W(z^n)z^n - f(z^n)$ is the column of right-hand sides. By going from inversion of the Jacobian to the solution of the system of linear equations the calculation time reduced threefold and the main storage capacity of a computer is reduced twofold.

4. Analysis of the Results of a Numerical Calculation. As follows from the calculations performed, the convergence of the solution, for example, for maximum discrepancy is rapid and requires 3-6 iterations for nonseparated flows in accordance with the required accuracy for the coefficients of the series. The number of iterations is increased to 10-15 for separated flows and flows with a complex configuration or large Reynolds

numbers. The calculation time for one iteration is 0.9 sec for N_{m1}, 1.8 sec for N_{m2}, and 6.3 sec for N_{m3} on an IBM PC/AT 286 12 MHz and this time can be reduced 1.5–2-fold. On average, obtaining the solution it required 5, 10, 30 sec, respectively. The time for obtaining the sought functions with known coefficients of the series should be regarded as the overhead of time needed for integrating the system of differential equations. But this time is usually small (to calculate functions at 200 points, about 1 sec is required for N_{m3}). Calculations of similar flows on the same computer by means of finite-difference methods require 1-2 orders more time.

For the case of nearly uniform entry of the flow into the channel at a Reynolds number of Re = 1000 the functions U and V shown in Fig. 1 were found with the approximation with N_{m3}. Calculations were also performed at Reynolds numbers up to 108 and showed satisfactory results in the sense of convergence of the iterative process to the solution and physicality of the latter.

As is seen from Fig. 1, the results for U and V conform quite satisfactorily with the theory, according to which a developed plane-parallel flow is formed at the outlet from the calculation section in the channel and the profile of the velocity U corresponds to a parabolic Poiseuille profile with a maximum of 1.5. It turned out that the approximation with N_{m2} provides acceptable results. For example, the defect of consumption for N_{m3} is 15% for 20 widths and for N_{m2} it is 1.7%.

The outlet conditions were put in the form of boundary conditions of the first or second kind, for which practically identical results were obtained. A much greater effect on the solution was produced by the location of the points within the calculation domain and the initial approximation of the coefficients of the expansion for z^0 in (8).

In this connection questions concerning global stability of the present method, its stability toward the initial approximation for the coefficients of the expansion and the initial and boundary conditions, convergence to the solution of the system of differential equations, and uniqueness and accuracy of the solution arise.

These questions fall outside the framework of the present article; we may, however, assume that with properly specified boundary conditions, approximation of the sought functions by multiply differentiable series, and smoothness of the solution, problems would be avoided.

5. Prediction of the Calculation Time. It is of interest to get to determine the time spent on one iteration step according to Newton's method which is used in the method of approximating series for different numbers of coefficients of the expansion. The number of coefficients of the expansion may characterize either the accuracy of the solution obtained or the complexity of the initial system of equations. It is convenient to express time in relative quantities, for example, t_N/t_{30}, where t_N is the calculation time for N coefficients and t_{30} is the calculation time for a system with 30 coefficients of expansion. Let us represent the total calculation time by the polynomial

$$t_N/t_{30} = AN^3 + BN^2 + CN. \tag{9}$$

Calculations by the method of approximating series show that $A = 2.454 \cdot 10^{-5}$, $B = -1.298 \cdot 10^{-4}$, $C = 0.01514$. The results of calculating t_N/t_{30} according to (9) are given in Fig. 2. It is considered here that the computations are performed on computers of equal speed.

It is possible to find t_N according to (9) or using Fig. 2:

$$t_N = Mt_{30}\, 10^{\log (t_N/t_{30})},$$

where M is the relative computer perfomance compared to an IBM PC/AT 286 12 MHz.

6. Estimation of the Potentialities of the Method. Proceeding from the above, we draw conclusions about the field of application of the method of approximating series and its accuracy and speed of computations, and we may compare these parameters with similar parameters for known and employed methods.

As was stated before, the method of approximating series is not limited to just one field of physics, which makes it similar to finite difference methods.

When estimating the accuracy and speed of computations we should distinguish between calculations for systems of linear and nonlinear differential equations by the approximating series method, since their solutions

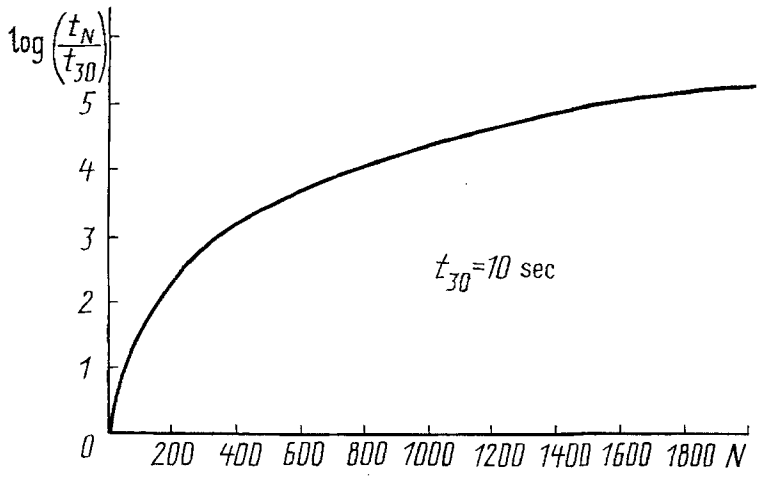

Fig. 2. Dependence of the calculation time for the method of approximating series t_N on the number of coefficients of the expansion of the sought functions N.

TABLE 1. Rought Time of Calculation by the Approximating Series Method for Different Flows of Liquid for a Cray X-MP/48 Computer

Type of flow	N	$\log t_N/t_{30}$	$T^{\text{Cray-X-MP}}$, sec
Two-dimensional incompressible, viscous, non-turbulent, P is calculated separately	30–60	0–0.8	$6\cdot10^{-3}$
Two-dimensional incompressible, viscous, non-turbulent, with calculation of P	47–75	0.4–1.0	$1\cdot10^{-2}$
Two-dimensional compressible, viscous, non-turbulent	75–100	1.0–1.4	$3\cdot10^{-2}$
Two-dimensional compressible, viscous, turbulent	100–130	1.4–1.7	$6\cdot10^{-2}$
Two-dimensional compressible, viscous, turbulent, nonstationary	500 –700	3.5–3.9	8
Three-dimensional incompressible, viscous, non-turbulent, stationary, 300–400	2.8–3.2	1.5	
Three-dimensional compressible, viscous, non-turbulent, stationary, 350–450	3.0–3.3	2.2	
Three-dimensional compressible, viscous, turbulent, stationary	600–700	3.7–3.9	8
Three-dimensional compressible, viscous, turbulent, nonstationary	10^3–$2\cdot10^3$, 4.4–5.3	25–200	

take significantly different times (a system of linear differential equations is solved 5–10 times more quickly due to the need for just one step in Newton's method).

It is possible to show that for systems of linear differential equations the calculation time for the method of approximating series at low accuracy is even less than for a theoretical solution represented in series for the Laplace, Helmholtz, diffusion, Schrödinger, Poisson, and wave equations and similar ones, if such solution exists (it exists for a limited set of initial and boundary conditions and configurations of calculation domain). Achieving similar accuracy by other methods requires by one-two orders more overhead of the processor time of a computer.

For systems of nonlinear differential equations the calculation time for the method of approximating series for any degree of accuracy of the calculated values is also one-two orders smaller than the calculation time for

other numerical methods. Examples of different types of flows of liquid for aerodynamic problems are presented in the Table 1. The number N of coefficients of the expansion and a rough calculation time for a Cray X-MP/48 supercomputer are given for the flows (it was considered that the Cray X-MP/48 perfomance is four orders higher than the IBM PC/AT 286 perfomance).

To provide evidence we compare the time of calculation of three-dimensional nonstationary flow of a viscous turbulent compressible liquid by a finite-difference method and the method of approximating series on a Cray X-MP/48 computer. The average calculation time for finite-difference methods is 1000-5000 sec [4. 5]. The expected calculation time for the method of approximating series is 25–200 sec with the same accuracy of determining the calculated quantities.

7. Description of the APPROX Program Package. To make the writting of programs using the method of approximating series easier, the APPROX program package is created and implemented on a computer of the IBM PC or VAX type. This package may easily be transferred to other types of computers. The APPROX program package makes it possible to write a program in the high-level language FORTRAN or Ada in 1-3 hours for a completely formalized problem (initial and boundary conditions are stated, the system of differential equation is written down, the approximation of all the unknown is selected, etc.). For example., every program with N_{m1}, N_{m2}, N_{m3} was done in less than 1 hour. The APPROX package allows one quickly and optimally to formulate boundary and initial conditions to select the system of differential equations and the approximating series for the unknown variables, etc.). In addition, the system allows one to output the results of calculations in a convenient form (multidimentional plots, sections, level lines, etc.) on a display screen or on paper (the graphs presented in the present work have been prepared by means of the system).

Conclusions. Thus, we may recommend the method of approximating series for wide use in calculations. The method allows one to save time and money, as compared to calculations performed by presently used methods. In addition the shorter calculation time for this method allows one to solve problems that are solved only experimentally at present.

You may receive information on the APPROX program package by telephone at the number (8-057) 40-08-30 (Kharkov).

NOTATION

x, y, coordinate axes; U, velocity component in the x direction; V, velocity component in the y direction; P, pressure; ρ, density; n, viscosity; l, channel width, Re, Reynolds number; m_1, m_2, m_3, degree of the approximating polynomial in the x direction; A_n, B_n, Z_k, D_k , coefficients of the expansion for U and V; N_{m1}, N_{m2}, N_{m3}, numbers of unknown coefficients of the expansion; z^n, column vector of coefficients of the expansion; $f(z^n)$, functions; $W(z^n)$, Jacobian; b^n, vector of right-hand sides.

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