http://mmg.tversu.ru ISSN 2311-1275

Mathematical Modelling and Geometry

Volume 14, No 2, pp. 11 – 20 (2026) doi:10.26456/mmg/2026-1422

A multi-stage Chebyshev collocation method for an approximate solution of a first-order ordinary differential equation

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Received 30 May 2026. Published 12 may 2026.

Abstract. A classical pseudospectral collocation method based on the expansion of the solution in a basis of Chebyshev polynomials is considered. This new approach to forming systems of linear algebraic equations for solving ordinary differential equations with variable coefficients and initial (and/or boundary) conditions allows for a significant simplification of the matrix structure, reducing it to a diagonal form. The solution is a two-step process. The basic algorithm is solving the problem of reconstructing a function from its known derivative and initial/boundary conditions. Reconstructing the expansion coefficients by the basic algorithm amounts to multiplying the transposed matrix of Chebyshev polynomial values on the selected collocation grid by the vector of function values describing the given derivative at the collocation points. Subsequently, multiplying the bidiagonal spectral "inverse" (with respect to the Chebyshev differentiation matrix) matrix by the resulting vector of interpolation coefficients yields all the expansion coefficients of the desired solution except the first one. This first coefficient is determined in the second stage based on the given initial (and/or boundary) condition. The novelty of this approach consists of first identifying a class of functions satisfying the differential equation. Only then solutions from this set that correspond to the given initial conditions are selected. The second stage is the calculation of the integrating factor of the ODE, based on the same basic algorithm, which allows us to reduce the solution of the general equation to an intermediate solution to the derivative recovery problem. To find the final solution, we again use the basic algorithm.

Keywords: initial value problems; pseudo spectral collocation method; Chebyshev polynomials; Gauss–Lobatto sets; numerical stability

MSC numbers: 65L60

1. Introduction

Spectral methods are a class of methods used in applied mathematics and scientific computing for the numerical solution of many differential equations [1, 2, 3, 4]. The basic idea of the method is to represent the desired solution of the differential equation as a weighted sum of certain "basis functions" [5] (for example, as a sum of power functions — a Taylor series, or a sum of sinusoids, which is a Fourier series), and then calculate the coefficients in the sum to satisfy the differential equation as best as possible.

Approximation of a continuous function by Chebyshev polynomials is the best in the uniform metric and almost the best in the quadratic metric. The set of polynomials $\{T_j(x)\}$ forms an orthonormal basis in $L^2([-1,1])$ with weight

$$\rho(x) = \frac{1}{\sqrt{1-x^2}}.$$

Denote by $P_p(x)$ the polynomial of degree p approximating the function $f(x)$ in the basis of Chebyshev polynomials of the first kind. The polynomials

$$\{T_0(x), T_1(x), \dots, T_p(x)\}$$

form a basis in the $(p+1)$-dimensional vector space V of polynomial functions. The function $f(x)$ does not necessarily belong to the space V and, therefore, differs from $P_p(x)$. Improvement of the approximation is provided by minimizing the residual.

$$v(x) = P_p(x) - f(x) = \sum_{j=0}^{p} c_j T_j(x) - f(x). \tag{1}$$

One method for minimizing the residual (1) is to project it onto a subspace orthogonal to the vector subspace

$$V = \mathrm{Span}\{T_0(x), T_1(x), \dots, T_p(x)\}$$

which is equivalent to the orthogonality of $v(x)$ to all basis functions:

$$c_j = \langle T_i(x), f(x) \rangle = 0, \quad i = 0, 1, \dots, p. \tag{2}$$

The collocation method consists of calculating the residual by its turning into zero at the points of the collocation grid:

$$v(x_k) = \sum_{j=0}^{p} c_j T_j(x_k) - f(x_k) = 0, \quad k = 0, \dots, p. \tag{3}$$

1.1 Numerical solution of ordinary differential equations

An exact solution of a trivial ordinary differential equation under the given initial (boundary) condition

$$y'(x) = f(x), \quad x \geq x_0, \quad y(x) = y_0, \tag{4}$$

the right-hand side of the equation being independent of y, can be presented as $y_0 + \int_{t_0}^{t} f(\tau)\,d\tau$. Since numerical methods for integrating functions are perfectly developed from theoretical and practical point of view, it seems natural to apply them to the numerical solution of ordinary differential equations of the general form

$$\boldsymbol{y}'(x) = \boldsymbol{f}(x, \boldsymbol{y}(\boldsymbol{x})), \quad x \geq x_0, \quad \boldsymbol{y}(x_0) = \boldsymbol{y}_0, \tag{5}$$

and this is exactly what naturally explains the development and popularity of Runge–Kutta-type methods. Such methods imply obtaining the solution in the interval $[x_0, x_0 + c_k h]$. The coefficients

$$0 \leq c_1 < c_2 < \cdots < c_n \leq 1$$

are chosen. Then using the polynomial collocation method the solution is approximated by polynomial p of degree n, which satisfies two types of conditions:

- initial condition: $p(x_0) = \boldsymbol{y}_0$, and
- differential equation $p'(x_k) = f(x_k, p(x_k))$ at all *collocation* points $[x_k = x_0 + c_k h]$, $k = 1, \ldots, n$.

Satisfying these $(n + 1)$ conditions allows calculating $(n + 1)$ coefficients of expansion of the desired polynomial p of degree n. Thus, some collocation methods are implicit Runge–Kutta methods.

In the given class of collocation (Runge–Kutta) methods, the approximation coefficients of the solution are found in a finite-dimensional subspace of piecewise linear functions (as in the trapezoidal rule) or cubic functions or other piecewise polynomial functions. The orthogonal collocation method instead uses a finite-dimensional subspace generated by the first n vectors in the Chebyshev polynomial basis.

In this case, linear ODEs transform into SLAEs. When transitioning to systems of linear algebraic equations, SLAEs are obtained with completely filled and often ill-conditioned matrices, necessitating the solution of systems using expensive Gaussian methods, LU decomposition, and other methods that require additional preconditioning, singular value decomposition, or regularization.

The choice of a suitable basis ensures high convergence rates and simple calculation of the spectral coefficients of the derivative and/or antiderivative functions from the expansion coefficients of the function under study.

Expansion in Chebyshev polynomials (compared to expansion in Legendre polynomials and others) offers advantages such as the simplicity of the spectral differentiation and integration matrices and the rapid recalculation of function values at collocation nodes: from the spectral representation to the representation in physical space and vice versa. These properties are particularly evident when choosing Chebyshev points of the first and second kind as collocation nodes, eliminating the labor-intensive SLAE solution for determining the expansion coefficients while taking into account the discrete orthogonality of the Chebyshev polynomials.

Using the Clenshaw summation method in matrix operations for calculating the expansion coefficients of the functions under study, their antiderivatives, and derivatives significantly (up to 10 times) increases the speed of such operations compared to traditional matrix-vector multiplication methods.

An additional advantage of using Chebyshev–Gauss–Lobatto grids is the disappearance of the Runge phenomenon, which occurs when using uniform grids [2].

It is important to note that solving the Cauchy problem does not necessarily require attempting to solve Eq. (1) while simultaneously satisfying both the initial condition and the differential equation at the collocation points. In some cases, a very fast and stable result can be achieved in two steps. It is much easier to first calculate those expansion coefficients of the desired solution that satisfy the differential equation at the collocation points. Only then can the missing expansion coefficients of the desired function be determined using the initial (final or intermediate) value.

2. Solving single-point problems for ODEs of the first order

Consider the solution of a Cauchy problem for the first-order ODE

$$y'(x) + g(x)y(x) = f(x) \tag{6}$$

under the additional condition

$$y(x_0) = y_0, \quad x \in [-1, 1].$$

Instead of ***merging all known conditions*** – differential (the equation itself) and initial (or boundary) – into ***a single system*** of approximate linear algebraic equations, we propose solving the problem in several stages.

Let us consider dividing the original problem of solving ODE (6) into simpler subproblems. The first of these is the problem of reconstructing a function from its given derivative and a fixed value at a predetermined point

$$y'(x) = f(x), \quad y(x_0) = y_0, \quad x \in [-1, 1], \tag{7}$$

which, in turn, is solved in two stages:

- polynomial interpolation of the derivative (calculation of the coefficients of the derivative expansion in basis functions) and

- calculation of the coefficients of the desired function expansion in terms of the boundary (boundary or other) condition and the coefficients of the derivative expansion.

First, the spectral coefficients characterizing the "general" solution to the original problem (7) are determined. Then, taking into account the initial/boundary conditions, we can identify the "particular" desired solution.

The spectral method of solving problem (7) consists in presenting the interpolating function as a series

$$p(x) = \sum_{k=0}^{n} c_k T_k(x), \quad x \in [-1, 1], \tag{8}$$

in the basis of Chebyshev polynomials of the first kind $\{T_k(x)\}_{k=0}^{\infty}$, specified in the Hilbert space of functions on the interval $[-1, 1]$. In this case, the expression for the derivative is

$$p'(x) = \sum_{k=0}^{n} c_k T_k'(x) = \sum_{k=0}^{n} b_k T_k(x). \tag{9}$$

Using three-term recurrence relations satisfied by Chebyshev polynomials and their derivatives [6, 7] and equating the coefficients of identical polynomials in Eq. (9), we arrive at the following dependence of the coefficients c_k on b_k [8]:

$$\begin{bmatrix} 1 & 0 & \frac{-1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & \frac{-1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{6} & 0 & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & \ddots & \frac{1/2}{(n-1)} & 0 \\ 0 & 0 & 0 & \ddots & 0 & \frac{1}{2n} \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{n-2} \\ b_{n-1} \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ \vdots \\ c_{n-1} \\ c_n \end{bmatrix}. \tag{10}$$

Calculating the coefficients $\{c_1, c_2, \dots, c_n\}$ of the desired function is reduced to multiplying a tridiagonal matrix by a vector, which can be implemented according to the following scheme:

$$\begin{cases} c_1 = b_0 - b_2/2, & k = 1 \\ c_k = \dfrac{b_{k-1} - b_{k+1}}{2k}, & k > 1,\ k < n-1 \\ c_k = \dfrac{b_{k-1}}{2k}, & k = n-1, n \end{cases} \tag{11}$$

Let us proceed to the calculation of coefficients $\{b_0, b_1, \dots, b_n\}$ of function $f(x)$ expansion in terms of Chebyshev polynomials of the first kind [3] on the interval $[-1, 1]$

$$\sum_{k=0}^{n} b_k T_k(x) = f(x).$$

The collocation method [5] consists in choosing such coefficients $\{b_0, b_1, \dots, b_n\}$ of the expansion of polynomial $p'(x)$, that the sought coefficients $b_k,\ k = 0, 1, \dots, n$ ensure satisfying the equalities

$$\sum_{k=0}^{n} b_k T_k(x_j) = f(x_j), \quad j = 0, \dots, n \tag{12}$$

at collocation points $\{x_0, x_1, \dots, x_n\}$.

The coefficients $b_k,\ k = 0, \dots, n$ must be solutions of SLAE (12). In the matrix form:

$$\boldsymbol{T}\boldsymbol{b} = \boldsymbol{f}. \tag{13}$$

The stability of the algorithm is achieved by using the property of discrete orthogonality of the Chebyshev matrix $\boldsymbol{T}$. The choice of the Gauss–Lobatto grid allows us to obtain an equivalent system $\widetilde{\boldsymbol{T}}\boldsymbol{b} = \widetilde{\boldsymbol{f}}$ when dividing by $\sqrt{2}$ the first and last equation in system (11). The condition of discrete orthogonality of the Chebyshev matrix of values of polynomials of the first kind allows us to obtain a system with a diagonal matrix when multiplying it from the left by the transposed matrix $\widetilde{\boldsymbol{T}}^{\boldsymbol{T}}$.

$$\begin{bmatrix} n & 0 & 0 & \dots & 0 \\ 0 & n/2 & 0 & \dots & 0 \\ 0 & 0 & n/2 & \dots & 0 \\ \dots & \dots & \dots & \ddots & \dots \\ 0 & 0 & 0 & \dots & n \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \dots \\ b_n \end{bmatrix} = \widetilde{\boldsymbol{T}}^{\boldsymbol{T}} \begin{bmatrix} \widetilde{f}_0 \\ \widetilde{f}_1 \\ \widetilde{f}_2 \\ \dots \\ \widetilde{f}_n \end{bmatrix}, \tag{14}$$

where $\widetilde{\boldsymbol{f}} = \widetilde{\boldsymbol{T}}^{\boldsymbol{T}}(f_0/\sqrt{2}, f_1, \dots, f_{n-1}, f_n/\sqrt{2})^T$.

The expansion coefficients of the function $f(x)$ can be easily written out in explicit form

$$b_0 = \widetilde{f}_0/n, \quad b_1 = 2\widetilde{f}_1/n, \quad b_2 = 2\widetilde{f}_2/n, \quad \dots, \quad b_n = \widetilde{f}_n/n. \tag{15}$$

Formulas (10),(11) uniquely determine the last n coefficients of the expansion of the desired polynomial $p(x)$ (see Eq. (8)). An additional condition is required to determine one more coefficient, c_0. The method under consideration makes it possible to solve both Cauchy problems with initial conditions and problems with general boundary conditions.

But even with this two-stage approach for a first-order ODE of the form

$$\frac{dy}{dx} + p(x)y = q(x)$$

the resulting SLAE turns out to be densely filled in the case of variable coefficients. To reduce the number of arithmetic operations in the implementation of the Chebyshev collocation algorithm and to increase the stability of the numerical methods used, K.P. Lovetskiy et al. proposed a multi-stage (modified) Chebyshev collocation method for solving a single-point problem for a first-order ODE [8].

2.1 Stage two: a linear first-order ODE of the general form

Consider a linear first-order ODE of a more general form:

$$\frac{dy}{dx} + p(x)y = q(x). \tag{16}$$

Assume $p(x)$ and $q(x)$ to be continuous functions. Then there exists an integrating factor $\mu(x)$, satisfying the equation

$$\mu(x)p(x) = \mu'(x). \tag{17}$$

Let us divide both sides of the equality by $\mu(x)$ and obtain the differential equation

$$\frac{\mu'(x)}{\mu(x)} = p(x) \tag{18}$$

or

$$(\ln \mu(x))' = p(x) \tag{19}$$

Let us introduce the notations

$$\ln \mu(x) \equiv u(x) = \sum_{k=0}^{n} c_k T_k(x), \quad x \in [-1, 1]. \tag{20}$$

Integrating both sides of Eq. (19), we determine the values of coefficients c_k, $k = 1, \dots, n$ in correspondence with Eq. (8) of the preceding Section. Let us write down the expression for the integrating factor logarithm in the form

$$\ln \mu(x) = c_0 + \sum_{k=1}^{n} c_k T_k(x), \quad x \in [-1, 1]. \tag{21}$$

The coefficient c_0 remains indefinite, and the integrating factor $\mu(x)$ is written in the form

$$\mu(x) = \exp\left(c_0 + \sum_{k=1}^{n} c_k T_k(x)\right) = \exp(c_0)\, \exp\left(\sum_{k=1}^{n} c_k T_k(x)\right), \tag{22}$$

where the factor $k = \exp(c_0)$ is an unknown coefficient.

Having calculated the integrating factor, we return to the solution of the initial equation (16). We multiply (16) by $\mu(x)$ and, taking relation (17) into account, arrive at a necessity to solve the equation

$$\mu(x)\frac{dy}{dx} + \mu'(x)y = \mu(x)q(x). \tag{23}$$

The left-hand side is a product derivative

$$(\mu(x)y(x))' = \mu(x)\frac{dy}{dx} + \mu'(x)y.$$

Therefore, replacing the sum on the left-hand side of (23) according to the rule for differentiating the product of functions, we obtain

$$(\mu(x)y(x))' = \mu(x)q(x). \tag{24}$$

From expression (22) for the integrating factor it follows (regardless of the value of the coefficient c_0, $\exp(c_0) > 0$) that the determination of the desired solution to problem (16) is reduced to solving the problem of reconstructing the coefficients $\{d_1, \dots, d_n\}$ of the expansion of the function $\mu(x)y(x)$ from the coefficients of its derivative expansion (8).

$$\mu(x)y(x) = d_0 + \sum_{k=1}^{n} d_k T_k(x), \tag{25}$$

and the general form of the solution is obtained by dividing equality (25) by $\mu(x)$.

$$y(x) = \frac{d_0 + \sum_{k=1}^{n} d_k T_k(x)}{\mu(x)}. \tag{26}$$

The value of the unknown constant d_0 is determined by the given initial or boundary conditions according to the formula

$$d_0 = y(x_0)\mu(x_0) - \sum_{k=1}^{n} d_k T_k(x_0). \tag{27}$$

3. Discussion

The modified Chebyshev collocation method for solving a single-point problem for a first-order ODE of the simplest form, i.e., the form of a total derivative, at the first stage of finding a general solution is divided into two stages:

- The construction step, based on the collocation points x_j and the values of the derivative $f(x_j)$ at the collocation points of the coefficients $\boldsymbol{b}$ of the Chebyshev decomposition of the interpolating polynomial, is performed by multiplying the diagonal Gram matrix $\widetilde{\boldsymbol{T}}^{\boldsymbol{T}}\widetilde{\boldsymbol{T}}$ of the Chebyshev collocation matrix $T_k(x)$ by the values of $\widetilde{\boldsymbol{f}}$. The coefficients c of the Chebyshev decomposition of the antiderivative of the derivative, i.e., the general solution of the simplest ODE problem (1.1.2), are obtained by multiplying the tridiagonal integration matrix $\boldsymbol{D}^{+}_{\text{Chebyshev}}$ by the resulting coefficient vector $\boldsymbol{b}$: $\boldsymbol{D}^{+}_{\text{Chebyshev}}\boldsymbol{b} = \boldsymbol{c}$.
- The step of calculating c_0 is performed by solving a single linear equation.

In the case of solving a single-point problem for a general ODE (16), the first step is to calculate the integrating factor $\mu(x)$ using the algorithm for solving the simplest ODE. Using the calculated integrating factor allows us to reduce the general ODE to a total derivative using the algorithm for solving the problem of reconstructing a function from its derivative.

- The integrating factor $\mu(x)$ satisfies the equation

$$\mu(x)p(x) = \mu'(x) \quad \Longleftrightarrow \quad (\mathbf{ln}(\boldsymbol{x}))' = \boldsymbol{p}(x)$$

  and allows reducing the ODE to the total derivative form

$$\mu(x)y'(x) + \mu'(x)y(x) = \mu(x)q(x) \quad \Longleftrightarrow \quad (\boldsymbol{\mu(x)y(x)})' = \boldsymbol{\mu(x)q(x)}.$$

- We calculate $\mathbf{ln}(\boldsymbol{x})$ using the method of solving the simplest equation.
- We calculate the product $\mu(x)y(x)$ using the method of solving the simplest equation.
- We calculate $y(x)$ by dividing the previous result by $\mu(x)$.

Thus, in the case of a single-point problem for a general-form ODE, the integrating multiplier method reduces the search for a general solution to a pair of successive elementary calculations in accordance with the basic algorithm for restoring a function from its derivative.

4. Conclusion

This paper proposes dividing the problem into independent subproblems and calculating the spectral components of the solution in parts – separately those that determine the overall solution and those determined by the boundary conditions. This divides the problem into independent subproblems, each solvable stably, reliably, and simply. In the simplest case, solving the first problem reduces to multiplying the right-hand side vector by the matrix of Chebyshev function values on a Gauss–Lobatto grid. In the next step, we solve a linear algebraic equation with a diagonal positive-definite matrix and, by multiplying the resulting left-hand vector by the bidiagonal "inverse" of the spectral Chebyshev differentiation matrix, obtain all but the first coefficient of the expansion of the desired solution. In the second, "most difficult" step, we determine the first coefficient of the expansion of solution in basis polynomials by solving a linear algebraic equation for this coefficient. A new approach to constructing systems of linear algebraic equations for solving ordinary differential equations with variable coefficients and initial (and/or boundary) conditions significantly simplifies the matrix structure, converting it to diagonal form. Solving the system is reduced to multiplying the matrix of Chebyshev polynomial values on the selected collocation grid by the vector of function values describing the given derivative at the collocation points. Subsequently, multiplying the resulting vector by the bidiagonal spectral "inverse" of the Chebyshev differentiation matrix yields all the expansion coefficients of the desired solution except the first coefficient. This first coefficient is determined in the second stage based on the given initial (and/or boundary) condition.

Solving a general LODE is reduced to a sequential calculation of the integrating factor using the basis method and then reapplying the basis method to calculate the desired general solution.

The novelty of this approach consists of first identifying a class (set) of functions satisfying the differential equation using a robust and computationally simple method of interpolating (collocating) the derivative of the future solution. Then, the coefficients of the expansion of the future solution (except the first one) are found based on the calculated coefficients of the derivative expansion using the integration matrix. Only then are solutions from this set selected that correspond to the given initial conditions.

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