

Review

A Review of Collocation Approximations to Solutions of Differential Equations

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Abstract: This review considers piecewise polynomial functions, that have long been known to be a useful and versatile tool in numerical analysis, for solving problems which have solutions with irregular features, such as steep gradients and oscillatory behaviour. Examples of piecewise polynomial functions used include splines, in particular B-splines, and Hermite functions. Spline functions are useful for obtaining global approximations whilst Hermite functions are useful for approximation over finite elements. Our aim in this review is to study quintic Hermite functions and develop a numerical collocation scheme for solving ODEs and PDEs. This choice of basis functions is further motivated by the fact that we are interested in solving problems having solutions with steep gradients and oscillatory properties, for which this approximation basis seems to be a suitable choice. We derive the quintic Hermite basis and use it to formulate the orthogonal collocation on finite element (OCFE) method. We present the error analysis for third order ODEs and derive both global and nodal error bounds to illustrate the super-convergence property at the nodes. Numerical simulations using the Julia programming language are performed for both ODEs and PDEs and enhance the theoretical results.



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1. Introduction

We begin this review by considering briefly various approximation strategies for continuous functions. The approximation of such continuous functions in Numerical Analysis is usually by a least squares approach or interpolation methods. In such cases a basis is chosen from an underlying approximation space. Depending on the problem this may be a polynomial, rational function or of the sinusoidal type. Specifically interpolation plays a key role in approximation of the unknown solution of differential equations. In such a case a polynomial basis is chosen, which serves as a trial function for the solution. For efficiency and stability a low order polynomial basis is used on a discretized domain. This approach is called the collocation method, and the trial functions are referred to as the collocation polynomial, or the interpolating polynomial. We review the background of collocation by looking at the criterion of the method. We then review different methods that are used to discretize both ODEs and PDEs. To do this, we go into detail about various collocation methods, as well as how they have been used over the years.

In particular we review the method of orthogonal collocation on finite elements (OCFE), where the domain is split into elements, and the latter mapped to the standard interval $[0, 1]$, thereafter Gauss points in $[0, 1]$ are used as collocation points. This approach is proved to yield optimal error bounds. In particular using spline approximation results in sub-optimal error bounds. For example using quintic spline approximation for

solving third order ODEs gives only third order convergence, whereas OCFE produces order six convergence. We solved the resulting DAEs using two approaches. Firstly we used DASSL to solve the DAEs resulting from OCFE in their original form. Secondly, we converted the DAEs to ODEs and used a stiff integrator to solve the resulting system of IVPs. These approaches are clearly superior to previous approaches, in which quasilinearization together with the second order Crank Nicolson method for the time integration is used. In Section 2 we show how the idea of collocation arises naturally from an approximation to the Galerkin method. Section 3 includes a literature review and the history of collocation. In Section 4 we derive the quintic Hermite basis functions and discuss their properties. Section 5 describes OCFE with respect to a quintic Hermite basis, and derives a simplified form of the trial functions, using the continuity conditions. In Section 6 we present a detailed error analysis for the linear ODE case using a quintic Hermite basis. In particular we show that the error is optimal when the collocation points are chosen as the Gauss points, and present nodal, and global error bounds. Finally in Section 7 we present numerical results for several linear, and non-linear differential equations, and validate the theorem in Section 6 by examining the global and nodal convergence orders.

2. Mathematical Setting

Here we review how collocation arises. We consider $L : \mathbb{C}(X) \rightarrow \mathbb{C}(X)$, where $\mathbb{C}(X)$ is the vector space of continuous functions on the domain X . Let L be a bounded linear operator. Let $\{\phi_1, \phi_2, \dots, \phi_N\}$ be a basis for a subspace Φ of $\mathbb{C}(X)$ of dimension N . Consider solving the linear equation

$$Ly = f(x).$$

If $Y \in \Phi$ is an approximation to y , then it follows that

$$Y = \sum_{i=1}^N a_i \phi_i(x),$$

where a_i are real coefficients. We also assume that $L(\Phi) \subseteq \Phi$. The quantity $r(x) = f(x) - LY$ is defined as the residual, and it can be shown that

$$\|Y - y\|_2 \leq \frac{K}{\|L\|_2} \|r\|_2,$$

where $K = \|L^{-1}\|_2 \|L\|_2$ is the condition number of L and $\|\cdot\|_2$ denotes compatible operator and function norms on $\mathbb{C}(X)$, with

$$\|f\|_2 = \left(\int_X |f(x)|^2 dx \right)^{\frac{1}{2}}.$$

For well conditioned problems $\|r\|_2 \rightarrow 0$ implies that $Y \rightarrow y$. Galerkin's method attempts to minimize the norm of the residual by requiring that $r \perp \Phi$, which is equivalent to

$$\langle r, \phi_k \rangle = \int_X r(x) \phi_k(x) dx = 0, \quad k = 1, 2, \dots, N. \quad (1)$$

This geometry in the Hilbert space $\mathbb{C}(X)$ is illustrated in Figure 1.

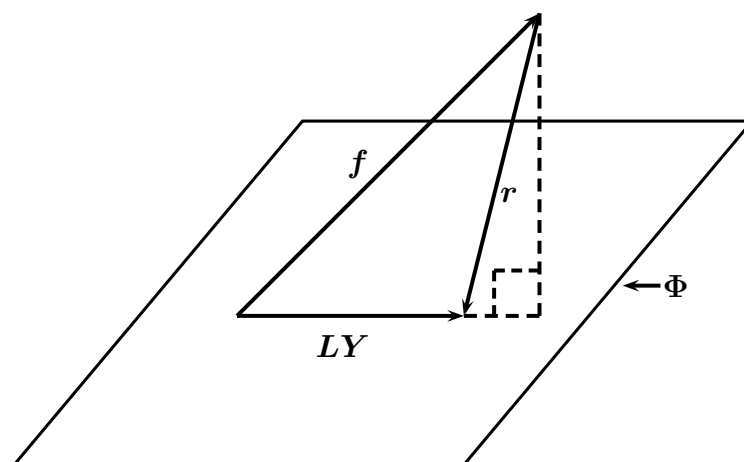


Figure 1. Geometry of Galerkin method.

But these integrals may be expensive to evaluate. The collocation method attempts to avoid this expensive calculation and is a simplification of the Galerkin method.

Integrals such as those mentioned in (1) can be evaluated using numerical quadrature, for instance,

$$\int_X r(x) \phi_k(x) dx \approx \sum_{i=1}^N w_{ik} r(x_i) \phi_k(x_i), \quad k = 1, 2, \dots, N,$$

where we have used the quadrature points x_i , $i = 1, 2, \dots, N$ and w_{ik} are the corresponding weights. If $\{\phi_1, \phi_2, \dots, \phi_N\}$ is a set of orthogonal polynomials then we may choose the x_i 's as the zeros of $\phi_N(x)$. This ensures that

$$\int_X r(x) \phi_N(x) dx \approx 0.$$

We note that the zeros of an orthogonal set of polynomials are real, unique and confined to the interval of orthogonality. Now

$$\int r(x) \phi_k(x) dx, \quad k = 1, 2, \dots, N-1,$$

would not approximate zero since $\phi_k(x_i) \neq 0$ for $k = 1, 2, \dots, N-1$. Hence, in order that this integral is approximately zero, we set $r(x_i) = 0$ for $i = 1, 2, \dots, N$. This is the criterion for the collocation method.

Remark

Whilst, theoretically the basis polynomials need not be orthogonal, it is advantageous to use an orthogonal basis and to exploit the properties of orthogonal polynomials mentioned previously. Furthermore, orthogonal polynomials satisfy a three term recurrence relation, which makes their evaluation simple. It must be stressed that the quadrature points x_i , henceforth called collocation points, may be chosen arbitrarily as long as they are confined to the domain of the problem. In what follows we shall always choose them as the zeros of a polynomial from an orthogonal family. This will then be referred to as the orthogonal collocation method.

3. Literature Review

There are three broad classes of methods for discretizing ODEs and PDEs in space.

- (a) Finite difference methods (FDM) are local methods which yield the numerical solution at mesh points in the spatial domain. They are easy to implement yielding matrices, which are sparse and computationally less expensive to compute. The main drawback

of finite difference methods are that they are not very accurate. The Crank-Nicholson method is the most popular FDM for solving PDEs. We refer to the books [1,2], and references therein, for a further exposition of these methods.

- (b) Finite element methods are derived using a variational/integral formulation and are global methods, which yield the numerical solution on intervals/sub-intervals in the spatial domain. Variants include the method of weighted residuals, Galerkin, Petrov-Galerkin method, Rayleigh Ritz method, Tau method, etc. These methods are mathematically robust but from a numerical point of view are not very practical, due to the need to evaluate integrals exactly. We refer to the classical text [3] for a more detailed description of these methods. Besides this, many other texts can be found in the literature.
- (c) Collocation methods have been developed to circumvent this shortfall. The collocation method is used to solve ordinary and partial differential equations, as well as integral equations. This is done by determining the approximate solution, by requiring the equation to be satisfied at specific points. These specific points are referred to as collocation points. These are chosen points that lie within the domain of the equation, and are used along with candidate solutions to check if the required conditions are met, such that the residual will be zero at these specific points.

Frazer et al. [4] was the first to use this method, in 1937. It was then used in 1941 by Bickley [5] in order to solve unstable heat condition problem. A low-order collocation method was used for a number of boundary-layer problems by Schetz [6], in 1963.

There are many variants of collocation methods and are mainly based on the application. Spectral/pseudo-spectral methods [7] are highly accurate methods and are mainly used in problems, which have very smooth solutions. Fourier Spectral methods are limited to problems posed on a periodic domain, such as when the basis functions are sinusoidal. If the basis functions are polynomials, then it is referred to as a polynomial collocation method. Chebyshev spectral methods have been developed to solve problems posed on a bounded domain. They yield very fast convergence algorithms known as spectral/exponential convergence. In most cases the matrices generated by these methods are dense and one has to resort to the Fast Fourier transform (FFT) to solve them.

Sinc collocation methods [8] are another example of collocation methods. By definition, the basis functions used in these methods are the Sinc functions, which are naturally posed on an unbounded domain, which is one of the drawbacks of this method. B-splines are by far the most popular choice of basis used in collocation methods to solve problems on a bounded domain. They have been successfully applied to solve many important problems including Burgers, KdV and Schrödinger equations [9,10]. The Hermite collocation method closely resembles the B-spline collocation method, but are computationally more efficient, and when used in conjunction with orthogonal collocation on finite elements, yield super convergence properties in algorithms similar to spectral convergence.

Orthogonal collocation arises from the polynomial collocation method, as the collocation points are chosen to be the roots of orthogonal polynomials. It can also be described as being an expansion to the method of weighted residuals.

Villadsen and Stewart were the first to use the orthogonal method, in 1967, after discovering that they yielded very good results, due to the roots of orthogonal polynomials having interesting properties [11]. Finlayson then used it for various applications in chemical engineering, in 1972 [12], and again for application to non-linear problems [13], in 1980. It was used by Fan, Chen and Erikson to solve problems from chemical reactions [14]. Orthogonal collocation is a method that has been widely used by many people for problems in chemical engineering [15–20] over the years. More recently, the method of orthogonal collocation using cubic Hermite basis has been developed, and applied successfully to solve parabolic partial differential equations, and models appearing in chemical engineer-

ing [21,22]. Traditionally a monomial basis $\{1, x, x^2, \dots, x^n\}$ was used to represent the trial functions or more efficiently the Lagrange basis $\{l_0(x), l_1(x), \dots, l_n(x)\}$, where

$$l_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^n \frac{(x - x_k)}{(x_i - x_k)} \quad (2)$$

The main focus in this review is to illustrate the use of orthogonal collocation using a quintic Hermite basis.

4. Quintic Hermite Basis Functions

We seek a basis for P_5 , the vector space of polynomials of degree ≤ 5 on the interval $[x_i, x_{i+1}]$. There are six such functions and we denote them by H_k , $k = 1, 2, \dots, 6$. We further stipulate their function and derivative values at the end points x_i and x_{i+1} as follows:

$$H_k^{(p)}(x_i) = \frac{\delta_{k,p+1}}{h^p}, \quad H_k^{(p)}(x_{i+1}) = 0, \quad H_{k+3}^{(p)}(x_i) = 0, \quad H_{k+3}^{(p)}(x_{i+1}) = \frac{\delta_{k,p+1}}{h^p}, \quad (3)$$

where $k, p + 1 \in \{1, 2, 3\}$ and $\delta_{i,j}$ is the well-known Kronecker delta symbol.

It is convenient to transform to the variable $z \in [0, 1]$ defined by

$$z = \frac{x - x_i}{x_{i+1} - x_i} = \frac{x - x_i}{h}, \quad (4)$$

where h is the uniform interval length. As x varies from x_i to x_{i+1} , z varies from 0 to 1. The interpolatory conditions in (3) transform naturally in the variable z to

$$H_k^{(p)}(0) = \delta_{k,p+1}, \quad H_k^{(p)}(1) = 0, \quad H_{k+3}^{(p)}(0) = 0, \quad H_{k+3}^{(p)}(1) = \delta_{k,p+1}.$$

These conditions enable the unique derivation of the $H_k(z)$, $k = 1, 2, \dots, 6$, however it is only necessary to derive $H_1(z), H_2(z)$ and $H_3(z)$ as by symmetry/anti-symmetry one may obtain the others. These polynomials are displayed in (5)–(10).

$$H_1(z) = (1 - z)^3(6z^2 + 3z + 1), \quad (5)$$

$$H_2(z) = (1 - z)^3(3z^2 + z), \quad (6)$$

$$H_3(z) = (1 - z)^3\left(\frac{1}{2}z^2\right), \quad (7)$$

$$H_4(z) = -H_1(1 - z), \quad (8)$$

$$H_5(z) = -H_2(1 - z), \quad (9)$$

$$H_6(z) = -H_3(1 - z). \quad (10)$$

If we write $H_4(z) = H_1(-(z - 1))$, then we note that $H_4(z)$ is a reflection of $H_1(z)$ about the vertical axis together with a shift of one unit to the right. $H_6(z)$ is related to $H_3(z)$ in a similar manner. Also, $H_5(z)$ may be interpreted as $H_2(z)$ rotated by 180° anticlockwise and then shifted one unit to the right.

5. Orthogonal Collocation on Finite Elements

Consider solving an ordinary differential equations in one spatial variable, x , and on the domain $[a, b]$. Firstly the domain $[a, b]$ is divided into N sub-intervals or elements of spacing $h = \frac{b-a}{N}$, by placing the dividing points or nodes, x_i , $i = 1, 2, \dots, N + 1$, as illustrated in Figure 2. We shall refer to this discretization as the mesh Δ .

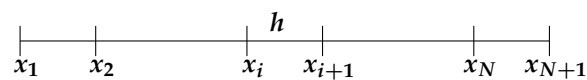


Figure 2. Mesh Δ .

Here $x_1 = a$ and $x_{N+1} = b$ coincide with the left and right hand boundaries, respectively. This differs from global orthogonal collocation where the domain is not subdivided and instead higher order polynomials are used to achieve greater accuracy.

The i th element $[x_i, x_{i+1}]$ is mapped to $[0, 1]$ by using a transformation of the form (4). We assume that the approximate solution in the i th element is given by

$$Y^i(x) = Y^i(z) = \sum_{k=1}^6 a_k^i H_k^i(z),$$

and is represented in the $(i+1)_{st}$ element by

$$Y^{i+1}(x) = Y^{i+1}(z) = \sum_{k=1}^6 a_k^{i+1} H_k^{i+1}(z).$$

The basis functions are plotted across both the i th and $(i+1)_{st}$ elements and illustrated in Figure 3.

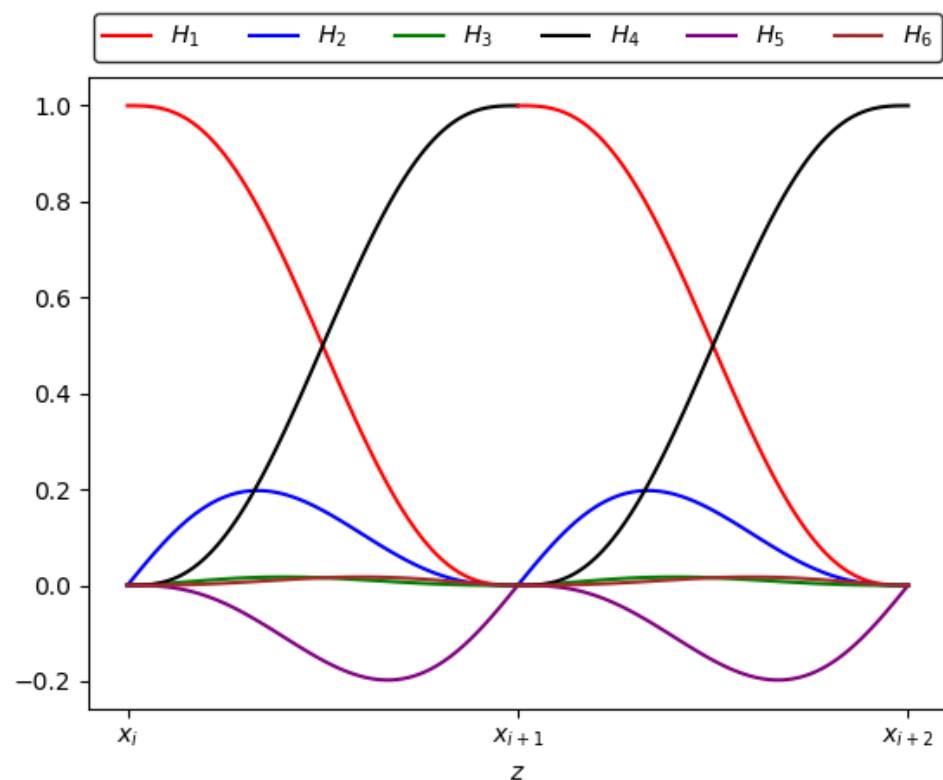


Figure 3. Basis functions on successive intervals.

We observe continuity at x_{i+1} for the basis functions. This is also true of their first and second derivatives. However the third derivative is discontinuous. This continuity has some interesting consequences on the coefficients of the solutions in the successive elements.

In order to obtain a smooth solution that is $\mathbb{C}^2$ continuous, we enforce the condition

$$Y^i(x_{i+1}) = Y^{i+1}(x_{i+1}),$$

which is equivalent, in the variable z , to

$$Y^i(1) = Y^{i+1}(0).$$

This implies that $a_1^{i+1} = a_4^i$. The continuity of the derivative at x_{i+1} is equivalent to

$$\left. \frac{dY^{(i)}}{dz} \right|_{z=1} = \left. \frac{dY^{(i+1)}}{dz} \right|_{z=0}$$

and yields $a_2^{i+1} = a_5^i$. Similarly the continuity of the second derivative at x_{i+1} is equivalent to

$$\left. \frac{d^2Y^{(i)}}{dz^2} \right|_{z=1} = \left. \frac{d^2Y^{(i+1)}}{dz^2} \right|_{z=0}. \quad (11)$$

This results in $a_3^{i+1} = a_6^i$. Hence the first three coefficients in the $(i+1)_{st}$ interval coincide with the last three coefficients in the i th interval. This repetitive pattern continues as we proceed to successive elements. Thus, we may represent the solution in the i th element by

$$Y(z) = \sum_{k=1}^6 a_{k+3(i-1)} H_k(z), \quad (12)$$

where we write $H_k(z)$ for $H_k^i(z)$ bearing in mind that $H_k(z)$ is a function of i , and that we have dropped the superscript i from $Y^i(z)$. With this labelling of the coefficients we are automatically ensuring that the solution, and its first and second derivatives are continuous at the nodes. There are $3N+3$ unknowns resulting from (12). Had we used a quintic Lagrange basis then we would have $6N$ unknowns, as it is not possible to build in the continuity conditions to get a simple form like in (12).

Remark

Substituting $z = 0$ and $z = 1$ into (12), its derivative and its second derivative, it can be shown that that $Y(x_i) = a_{3i-2}$, $hY'(x_i) = a_{3i-1}$ and $h^2Y''(x_i) = a_{3i}$, $i = 1, 2, \dots, N+1$. Thus every third coefficient beginning from a_1 is an approximation to the solution at the nodes. Similarly every third coefficient beginning from a_2 scaled by h , is an approximation to the derivative at the nodes. Likewise, every third coefficient beginning from a_3 scaled by h^2 represents an approximation to the second derivative at the nodes.

6. Error Analysis

The following is an adaptation of the work done by de Boor and Swartz [23] to quintic Hermite collocation. A third order differential equation, defined on $[a, b]$, can be written in the form

$$Ly(x) = f(x),$$

where the operator $L = \sum_{k=0}^3 a_k(x)D^k$ and D denotes the derivative operator. Then, the error is given by

$$\begin{aligned} y(x) - Y(x) &= L^{-1}f(x) - Y(x) \\ &= L^{-1}[f(x) - LY(x)] \\ &= L^{-1}r(x), \end{aligned}$$

where $r(x)$ is the residual. Hence,

$$y(x) - Y(x) = \int_a^b G(x, \xi) r(\xi) d\xi$$

where $G(x, \xi)$ is the Green's function, or integral kernel, associated with the linear problem. Now,

$$D^p(y(x) - Y(x)) = \int_a^b G_p(x, \xi) r(\xi) d\xi \quad (13)$$

$$\begin{aligned} &= \sum_{j=1}^N \int_{x_j}^{x_{j+1}} G_p(x, \xi) r(\xi) d\xi \\ &= \sum_{j=1}^N E_j(x), \end{aligned} \quad (14)$$

where $G_p(x, \xi) = D^p G(x, \xi)$ and

$$E_j(x) = \int_{x_j}^{x_{j+1}} G_p(x, \xi) r(\xi) d\xi, \quad p = 0, 1, 2. \quad (15)$$

Consider one of the intervals $[x_j, x_{j+1}]$ of Δ . Denote the collocation points by

$$\begin{aligned} x_{j,i} &= \frac{x_j + x_{j+1}}{2} + r_i \frac{h}{2} \\ &= x_j + \frac{h}{2} + r_i \frac{h}{2}, \quad i = 1, 2, 3. \end{aligned}$$

Approximate the residual $r(\xi)$ on $[x_j, x_{j+1}]$ by a quadratic interpolant $p_2(\xi)$ such that

$$r(\xi) = p_2(\xi) + \frac{r^3(\theta_\xi)}{6} (\xi - x_{j,1})(\xi - x_{j,2})(\xi - x_{j,3}), \quad (16)$$

where $\theta_\xi \in (x_j, x_{j+1})$.

Since $r(\xi)$ vanishes at the collocation points, we have $p_2(\xi) = 0$ and hence (16) can be written as

$$r(\xi) = p_3(\xi) r[x_{j,1}, x_{j,2}, x_{j,3}, \xi],$$

where $p_3(\xi) = \prod_{i=1}^3 (\xi - x_{j,i})$ and $r[x_{j,1}, x_{j,2}, x_{j,3}, \xi]$ denotes the third divided difference of r . Hence the integrand in (13) can be written in the form

$$\begin{aligned} G_p(x, \xi) r(\xi) &= p_3(\xi) G_p(x, \xi) r[x_{j,1}, x_{j,2}, x_{j,3}, \xi] \\ &= p_3(\xi) g(x, \xi), \end{aligned} \quad (17)$$

where $g(x, \xi) = G_p(x, \xi) r[x_{j,1}, x_{j,2}, x_{j,3}, \xi]$.

Interpolate $g(x, \xi)$ by a polynomial $q_{n-1}(x, \xi)$ of degree $\leq n-1$, in the variable ξ at any points $\sigma_i, i = 1, 2, \dots, n$ in $[x_j, x_{j+1}]$, to obtain

$$g(x, \xi) = q_{n-1}(x, \xi) + \frac{g^n(x, \xi_\sigma)}{n!} \prod_{i=1}^n (\xi - \sigma_i), \quad (18)$$

where $\xi_\sigma \in (x_j, x_{j+1})$. Equation (17) then becomes

$$G_p(x, \xi)r(\xi) = p_3(\xi) \left[q_{n-1}(x, \xi) + \frac{g^n(x, \xi_\sigma)}{n!} \prod_{i=1}^n (\xi - \sigma_i) \right]. \quad (19)$$

Substituting (19) into (15) results in

$$E_j(x) = \int_{x_j}^{x_{j+1}} p_3(\xi) q_{n-1}(x, \xi) d\xi + \int_{x_j}^{x_{j+1}} p_3(\xi) \frac{g^n(x, \xi_\sigma)}{n!} \prod_{i=1}^n (\xi - \sigma_i) d\xi.$$

If the collocation points are chosen so that $p_3(\xi)$ is orthogonal to $q_{n-1}(x, \xi)$, that is

$$\int_{x_j}^{x_{j+1}} p_3(\xi) q_{n-1}(x, \xi) d\xi = 0$$

for all polynomials $q_{n-1}(x, \xi)$ of degree $\leq n-1$, then

$$\begin{aligned} E_j(x) &= \int_{x_j}^{x_{j+1}} \prod_{i=1}^3 (\xi - x_{j,i}) \frac{g^n(x, \xi_\sigma)}{n!} \prod_{i=1}^n (\xi - \sigma_i) d\xi \\ &= O(h^{n+4}). \end{aligned} \quad (20)$$

Equation (20) follows since $|\xi - x_{j,i}|, |\xi - \sigma_i| \leq h$ and we have assumed that $D^n g(x, \xi)$ can be bounded independently of Δ . If we now sum $E_j(x)$ in (14), we obtain

$$D^p(y(x) - Y(x)) = O(h^{n+3}).$$

If $n = 0$, we forgo the interpolation of $g(x, \xi)$ and assume that $g(x, \xi)$ can be bounded on Δ such that

$$D^p(y(x) - Y(x)) = O(h^3).$$

We follow this idea to obtain higher order convergence in the case that $D^n g(x, \xi)$ cannot be bounded independent of Δ . In order to achieve this we prove the following theorem.

Theorem 1. Let $k_j, j = 0, 1, \dots, 8$ be constants independent of Δ and assume that there exists a constant k_1 such that $\forall x \in [a, b]$

$$\|D^j G_p(x, \xi)\| \leq k_1, \quad p = 0, 1, 2, \quad j = 0, 1, 2, 3, \quad (21)$$

where we consider $G_p(x, \xi)$ to be an element of $\mathbb{C}^3[a, x] \times \mathbb{C}^3[x, b]$. If the coefficients of L are smooth enough, specifically $a_i(x) \in \mathbb{C}^6[a, b]$, $i = 0, 1, 2, 3$ and $y(x) \in \mathbb{C}^9[a, b]$, then there exists a constant k_2 such that for each j

$$\|D^{3+p} r\|_{(j)} \leq k_2 \quad p = 0, 1, 2, 3, \quad (22)$$

where

$$\|f\|_{(j)} = \sup_{\xi \in (x_j, x_{j+1})} |f(\xi)|.$$

Proof. Since $r = f - LY = L(y - Y)$, it follows that $D^{3+p} r$ on $[x_j, x_{j+1}]$ is a combination of the derivatives of the coefficients of L , up to the order $3 + p$, with the derivatives of $y - Y$ up to the order $6 + p$ (recall L is third order). It is therefore sufficient to prove the existence of a constant k_3 such that

$$\|D^p(y - Y)\|_{(j)} \leq k_3, \quad p = 0, 1, \dots, 9. \quad (23)$$

The following result, namely.

$$\|D^p(y - Y)\|_{(j)} \leq k_0 h^3, \quad p = 0, 1, 2, 3, \quad (24)$$

is proved by de Boor and Swartz [23].

We now consider the case $p = 4, 5$. Expand y at some point $\sigma \in [x_j, x_{j+1}]$ in a Taylor series y_j of order < 6 to obtain

$$y - y_j = \frac{y^{(6)}(\xi_j)}{6!} (\xi - \sigma)^6,$$

where $\xi_j \in (x_j, x_{j+1})$, from which it is simple to show that

$$D^p(y - y_j) = \frac{y^{(6)}(\xi_j)}{(6-p)!} (\xi - \sigma)^{6-p}. \quad (25)$$

From (25), we deduce that

$$\|D^p(y - y_j)\|_{(j)} \leq k_4 h^{6-p}. \quad (26)$$

If X is a non-negative discrete random variable and t is a positive real number then, by Markov's inequality

$$P[X > t] \leq \frac{E(X)}{t}$$

where $E(X)$ denotes the expectation of X and P , the probability. With $X = X_1 = \frac{\|D^3(y_j - Y)\|_{(j)}}{h}$ and $t = t_1 = \|D^4(y_j - Y)\|_{(j)}$, we obtain

$$P[X_1 > t_1] \leq \frac{\|D^3(y_j - Y)\|_{(j)}}{h \|D^4(y_j - Y)\|_{(j)}},$$

and with $X = X_2 = \frac{\|D^3(y_j - Y)\|_{(j)}}{h^2}$ and $t = t_2 = \|D^5(y_j - Y)\|_{(j)}$ we obtain

$$P[X_2 > t_2] \leq \frac{\|D^3(y_j - Y)\|_{(j)}}{h^2 \|D^5(y_j - Y)\|_{(j)}},$$

which allows us to write

$$\|D^p(y_j - Y)\|_{(j)} \leq k_7 h^{3-p} \|D^3(y_j - Y)\|_{(j)}, \quad (27)$$

for $p = 4, 5$, where

$$k_7 = \max \left\{ \frac{1}{P[X_1 > t_1]}, \frac{1}{P[X_2 > t_2]} \right\}.$$

We also have that

$$\begin{aligned} \|D^3(y_j - Y)\|_{(j)} &\leq \|D^3(y_j - y)\|_{(j)} + \|D^3(y - Y)\|_{(j)} \\ &\leq k_4 h^3 + k_0 h^3, \end{aligned} \quad (28)$$

where we have used both (24) and (26). Substituting (28) into (27) yields

$$\begin{aligned} \|D^p(y_j - Y)\|_{(j)} &\leq k_7 (k_4 + k_0) h^{6-p} \\ &= k_5 h^{6-p}. \end{aligned} \quad (29)$$

Hence, for $p = 4, 5$ we have that

$$\begin{aligned}\|D^p(y - Y)\|_{(j)} &\leq \|D^p(y - y_j)\|_{(j)} + \|D^p(y_j - Y)\|_{(j)} \\ &\leq k_4 h^{6-p} + k_5 h^{6-p} \\ &\leq k_6 h^{6-p},\end{aligned}\quad (30)$$

where we have used (26) and (29).

For $p = 6, 7, 8, 9$

$$D^p(y - Y) = D^p y \quad (\text{recall } Y \text{ has degree } < 6)$$

so that

$$\begin{aligned}\|D^p(y - Y)\|_{(j)} &= \|D^p y\|_{(j)} \\ &\leq \max\{\|D^p y\|_{(j)} \mid 6 \leq p \leq 9\} \\ &= k_8.\end{aligned}\quad (31)$$

Hence (24), (30) and (31) proves (23). $\square$

The following theorem establishes the order of convergence.

Theorem 2. Let $k_j, j = 9, 10, \dots, 13$ be constants independent of Δ . Assume that the coefficients $a_i(x)$ of L satisfy $a_i(x) \in \mathbb{C}^6$ for all i , that Equation (21) holds and that $y(x) \in \mathbb{C}^9[a, b]$. If the collocation points are chosen such that $q_2(x, \xi)$ is orthogonal to $p_3(\xi)$ for every $q_2(x, \xi) \in \mathbb{P}_2$ then there exists a constant c_1 such that

$$|D^p(y - Y)(x_j)| \leq c_1 h^6, \quad p = 0, 1, 2, \quad (32)$$

and a constant c_2 such that

$$\|D^p(y - Y)\|_\infty \leq c_2 h^{6-p}, \quad p = 0, 1, 2, 3. \quad (33)$$

Proof. We write

$$G_p(x, \xi) r(\xi) = p_3(\xi) \left[q_2(x, \xi) + (\xi - x_j)^3 \frac{(D^3 g(x, \xi))(\theta_\xi)}{3!} \right] \quad (34)$$

with $q_2(x, \xi)$ the Taylor series for $g(x, \xi)$, with terms of order ≤ 2 (see (17) and (18)). Choosing the collocation points so that

$$\int_{x_j}^{x_{j+1}} q_2(x, \xi) p_3(\xi) d\xi = 0 \quad (35)$$

for every polynomial $q_2 \in \mathbb{P}_2$. We have

$$\begin{aligned}E_j(x) &= \int_{x_j}^{x_{j+1}} G_p(x, \xi) r(\xi) d\xi \quad j = 1, \dots, N \\ |E_j(x)| &= \left| \int_{x_j}^{x_{j+1}} p_3(\xi) (\xi - x_j)^3 \frac{(D^3 g(x, \xi))(\theta_\xi)}{3!} d\xi \right| \\ &\leq k_9 h^7 \|D^3 g(x, \xi)\|_{(j)}.\end{aligned}\quad (36)$$

$$\leq k_9 h^7 \|D^3 g(x, \xi)\|_{(j)}. \quad (37)$$

Now

$$D^3(g_1 g_2) = \sum_{s=0}^3 \binom{3}{s} D^{3-s} g_1 D^s g_2.$$

We let $g_1 = G_p(x, \xi)$ and $g_2 = r[x_{j,1}, x_{j,2}, x_{j,3}, \xi]$. From

$$\begin{aligned} Dg_2 &= r[x_{j,1}, x_{j,2}, x_{j,3}, \xi, \xi] = \frac{(D^{3+1}r)(\theta_{x,1})}{4!}, \\ D^2g_2 &= r[x_{j,1}, x_{j,2}, x_{j,3}, \xi, \xi, \xi] = \frac{(D^{3+2}r)(\theta_{x,2})}{5!}, \end{aligned}$$

we infer that

$$D^s g_2 = \frac{(D^{3+s}r)(\theta_{x,s})}{(s+3)!}.$$

Hence

$$D^3 g(x, \xi) = \sum_{s=0}^3 \binom{3}{s} D^{3-s} G_p(x, \xi) \frac{(D^{3+s}r)(\theta_{x,s})}{(s+3)!}. \quad (38)$$

We now consider three cases:

- (i) If $x \notin (x_j, x_{j+1})$ then from (21)

$$\|D^{3-s} G_p(x, \xi)\|_{(j)} \leq k_1 \quad s = 0, 1, 2, 3$$

while

$$\|D^{3+s}r\|_{(j)} \leq k_2$$

from (22). Hence from (38), we have

$$\|D^3 g(x, \xi)\|_{(j)} \leq k_{10},$$

and (37) gives

$$|E_j(x)| \leq k_{11} h^7. \quad (39)$$

- (ii) If $x \in (x_j, x_{j+1})$ then $G_p(x, \xi) \in \mathbb{C}^{2-p}[x_j, x_{j+1}]$. Now consider say $p = 0$. Equation (34) is then rewritten as

$$G_0(x, \xi) r(\xi) = p_3(\xi) \left[q_1(x, \xi) + (\xi - x_j)^2 \frac{D^2 g(x, \xi)(\theta_{\xi})}{2!} \right],$$

where $q_1(x, \xi)$ is the Taylor series for $g(x, \xi)$ of order one. Once again, we choose the collocation points so that

$$\int_{x_j}^{x_{j+1}} q_1(x, \xi) p_3(\xi) d\xi = 0.$$

Hence the equivalent equation to (36) is

$$\begin{aligned} |E_j(x)| &= \left| \int_{x_j}^{x_{j+1}} p_3(\xi) (\xi - x_j)^2 \frac{D^2(g(x, \xi))(\theta_{\xi})}{2!} d\xi \right| \\ &\leq k_9 h^6 \|D^2 g(x, \xi)\|_{(j)}. \end{aligned} \quad (40)$$

The equivalent equation to (38) is then

$$D^2g(x, \xi) = \sum_{s=0}^2 \binom{2}{s} D^{2-s}G_0(x, \xi) \frac{D^{3+s}r(\theta_{x,s})}{(s+3)!}$$

and $\|D^2g(x, \xi)\|_{(j)} \leq k_{10}$. Hence (40) reduces to

$$|E_j(x)| \leq k_{12}h^6.$$

Similarly, by considering $p = 1, 2$ we may show that

$$\|D^s g(x, \xi)\|_{(j)} \leq k_{10}, \quad s \leq 2 - p$$

and

$$|E_j(x)| \leq k_{12}h^{6-p}. \quad (41)$$

(iii) If $x \in \Delta$ so that $x \notin (x_j, x_{j+1})$ for all j then, from summing (39) (recall (14)) we obtain

$$|D^p(y - Y)(x)| \leq c_1 h^6, \quad p = 0, 1, 2$$

for x coinciding with the nodes x_j . Otherwise $x \in (x_j, x_{j+1})$ for exactly one of the sub-intervals of Δ . So, by (39) and (41) and summing over j we obtain

$$\begin{aligned} |D^p(y - Y)(x)| &\leq k_{11}h^6 + k_{12}h^{6-p} \\ &\leq k_{13}h^{6-p} \end{aligned}$$

This implies (33).

□

The following theorem establishes the optimal choice for the collocation points.

Theorem 3. *The optimal choice for the collocation points are the Gauss points.*

Proof. The orthogonality of $q_2(x, \xi)$ and $p_3(\xi)$ from (35) is equivalent to

$$\int_{x_j}^{x_{j+1}} (\xi - x_{j,1})(\xi - x_{j,2})(\xi - x_{j,3})\xi^p d\xi = 0, \quad p = 0, 1, 2. \quad (42)$$

Change the integral in (42) to the interval $[-1, 1]$ by using the linear transformation

$$\xi = \frac{h}{2}\xi' + x_j + \frac{h}{2},$$

to yield

$$\int_{-1}^1 (\xi' - r_1)(\xi' - r_2)(\xi' - r_3) \left(\frac{h}{2}\xi' + x_j + \frac{h}{2} \right)^p d\xi' = 0, \quad p = 0, 1, 2. \quad (43)$$

Equation (43) is equivalent to the following three equations

$$\int_{-1}^1 (\xi' - r_1)(\xi' - r_2)(\xi' - r_3) d\xi' = 0, \quad (44)$$

$$\int_{-1}^1 (\xi' - r_1)(\xi' - r_2)(\xi' - r_3)\xi' d\xi' = 0, \quad (45)$$

$$\int_{-1}^1 (\xi' - r_1)(\xi' - r_2)(\xi' - r_3)\xi'^2 d\xi' = 0. \quad (46)$$

Integrating (44)–(46), we get

$$r_1 + r_2 + r_3 + 3r_1r_2r_3 = 0 \quad (47)$$

$$r_1r_2 + r_2r_3 + r_1r_3 = -\frac{3}{5} \quad (48)$$

$$r_1 + r_2 + r_3 + \frac{5}{3}r_1r_2r_3 = 0. \quad (49)$$

Equations (47) and (49) implies that $r_1r_2r_3 = 0$, hence we choose $r_2 = 0$. without loss of generality. This implies that $r_3 = -r_1$ and $r_1^2 = \frac{3}{5}$, so that $r_1 = -\sqrt{\frac{3}{5}}$, $r_3 = \sqrt{\frac{3}{5}}$. These are the Gauss points, or zeros, of the third degree Legendre Polynomial. $\square$

7. Numerical Examples

Example 1. We now consider the ODE

$$\begin{aligned} y'''(x) + 2y'(x) &= -980 \cos(10x) \\ y(0) = 0, \quad y'(0) &= 10, \quad y(1) = \sin(10). \end{aligned}$$

Substituting (12) in the given ODE results in the following system of equations:

$$\sum_{k=1}^6 \left[\frac{1}{h^3} H_k'''(z) + \frac{2}{h} H_k'(z) \right] a_{k+3(i-1)} = -980 \cos(10(x_i + zh)), \quad i = 1, 2, \dots, N. \quad (50)$$

The boundary condition

$$y(0) = Y(0) = \sum_{k=1}^6 a_k H_k(0) = 0$$

yields $a_1 = 0$ whilst the derivative condition

$$y'(0) = Y'(0) = \frac{1}{h} \sum_{k=1}^6 a_k H_k'(0) = 10$$

yields $a_2 = 10h$ and

$$y(1) = Y(1) = \sum_{k=1}^6 a_{k+3(N-1)} H_k(1) = \sin(10)$$

yields $a_{3N+1} = \sin(10)$.

There are $3N + 3$ unknowns. Given that we have three boundary conditions, we thus require $3N$ conditions in order to solve the problem uniquely. We therefore choose three collocation points r_1, r_2, r_3 in each element. The r_j are chosen as the zeros of the third degree Legendre polynomial, shifted to the interval $[0, 1]$. These were shown to be the optimal choice for collocation points. The collocation points are then substituted into Equation (50) to give the $3N$ linear equations. The matrix vector system, of size $(3N + 3) \times (3N + 3)$, has the form $Aa = f$ where A has the form (illustrated for $N = 3$)

and

$$|y(x_j) - Y(x_j)|_{\frac{h}{2}} = O\left(\left(\frac{h}{2}\right)^n\right). \quad (53)$$

By taking the ratio of (52) to (53) we obtain

$$\alpha = \frac{|y(x_j) - Y(x_j)|_h}{|y(x_j) - Y(x_j)|_{\frac{h}{2}}} \approx 2^n,$$

from which the order of convergence $n(h) \approx \frac{\ln(\alpha)}{\ln(2)}$.

The conditions of Theorem 2 are satisfied. We have solved the problem with $N = 20$ and $N = 40$ and summarise in Table 1 the convergence orders at the common nodes for $p = 0, 1, 2$ according to Equation (32). The orders agree remarkably with Equation (32), the difference being attributed to numerical error. The global order is shown in Table 2 and illustrates the validity of Equation (33).

Table 1. Nodal convergence rates at the common nodes for Example 1.

$ D^p(y - Y)(x_j) $				$ D^p(y - Y)(x_j) $			
x_j	$p = 0$	$p = 1$	$p = 2$	x_j	$p = 0$	$p = 1$	$p = 2$
0.05	6.0178	6.0180	6.0107	0.55	6.0102	6.0133	6.0231
0.10	6.0177	6.0151	6.0109	0.60	6.1360	6.0133	6.0130
0.15	6.0175	6.0146	6.0112	0.65	6.0155	6.0133	6.0116
0.20	6.0171	6.0144	6.0118	0.70	6.0166	6.0130	6.0113
0.25	6.0164	6.0143	6.0126	0.75	6.0172	6.0125	6.0114
0.30	6.0150	6.0142	6.0142	0.80	6.0175	6.0105	6.0117
0.35	6.0125	6.0142	6.0185	0.85	6.0177	6.0442	6.0123
0.40	6.0082	6.0142	6.0543	0.90	6.0177	6.0179	6.0134
0.45	6.0038	6.0146	6.9835	0.95	6.0177	6.0174	6.0163
0.50	6.0053	6.0119	6.9829				

Table 2. Global convergence rates for Example 1.

p	$\ D^p(y - Y)(x)\ _\infty$
0	6.0214
1	5.0000
2	4.0125
3	2.9963

Example 2. Consider the problem

$$y'' + \frac{y'}{x} = \left(\frac{2}{8 - x^2}\right)^2, \quad 0 < x < 1, \quad y'(0) = y(1) = 0,$$

which has the exact solution

$$y(x) = 2 \ln\left(\frac{7}{8 - x^2}\right).$$

As there are two boundary conditions, we choose an additional collocation point in the first element. Hence the collocation points in the first element are the zeros of the fourth degree Legendre polynomial shifted to $[0, 1]$, whilst in the rest it is the zeros of the third degree Legendre polynomial. The solution is smooth on $[0, 1]$, but the coefficient $\frac{1}{x}$ is unbounded at $x = 0$. This, however, is not a problem since the collocation points are chosen in $(0, 1)$, which avoids the endpoints. The errors at the common nodes as well as the convergence order is displayed in Table 3. Clearly convergence is $O(h)$. Theorem 2 does not apply here as there is a coefficient with a singularity at $x = 0$.

In the next example we consider the application of the method to partial differential equations.

Table 3. Nodal errors and convergence rates at the common nodes for Example 2.

x_j	$ (y - Y)(x_j) $				
	$N = 10$	$N = 20$	$N = 40$	$n(h)$	$n(\frac{h}{2})$
0.1	3.851338×10^{-3}	1.881677×10^{-3}	9.307417×10^{-4}	1.0333	1.0156
0.2	3.409223×10^{-3}	1.677216×10^{-3}	8.302827×10^{-4}	1.0234	1.0144
0.3	3.005355×10^{-3}	1.474348×10^{-3}	7.303313×10^{-4}	1.0275	1.0135
0.4	2.582037×10^{-3}	1.271405×10^{-3}	6.301073×10^{-4}	1.0221	1.0128
0.5	2.172848×10^{-3}	1.067288×10^{-3}	5.291418×10^{-4}	1.0256	1.0122
0.6	1.747602×10^{-3}	8.611265×10^{-4}	4.270521×10^{-4}	1.0211	1.0118
0.7	1.327715×10^{-3}	6.521262×10^{-4}	3.234758×10^{-4}	1.0257	1.0115
0.8	8.915583×10^{-4}	4.394996×10^{-4}	2.180437×10^{-4}	1.0205	1.0112
0.9	4.548230×10^{-4}	2.224223×10^{-4}	1.103623×10^{-4}	1.0320	1.0111

Example 3. We illustrate the full spatial discretization process involved in the collocation procedure on this example.

$$u_t - u_{xxx} = 27\pi^3 \cos(t) \cos(3\pi x) - \sin(t) \sin(3\pi x), \quad 0 < x < 1, t \geq 0 \quad (54)$$

with boundary conditions

$$u(0, t) = 0, \quad u(1, t) = 0, \quad u_x(0, t) = 3\pi \cos(t)$$

and initial condition

$$u(x, 0) = \sin(3\pi x).$$

The exact solution is given by

$$u(x, t) = \cos(t) \sin(3\pi x).$$

In the variable z Equation (54) becomes

$$u_t - \frac{1}{h^3} u_{zzz} = 27\pi^3 \cos(t) \cos(3\pi(zh + x_i)) - \sin(t) \sin(3\pi zh + x_i). \quad (55)$$

Analogous to Equation (12), the trial solution, in the i th element, is written as

$$U^i(z) = \sum_{k=1}^6 a_{k+3(i-1)}(t) H_k(z). \quad (56)$$

Here the time dependence is reflected in the coefficients a . Substituting (56) into (55), we obtain

$$\begin{aligned} & \sum_{k=1}^6 a'_{k+3(i-1)}(t) H_k(z_j) - \frac{1}{h^3} \sum_{k=1}^6 a_{k+3(i-1)}(t) H_k'''(z_j) - 27\pi^3 \cos(t) \cos(3\pi(z_j h + x_i)) \\ & + \sin(t) \sin(3\pi(z_j h + x_i)) = 0. \end{aligned} \quad (57)$$

We then substitute three collocation points from each sub-interval into Equation (57) to obtain $3N$ conditions. Using these, along with the boundary conditions, we get a linear differential algebraic system of size $3N + 3$. In particular, the boundary conditions imply that $a_1(t) = a_{3N+1}(t) = 0$ and $a_2(t) = 3\pi h \cos(t)$. Differential algebraic systems are solved using the classical DASSL solver [24]. DASSL is designed for the numerical solution of implicit systems of differential/algebraic equations written in the form $F(t, y, y') = 0$, where F, y and y' are vectors, and initial values for y and y' are given. It is a classic DAE solver released as open source in 1982 and has been ported to Julia

recently. (<https://github.com/JuliaLang/julia>, accessed on 1 November 2022) was released in 2012 by MIT.

It is an open-source, multi-paradigm, high-level, high-performance, and incredibly dynamic scripting language. For scientific computing it resembles Matlab in syntax. It comes close to C in speed. It allows interaction with other scientific languages like Fortran, Python and R. There are over 2000 modules that can be added to it. One can interface with many plotting modules, but we have elected to use pyplot from matplotlib.

The graphs of both the solution and error are depicted in Figures 5 and 6, respectively. The numerical results indicate that the present method is successful in capturing the oscillatory nature of the solution in both space and time with a reasonable accuracy. The drop in accuracy as compared to the ode case can be attributed to the error in the time integration process.

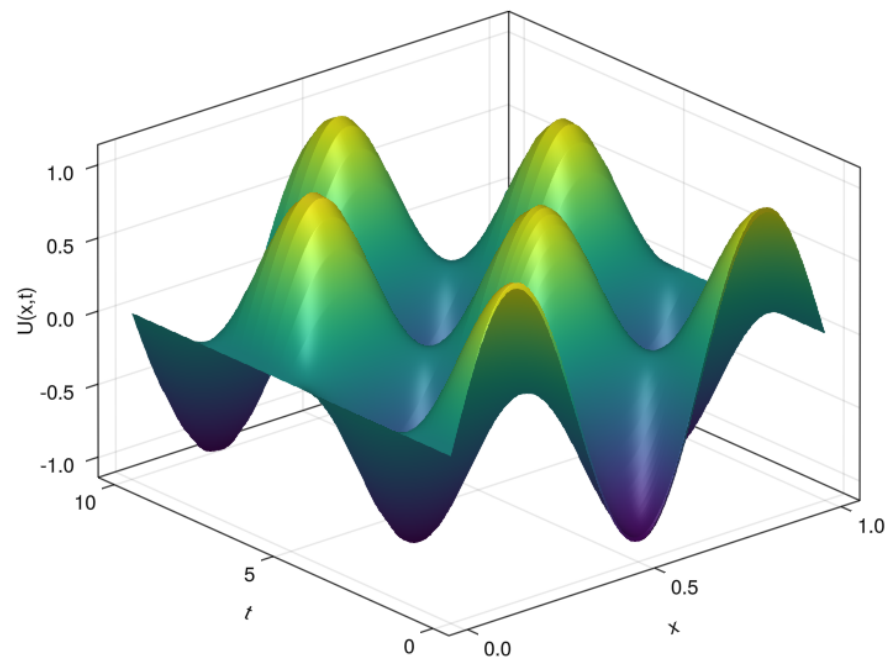


Figure 5. Approximate solution with $N = 100$ for Example 3.

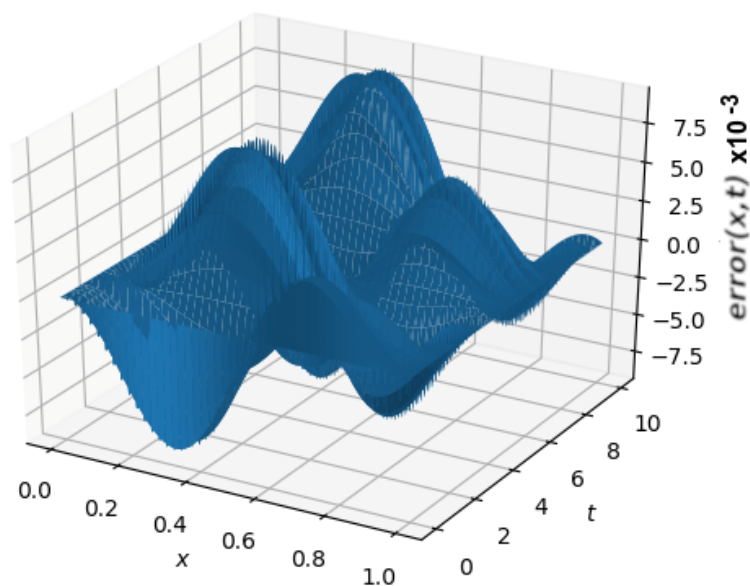


Figure 6. Error with $N = 100$ for Example 3.

We now solve the Korteweg–de Vries (KdV) equation [10]. The semi-discretization in space results in a system of DAEs which can be converted into a system of IVPs and be solved along similar lines as the ODE case discussed in Section 5. For the time integration we use a suitable high order stiff integrator. In contrast, most methods developed in previous studies used quasi-linearization with second order Crank Nicolson method for the time integration.

Example 4. We consider the following form of the KdV equation and illustrate the spatial discretization process involved in the collocation process below:

$$u_t + \epsilon uu_x + \mu u_{xxx} = 0, \quad 0 < x < 2. \quad (58)$$

It has boundary conditions

$$u_x(0, t) = u_x(2, t) = 0, \quad u(2, t) = 0$$

and an initial condition

$$u(x, 0) = 3C \operatorname{sech}^2(Ax + D),$$

where $\epsilon = 1$, $\mu = 4.84 \times 10^{-4}$, $C = 0.3$, $D = -6$, $A = 0.5\sqrt{\frac{\epsilon C}{\mu}}$. The exact solution is given by, (see [10])

$$u(x, t) = 3C \operatorname{sech}^2(Ax - Bt + D),$$

We use the exact same method as before, switching to the variable z so that (58) becomes

$$u_t + \frac{\epsilon}{h} uu_z + \frac{\mu}{h^4} u_{zzz} = 0. \quad (59)$$

We then substitute (56) into (59), to get

$$\begin{aligned} & \sum_{k=1}^6 a'_{k+3(i-1)}(t) H_k(z) + \left[\frac{\epsilon}{h} \sum_{k=1}^6 a_{k+3(i-1)}(t) H_k(z) \right] \left[\sum_{k=1}^6 a_{k+3(i-1)}(t) H'_k(z) \right] \\ & + \frac{\mu}{h^4} \sum_{k=1}^6 a_{k+3(i-1)}(t) H'''_k(z) = 0. \end{aligned} \quad (60)$$

We substitute three collocation points per element into Equation (60) to obtain $3N$ conditions. Together with the boundary conditions, we obtain a non-linear differential algebraic system of size $3N + 3$. In particular, the boundary conditions imply that $a_2(t) = a_{3N+1}(t) = a_{3N+2}(t) = 0$.

In order to obtain the initial conditions for the coefficients, that is $a_{k+3(i-1)}(0)$, we let

$$u(z, 0) = U(z, 0) = \sum_{k=1}^6 a_{k+3(i-1)}(0) H_k(z) = 3C \operatorname{sech}^2(A(x_i + zh) + D), \quad i = 1, 2, \dots, N. \quad (61)$$

We substitute the $3N$ collocation points into (61) to obtain a $3N \times 3N$ matrix vector system whose solution yields the value of the coefficients at $t = 0$. Equations (60) and (61) is easily converted to a system of IVPs which can be efficiently solved using the Julia QNDF solver (which is equivalent to the ODE15s in Matlab). Thereafter the PDE solution over the domain is obtained from Equation (56). Figure 7 depicts the solution profiles for various t values. This example describes a wave propagating in the positive x direction. In this figure the solid line represents the exact solution and the circles the approximate solution. It is clear the approximate solution closely matches the exact solution. The 3D solution and error are shown in Figures 8 and 9, respectively. We see that applying the quintic OCFE method in space combined with a powerful stiff ODE solver in time is capable of producing a very smooth and accurate solution.

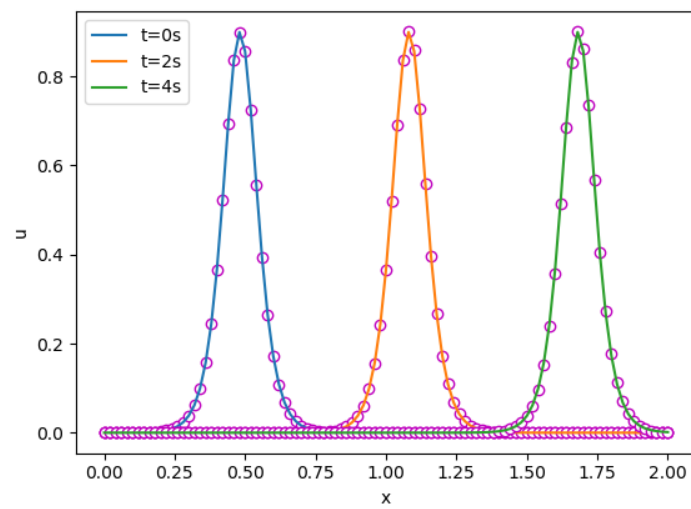


Figure 7. Approximate solution $N = 100$ for Example 4.

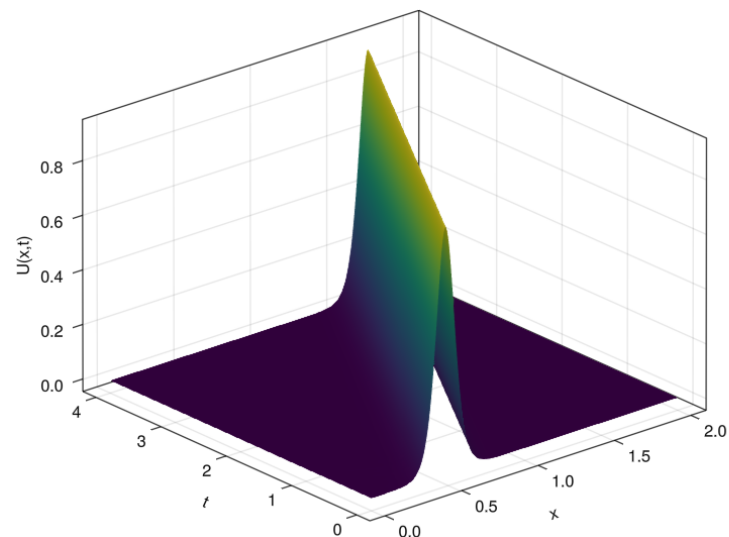


Figure 8. 3D surface plot for the approximate solution for Example 4.

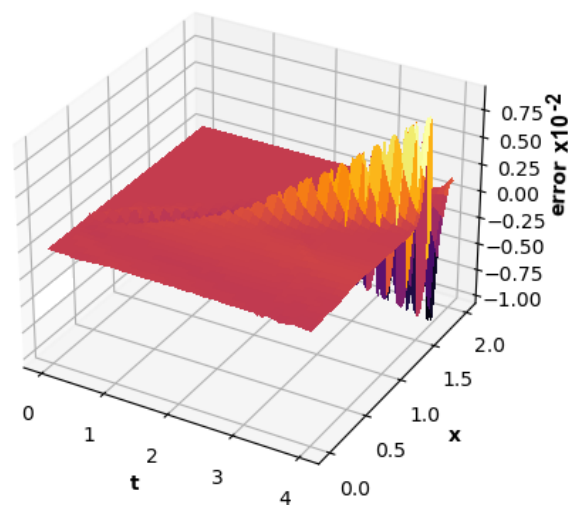


Figure 9. Error $N = 100$ for Example 4.

8. Conclusions

We have reviewed the numerical approximation of the solution of differential equations, using collocation methods, with a bias towards a quintic Hermite basis. In Lagrange collocation, the continuity conditions have to be satisfied, as well as the residual set to zero at the collocation points. This results in a much larger system of equations to solve. By using a Hermite basis the continuity conditions are automatically satisfied, as reflected in the coefficients of the trial solution. Thus only the collocation equations have to be solved. This is a huge computational advantage. In addition we have provided a useful error analysis, which is also applicable to the non-linear case. Collocation on finite elements is essentially equivalent to minimizing the residual over the domain of the problem. It is a powerful and versatile tool that rivals finite difference approximations, especially when the solution is oscillatory in nature.

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