

Heptic Hermite Collocation on Finite Elements



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Abstract We present the solution of linear and nonlinear ordinary differential equations using collocation on finite elements. A heptic (septic) basis is derived and its properties are discussed. The phenomenon of superconvergence at the nodes is illustrated. An investigation of the global and nodal rates of convergence reveals remarkable agreement with a theorem proved by Carl R. de Boor in 1973.

Keywords Heptic collocation · Superconvergence · Differential equations

1 Introduction

Orthogonal Collocation (OC) is an approximation method for solving differential equations. It is similar to the Pseudospectral Method (PS) and is also referred to as the Differential Quadrature Method (DQ). In contrast to finite difference methods, the solution by OC is defined as a continuous or piecewise continuous function.

The collocation method is employed in two different ways, either globally or locally. In the global collocation method, the method finds the solution for various numbers of collocation points. In the local collocation method, the domain is divided into equal-width subintervals called finite elements, and each element has a fixed number of collocation points within its boundaries. The solutions are then computed from the collocation points within each element.

The collocation method was introduced in the 1930s [1–4]. It was named the interpolation method by Kantorovich [1]; Lanczos called it the method of selected points [3] while Frazer et al. called it collocation [2]. From these three names, it can

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be inferred that the method interpolates the residual to zero at chosen points. The most attractive feature of the method is that it is easier to implement, since it does not require integration to determine the unknown coefficients.

The collocation might lead to the Runge phenomenon [5] because it is primarily a residual interpolation method. Bert and Malik [6] provided several examples of problems related to collocation with equal intervals.

Lanczos used Chebyshev polynomials for the basis functions and collocated at the zeros of Chebyshev polynomials of the second kind. Wright [7] chose to collocate at the zeros of Chebyshev polynomials of the first kind. The application of Chebyshev roots was a great improvement because the Runge phenomenon does not occur.

Another advancement to the method was the usage of Gaussian or Lobatto quadrature points by Villadsen and Stewart [8]. These are simply the roots of Jacobi polynomials. They referred to this as Orthogonal Collocation. By constructing the method with nodal values they further enhanced it. These adjustments gave rise to finite difference-like methods.

The phenomenon of collocation method in the 1970s happens in three branches, namely Orthogonal Collocation (OC), Pseudospectral (PS), and Differential Quadrature (DQ). Villadsen and Stewart introduced the OC branch in their paper, and further improvements to the method which outline collocation at Gauss, Radau, and Lobatto points were mentioned in Villadsen [8], Finlayson [9], and Villadsen and Michelsen [10]. It was proved that the numerical quadrature of the method of moments is equivalent to collocation at Gauss points.

They further applied the method for problems symmetric about an axis, using cylindrical, spherical, and planar coordinates. They exclusively used the nodal differentiation matrices. Early papers indicated that the method compared favourably with finite differences [11–14].

Orzag was the first to start the Pseudospectral thread [15] which was later improved by Gottlieb and Orzag [16]. Although the pseudospectral method is similar to collocation, it is seldom used to refer to approximations of integration in MWR. Orzag solved periodic problems using trigonometric basis functions. His work includes collocation at the zeros of Chebyshev polynomials of the second kind for non-periodic first-order linear hyperbolic problems. He showed that collocation can accurately approximate the Galerkin method. Here, he used Chebyshev trial functions and did not consider nodal approximations. His main contribution was the application of fast Fourier transforms (FFT) to perform calculations.

The Differential Quadrature Method thread was initially presented in Bellman and Casti [17], Bellman et al. [18], and Bellman [19]. Here Bellman et al. introduced the idea of a nodal differential matrix applied to first- and second-order differential equations. Although the paper does not give much details with respect to boundary condition treatment. The idea to apply a nodal differentiation matrix was not new, it has been applied before. In Bellman et al. [18], Bellman proposed the method of differentiation matrices based on collocation at Gauss points. In Nielson [20], the formulas for the nodal differentiation matrix with arbitrary nodal locations were introduced. The method was adopted for the solution of engineering problems.

When one uses a global polynomial, the solution is represented by a single polynomial on the domain. This approach is fairly accurate when low-order polynomials can represent the solution.

Finite element methods can accurately represent complex geometries. The interest in finite element methods erupted in the 1970s [21–23]. There was a huge interest for other applications because of the initial success in structural mechanics. The idea by Villadsen and Stewart of using quadrature points globally was extended to finite elements.

Unlike the global method, a finite element method divides the domain into a collection of subdomains, with a polynomial representation over each subdomain. The two methods are identical when using a single element hence the finite element method is more general. The degree of continuity at the element boundaries is denoted by C^n .

There are two alternatives to dealing with the continuity conditions at the boundary of the elements. Firstly we could enforce the continuity of the trial functions at the boundary of the elements. This also applies to the continuity of the derivatives depending on the smoothness requirement. Alternatively, we could choose trial functions like the Hermite polynomials which have built-in continuity. The latter approach results in fewer unknowns to solve for. To a large extent the solution of chemical engineering problems, namely two point boundary value problems have been achieved by the Galerkin finite element method [24, 25] with far greater accuracy than the collocation method, though with slightly more numerical effort. For the solution of reaction-diffusion models, see [26, 27].

C^1 Collocation at Gauss Points This was described by de Boor and Swartz [28] and Douglas and Dupont [29]. Carey and Finlayson [30] employed a Lagrange basis.

C^0 Collocation at Lobatto Points This method based on Lobatto points is also used in the finite element approach. One method is C^0 , which uses Lagrange basis functions and called the Hybrid-Collocation-Galerkin method [31–33]. Another approach described in Gray [34], Young [35], Young [36], Hennart [37], and Leyk [38, 39] uses a Lagrange basis and a simple Galerkin method with integration effected using Lobatto quadrature. Young called this the Lobatto-Galerkin method. Gray and Hennart only used quadratic trial functions with integration using Simpson's rule. This was referred to as the *hp* Spectral element in Maday and Patera [40], Canuto et al. [41], Karniadakis and Sherwin [42], and Vosse and Mineev [43].

Convergence Rate and Efficiency The approximate solution for orthogonal collocation and the finite element methods they approximate have the same convergence and superconvergence rates. Finite element methods and collocation at Gauss points require much less numerical effort than the contrasting Galerkin method when using the same trial functions especially in several dimensions.

2 Heptic Hermite Basis Functions

We seek a basis for \mathcal{P}_7 , the vector space of polynomials of degree ≤ 7 on the interval $[x_i, x_{i+1}]$. There are eight such functions and we denote them by $H_k, k = 1, 2, \dots, 8$. We further stipulate their function and derivative values at the end points x_i and x_{i+1} as follows:

$$H_k^{(p)}(x_i) = \frac{\delta_{k,p+1}}{h^p}, H_k^{(p)}(x_{i+1}) = 0, H_{k+4}^{(p)}(x_i) = 0, H_{k+4}^{(p)}(x_{i+1}) = \frac{\delta_{k,p+1}}{h^p}, \quad (1)$$

where $k, p + 1 \in S = \{1, 2, 3, 4\}$ 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

$$z = \frac{(x - x_i)}{(x_{i+1} - x_i)} = \frac{(x - x_i)}{h} \quad (2)$$

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 (1) transform naturally in the variable z to

$$H_k^{(p)}(0) = \delta_{k,p+1}, H_k^{(p)}(1) = 0, H_{k+4}^{(p)}(0) = 0, H_{k+4}^{(p)}(1) = \delta_{k,p+1} \quad k, p + 1 \in S.$$

These conditions enable the unique derivation of the $H_k(z), k = 1, 2, \dots, 8$. The polynomial $H_3(z)$ has a zero of multiplicity four at $z = 1$ and a zero of multiplicity two at $z = 0$ and therefore has the form of $H_3(z) = (Az + B)z^2(z - 1)^4$. The remaining conditions $H_3''(0) = 1$ and $H_3'''(0) = 0$ are used to evaluate A and B . Using this approach, the polynomials $H_1(z), H_2(z), H_3(z)$, and $H_4(z)$ are derived and displayed in Eqs. (3)–(6).

$$H_1(z) = (20z^3 + 10z^2 + 4z + 1)(z - 1)^4 \quad (3)$$

$$H_2(z) = z(10z^2 + 4z + 1)(z - 1)^4 \quad (4)$$

$$H_3(z) = \frac{z^2}{2}(4z + 1)(z - 1)^4 \quad (5)$$

$$H_4(z) = \frac{z^3}{6}(z - 1)^4. \quad (6)$$

By using symmetry/antisymmetry, one can show that

$$H_5(z) = H_1(1 - z) \quad (7)$$

$$H_6(z) = -H_2(1 - z) \quad (8)$$

$$H_7(z) = H_3(1 - z) \quad (9)$$

$$H_8(z) = -H_4(1 - z). \quad (10)$$

From (7)–(10), we may write

$$H_{j+4}^{(p)}(z) = (-1)^{j-1+p} H_j^{(p)}(1 - z), \quad j = 1, 2, 3, 4. \tag{11}$$

The uniqueness of the interpolatory conditions ensures that the polynomials $H_i(z)$ are independent. Consider $p = 0$, if $H_j(z)$ is shifted to the $(i + 1)_{st}$ interval the equation of the curve becomes $H_j(z - 1)$. When evaluated at $z = 1$ we get $H_j(0)$. Now $H_{j+4}(1) = (-1)^{j-1} H_j(0)$ and for $j = 1, 3$ $H_{j+4}(1) = H_j(0)$, also for $j = 2, 4$ we have $H_{j+4}(1) = -H_j(0) = 0 = H_j(0)$. Similar relationships apply for the derivatives of order up to three. Hence $H_{j+4}(z)$ and its derivatives up to order three are continuous at the element boundary with $H_j(z)$ and its derivatives of order up to three in the $(i + 1)_{st}$ interval. If we write $H_5(z) = H_1(-(z - 1))$, then we note that $H_5(z)$ is a reflection of $H_1(z)$ about the vertical axis together with a shift of one unit to the right. $H_7(z)$ is similarly related to $H_3(z)$. Also, $H_6(z)$ may be interpreted as $H_2(z)$ rotated by 180° anticlockwise and then shifted one unit to the right. $H_8(z)$ is also related to $H_4(z)$ in a similar manner.

3 Collocation on Finite Elements

Consider solving a fourth-order linear ordinary differential equation in one spatial variable, x , and on the domain $[a, b]$. Firstly, the domain $[a, b]$ is divided into N subintervals 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 Fig. 1. We shall refer to this discretization as the 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 (2). We assume that the approximate solution in the i_{th} element is given by

$$U^i(x) = U^i(z) = \sum_{k=1}^8 C_k^{(i)} H_k^i(z)$$

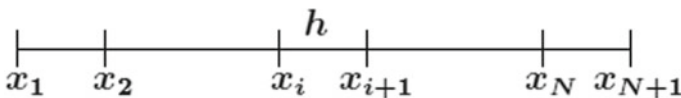


Fig. 1 Mesh points on the global domain

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

$$U^{i+1}(x) = U^{i+1}(z) = \sum_{k=1}^8 C_k^{i+1} H_k^{i+1}(z).$$

The continuity of the basis functions and their first three derivatives have some interesting consequences on the coefficients of the solutions in the successive elements. In order to obtain a smooth solution that is C^3 continuous, we enforce the condition

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

which is equivalent, in the variable z , to $U^i(1) = U^{i+1}(0)$. This implies that $C_1^{i+1} = C_5^i$. The continuity of the derivative at x_{i+1} is equivalent to

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

and this yields $C_2^{i+1} = C_6^i$. Similarly, the continuity of the second derivative at x_{i+1} yields $C_3^{i+1} = C_7^i$ and that of the third derivative yields $C_4^{i+1} = C_8^i$. Thus, the first four coefficients in interval $i + 1$ are a repetition of the last four coefficients in interval i . Thus, we can write the trial solution as

$$U(z) = \sum_{k=1}^8 C_{k+4(i-1)} H_k(z), \tag{12}$$

where we write $H_k(z)$ for $H_k^i(z)$ bearing in mind that $H_k(z)$ is a function of i and we have dropped the superscript i from $U^i(z)$. With this labelling of the coefficients, we are automatically ensuring that the solution and its first, second, and third derivatives are continuous at the nodes.

Remark 1 Substituting $z = 0$ and $z = 1$ into (12), its derivative, its second and its third derivative, we can show that $U(x_i) = C_{4i-3}$, $hU'(x_i) = C_{4i-2}$, $h^2U''(x_i) = C_{4i-1}$, and $h^3U'''(x_i) = C_{4i}$, $i = 1, 2, \dots, N + 1$. Thus, every fourth coefficient beginning from C_1 is an approximation to the solution at the nodes. Similarly, every fourth coefficient beginning from C_2 scaled by h is an approximation to the derivative at the nodes. Likewise, every fourth coefficient beginning from C_3 scaled by h^2 represents an approximation to the second derivative at the nodes, and every fourth coefficient beginning from C_4 scaled by h^3 represents an approximation to the third derivative at the nodes.

We find it more instructive to apply the error bounds derived in [28] and to illustrate the numerical validity of the bounds in the present context on two examples. Consider the fourth-order linear differential equation, defined on $[a, b]$, which can be written in the form $Lu(x) = f(x)$, where the operator $L = \sum_{k=0}^4 a_k(x)D^k$ and D denotes the derivative operator.

The following theorem establishes the order of convergence for very smooth solutions [28].

Theorem 1 ([28]) *Assume that the coefficients $a_i(x)$ of L satisfy $a_i(x) \in C^8[a, b]$ for all i and that $u(x) \in C^{12}[a, b]$. If the collocation points are chosen as the Gauss points, then there exists a constant c_1 such that*

$$|D^p(u - U)(x_j)| \leq c_1 h^8, \quad p = 0, 1, 2, 3 \tag{13}$$

and a constant c_2 such that

$$\|D^p(u - U)\|_\infty \leq c_2 h^{8-p}, \quad p = 0, 1, 2, 3, 4. \tag{14}$$

Here, $U(x)$ represents the collocation approximation of $u(x)$. Similar error bounds hold for nonlinear ODEs [28] and will be illustrated with an example below.

This effectively means that at the nodes the error of the collocation solution and its derivatives of order up to three should be $O(h^8)$. Also, the infinity norm of the error and its derivatives of order up to four should be $O(h^{8-p})$.

4 Numerical Example

Example 1 Consider the fourth-order ODE

$$u^{(iv)} - (10\pi)^3 u = (10\pi)^3 (10\pi - 1) \sin(10\pi x) = f(x) \tag{15}$$

with analytical solution $u(x) = \sin(10\pi x)$ and boundary conditions $u(0) = 0 = u(1)$ and $u'(0) = 10\pi = u'(1)$

We substitute the trial solution (12) into the differential equation (15) to obtain

$$\sum_{k=1}^8 \left[H_k^{(iv)}(z)/h^4 - (10\pi)^3 H_k(z) \right] C_{k+4(i-1)} = f(x_i + zh), \quad i = 1, 2, \dots, N. \tag{16}$$

The boundary condition $u(0) = U(0) = \sum_{k=1}^8 C_k H_k(0) = 0$ yields $C_1 = 0$ while the boundary condition $u(1) = U(1) = \sum_{k=1}^8 C_{k+4(N-1)} H_k(1) = 0$ yields $C_{4N+1} = 0$. The boundary condition $u'(0) = U'(0) = \frac{1}{h} \sum_{k=1}^8 C_k H'_k(0) = 10\pi$ yields $C_2 = 10\pi h$. Similarly, $u'(1) = U'(1) = \frac{1}{h} \sum_{k=1}^8 C_{k+4(N-1)} H'_k(1) = 10\pi$ yields $C_{4N+2} = 10\pi h$.

There are $4N + 4$ unknowns in Eq. (12). Given that we have two boundary conditions on the left and two boundary conditions on the right, we thus require $4N$ conditions in order to solve the problem uniquely. We choose four collocation points denoted by s_1, s_2, s_3, s_4 , in each interval. The s_j are chosen as the zeros of the fourth

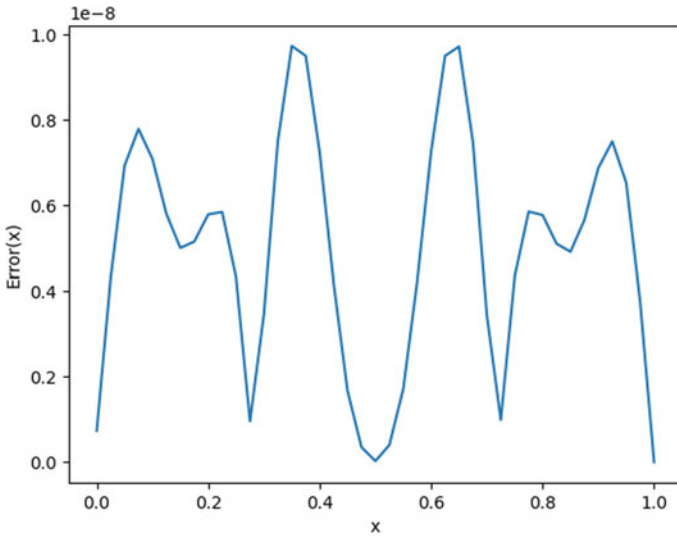


Fig. 2 Error plot with $N = 20$ for example 2.1

The non-zero blocks of matrix A are shifted four places to the right and account for the repetition of the coefficients. The position of the ones accounts for the boundary conditions. The sparse nature of the matrix and the repetitive pattern can easily be exploited to solve the linear system efficiently with minimum CPU storage requirements.

After solving (17), the solution is constructed on each subinterval using the appropriate coefficients and can then be plotted.

Since there is very good agreement between the approximate solution and the exact solution, we choose to show the error plot in Fig. 2 for $N = 20$. We point out that in contrast to global collocation the numerical results are much more acceptable.

We use the following technique to approximate the convergence order. If the discrete error at the nodes x_j is $O(h^n)$ then

$$|D^p(u - U)(x_j)|^{(h)} = O(h^n) \tag{19}$$

and

$$|D^p(u - U)(x_j)|^{(\frac{h}{2})} = O\left(\left(\frac{h}{2}\right)^n\right). \tag{20}$$

By taking the ratio of (19)–(20), we obtain

$$\alpha_1 = \frac{|D^p(u - U)(x_j)|^{(h)}}{|D^p(u - U)(x_j)|^{(\frac{h}{2})}} \approx 2^n \tag{21}$$

Table 1 Convergence order $n(h)$ at nodes from (21)

x_i	$p = 0$	$p = 1$	$p = 2$	$p = 3$	x_i	$p = 0$	$p = 1$	$p = 2$	$p = 3$
0.05	8.3581	8.2630	8.3306	8.2909	0.55	8.7506	8.2487	8.7841	8.2493
0.10	8.3486	8.1682	8.3474	8.2273	0.60	8.3179	8.2433	8.3184	8.8037
0.15	8.3358	9.0963	8.3618	8.0691	0.65	8.2625	8.4625	8.2502	8.4620
0.20	8.2448	8.2739	8.2377	8.3273	0.70	8.1744	8.7793	8.1824	8.4068
0.25	8.1592	8.3138	8.1167	8.3128	0.75	8.3788	8.2916	8.3458	8.2867
0.30	8.4366	8.5032	8.4341	8.2856	0.80	8.3677	8.2011	8.3593	8.2233
0.35	8.3041	8.1579	8.2915	8.1548	0.85	8.3613	7.8613	8.3673	6.4756
0.40	8.2843	7.9236	8.2846	7.5945	0.90	8.2783	8.2569	8.2282	8.3518
0.45	8.1588	8.3554	8.2455	8.3554	0.95	8.2408	8.2857	8.0558	8.3496

Table 2 Global convergence orders from (22)

p	0	1	2	3	4
$n(h)$	7.9596	6.8907	5.6224	4.6626	3.7390

from which the order of convergence $n(h) \approx \frac{\ln(\alpha_1)}{\ln(2)}$. Similarly, we obtain

$$\alpha_2 = \frac{\|D^p(u - U)(x)\|_\infty^{(h)}}{\|D^p(u - U)(x)\|_\infty^{(\frac{h}{2})}} \approx 2^n. \tag{22}$$

These results are summarized in Tables 1 and 2. It is seen that the nodal order is approximately 8, while the global order seems to satisfy (14). The error in the global convergence order is attributed to the conditioning of the matrix for this problem as well as the low value of N used. The pointwise error in the domain is least and of order 8 only at the nodes, a phenomenon known as superconvergence.

Example 2 As a second example, we solve a nonlinear BVP.

$$u^{(iv)}(x) + u'''(x) + u''(x) + u(x)u'(x) = f(x), \quad -2 < x < 2, \tag{23}$$

with exact solution $u(x) = e^{-x^2}$.

The right-hand side $f(x)$ and boundary conditions are extracted from the exact solution. Clearly, the exact solution $u(x)$ satisfies the hypothesis of Theorem (1) and therefore we expect nodal and global errors of $O(h^8)$. If the global error $\|D^p(u - U)(x)\|_\infty^N$ is $O(h^{-n})$ then

$$\alpha_3 = \frac{\|D^p(u - U)(x)\|_\infty^N}{\|D^p(u - U)(x)\|_\infty^{N+1}} \approx \left(\frac{N+1}{N}\right)^n \tag{24}$$

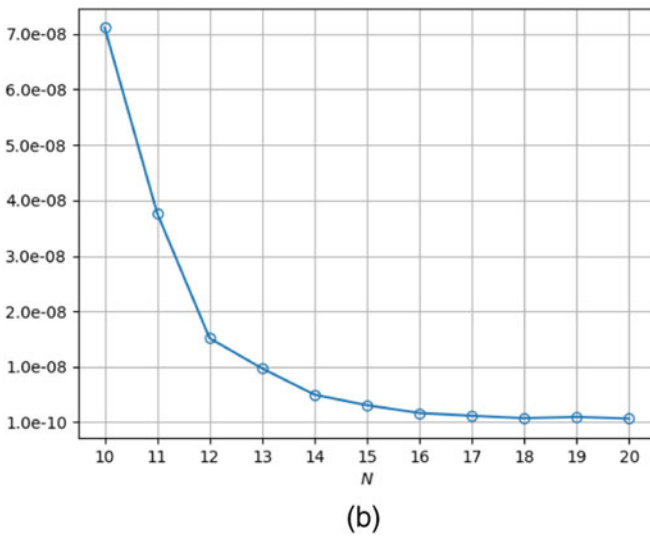
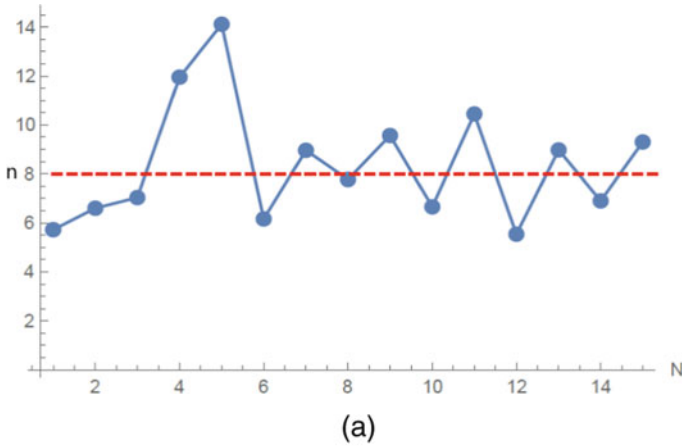


Fig. 3 a Global error order. b Global error

and the global convergence order is given by

$$n \approx \frac{\ln \alpha_3}{\ln \left(\frac{N+1}{N} \right)}. \tag{25}$$

We use Eq.(25) to estimate this order as it is computationally inefficient to use (22) in this case. For a nonlinear problem, the nonlinear solver consumes much CPU time as the number of equations increases. For example for $N = 10$, if we had used

Table 3 Nodal order and error for $N = 8$

i	x_i	n	$ (u - U)(x_i) $
2	-1.5	8.218	9.73e-8
3	-1.0	11.257	3.75e-8
4	-0.5	8.463	1.32e-7
5	0.0	8.523	2.59e-7
6	0.5	8.929	2.85e-8
7	1.0	7.995	7.21e-8
8	1.5	8.671	6.68e-8

(22) then this will require solving additionally 84 ($N = 20$) nonlinear equations as compared to 48 ($N = 11$) nonlinear equations.

In Fig. 3a, we plot the global order ($p = 0$) as a function of N for small values of N . These orders seem to oscillate about the horizontal red line ($N = 8$). Those below the line are attributed to numerical errors arising from the Julia nonlinear solver `nlsolve`. For larger values of N , the actual global errors are illustrated in Fig. 3b and agree remarkably with the theoretical bound of Theorem (1).

For ($N = 8$) the nodal orders using (21) as well as the nodal errors are tabulated in Table 3. Again this reinforces the validity of Theorem (1).

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