

## A WELL-CONDITIONED COLLOCATION METHOD USING A PSEUDOSPECTRAL INTEGRATION MATRIX\*

LI-LIAN WANG<sup>†</sup>, MICHAEL DANIEL SAMSON<sup>†</sup>, AND XIAODAN ZHAO<sup>‡</sup>

**Abstract.** In this paper, a well-conditioned collocation method is constructed for solving general  $p$ th order linear differential equations with various types of boundary conditions. Based on a suitable Birkhoff interpolation, we obtain a new set of polynomial basis functions that results in a collocation scheme with two important features: the condition number of the linear system is independent of the number of collocation points, and the underlying boundary conditions are imposed exactly. Moreover, the new basis leads to an exact inverse of the pseudospectral differentiation matrix of the highest derivative (at interior collocation points), which is therefore called the pseudospectral integration matrix (PSIM). We show that PSIM produces the optimal integration preconditioner and stable collocation solutions with even thousands of points.

**Key words.** Birkhoff interpolation, integration preconditioning, collocation method, pseudospectral differentiation matrix, pseudospectral integration matrix, condition number

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**1. Introduction.** The spectral collocation method is implemented in physical space and approximates derivative values by direct differentiation of the Lagrange interpolating polynomial at a set of Gauss-type points. Its fairly straightforward realization is akin to the high-order finite difference method (cf. [21, 46]). This marks its advantages over the spectral method using modal basis functions in dealing with variable coefficient and/or nonlinear problems (see various monographs on spectral methods [24, 26, 3, 6, 30, 42]). However, practitioners are plagued with the involved ill-conditioned linear systems (e.g., the condition number of the  $p$ th order differential operator grows like  $N^{2p}$ ). This longstanding drawback causes severe degradation of expected spectral accuracy [47], while the accuracy of machine zero can be well observed from the well-conditioned spectral-Galerkin method (see, e.g., [40]). In practice, it becomes rather prohibitive to solve the linear system by a direct solver or even an iterative method when the number of collocation points is large.

One significant attempt to circumvent this barrier is the use of suitable *preconditioners*. Preconditioners built on low-order finite difference or finite element approximations can be found in, e.g., [13, 14, 7, 32, 33, 5]. The *integration preconditioning* (IP) proposed in [11, 12, 19] (with ideas from Clenshaw [9]) has proved to be efficient. We highlight that the IP in Hesthaven [29] led to a significant reduction of the condition number from  $O(N^4)$  to  $O(\sqrt{N})$  for second-order differential linear operators with Dirichlet

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<sup>†</sup>Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, 637371, Singapore (lilian@ntu.edu.sg, michael.daniel.samson@gmail.com).

<sup>‡</sup>Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, 637371, Singapore, and National Heart Center Singapore, 5 Hospital Drive, 169609, Singapore (zhaoxd0722@gmail.com).

boundary conditions (which were imposed by the penalty method [22]). Elbarbary [18] improved the IP in [29] through carefully manipulating the involved singular matrices and imposing the boundary conditions by some auxiliary equations. Another remarkable approach is the *spectral integration method* proposed by Greengard [25] (also see [53]), which recasts the differential form into integral form and then approximates the solution by orthogonal polynomials. This method was incorporated into the `chebop` system [16, 15]. A relevant approach by El-Gendi [17] is not based on reformulating the differential equations but uses the integrated Chebyshev polynomials as basis functions. Then the spectral integration matrix is employed in place of the pseudospectral differentiation matrix (PSDM) to obtain much better conditioned linear systems (see, e.g., [37, 23, 38, 19] and the references therein).

In this paper, we take a very different route to construct well-conditioned collocation methods. The essential idea is to associate the highest differential operator and underlying boundary conditions with a suitable *Birkhoff interpolation* (cf. [35, 44]) that interpolates the derivative values at interior collocation points, and interpolate the boundary data at endpoints. This leads to the *Birkhoff interpolation basis polynomials* with the following distinctive features:

- (i) Under the new basis, the linear system of a usual collocation scheme is well-conditioned, and the matrix of the highest derivative is diagonal or identity. Moreover, the underlying boundary conditions are imposed exactly. This technique can be viewed as the collocation analogue of the well-conditioned spectral-Galerkin method (cf. [40, 41, 27]), where the matrix of the highest derivative in the Galerkin system is diagonal under certain modal basis functions.
- (ii) The new basis produces the *exact inverse* of PSDM of the highest derivative (involving only interior collocation points). This inspires us to introduce the concept of the PSIM. The integral expression of the new basis offers a stable way to compute PSIM and the inverse of PSDM even for thousands of collocation points.
- (iii) This leads to optimal integration preconditioners for the usual collocation methods and enables us to have insights into the IP in [29, 18]. Indeed, the preconditioning from Birkhoff interpolation is natural and optimal.

We point out that Costabile and Longo [10] touched on the application of Birkhoff interpolation (see (3.1)) to second-order boundary value problems (BVPs), but the focus of their work was largely on the analysis of interpolation and quadrature errors. Zhang [54] considered the Birkhoff interpolation (see (4.1)) in a very different context of superconvergence of polynomial interpolation. Collocation methods based on a special Birkhoff quadrature rule for Neumann problems were discussed in [20, 48] and were extended to mixed boundary conditions in [49]. It is also noteworthy to point out recent interest in developing spectral solvers (see, e.g., [34, 8, 39, 28]).

The rest of the paper is organized as follows. In section 2, we review several topics that are pertinent to the forthcoming development. In section 3, we elaborate on the new methodology for second-order BVPs. In section 4, we present miscellaneous extensions of the approach to first-order initial value problems (IVPs), higher-order equations, and multiple dimensions.

**2. Birkhoff interpolation and pseudospectral differentiation matrix.** We briefly review several topics directly bearing on the subsequent algorithm. We introduce the pseudospectral integration matrix, which is a central piece of the puzzle for our new approach.

**2.1. Birkhoff interpolation.** Let  $\{x_j\}_{j=0}^N$  be a set of distinct interpolation points such that

$$(2.1) \quad -1 \leq x_0 < x_1 < \cdots < x_{N-1} < x_N \leq 1.$$

Let  $\mathbb{P}_K$  be the set of all algebraic polynomials of degree at most  $K$ . Given  $K+1$  data  $\{y_j^m\}$  (with  $K \geq N$ ), we consider the interpolation problem (cf. [35, 44]):

$$(2.2) \quad \text{Find } p_K \in \mathbb{P}_K \text{ such that } p_K^{(m)}(x_j) = y_j^m \quad (K+1 \text{ equations}).$$

We have the Hermite interpolation if for each  $j$ , the orders of derivatives in (2.2) form an unbroken sequence,  $m = 0, 1, \dots, m_j$ . In this case, the interpolation polynomial  $p_K$  uniquely exists. On the other hand, if some of the sequences are broken, we have the Birkhoff interpolation. However, the existence and uniqueness of the Birkhoff interpolation polynomial are not guaranteed (cf. [35, 44]). For example, for (2.2) with  $K = N = 2$ , and given data  $\{y_0^0, y_1^1, y_2^0\}$ , the quadratic polynomial  $p_2(x)$  does not exist, when  $x_1 = (x_0 + x_2)/2$ . This happens to Legendre/Chebyshev–Gauss–Lobatto points, where  $x_0 = -1, x_1 = 0$  and  $x_2 = 1$ .

In this paper, we consider special Birkhoff interpolation at Gauss-type points and some variants that incorporate mixed boundary data, for instance,  $ap'_K(-1) + bp_K(-1) = y_0$  with constants  $a, b$  (see section 3.5).

**2.2. Legendre and Chebyshev polynomials.** Without loss of generality, we present the new collocation approach at Legendre and Chebyshev points, but it is straightforward to extend the idea to Jacobi polynomials.

Let  $P_k(x)$  and  $T_k(x)$  (with  $x \in I := (-1, 1)$ ) be respectively the Legendre and Chebyshev polynomials (cf. [45]). They are mutually orthogonal:

$$(2.3) \quad \int_{-1}^1 P_k(x)P_j(x) dx = \gamma_k \delta_{kj}, \quad \int_{-1}^1 \frac{T_k(x)T_j(x)}{\sqrt{1-x^2}} dx = \frac{c_k \pi}{2} \delta_{kj},$$

where  $\gamma_k = 2/(2k+1)$ ,  $c_0 = 2$ , and  $c_k = 1$  for  $k \geq 1$ . There hold

$$(2.4) \quad \begin{aligned} P_k(x) &= \frac{1}{2k+1} (P'_{k+1}(x) - P'_{k-1}(x)), \\ T_k(x) &= \frac{1}{2(k+1)} T'_{k+1}(x) - \frac{1}{2(k-1)} T'_{k-1}(x) \end{aligned}$$

for  $k \geq 1$  and  $k \geq 2$ , respectively. Moreover, we have

$$(2.5) \quad \begin{aligned} P_k(\pm 1) &= (\pm 1)^k, \quad P'_k(\pm 1) = \frac{1}{2} (\pm 1)^{k-1} k(k+1), \\ T_k(\pm 1) &= (\pm 1)^k, \quad T'_k(\pm 1) = (\pm 1)^{k-1} k^2. \end{aligned}$$

Let  $\{x_j, \omega_j\}_{j=0}^N$  be the Gauss–Lobatto (GL) points (with  $x_0 = -1, x_N = 1$ ) and quadrature weights. (i) The Legendre–Gauss–Lobatto (LGL) points are zeros of  $(1-x^2)P'_N(x)$ , and

$$(2.6) \quad \omega_j = \frac{2}{N(N+1)} \frac{1}{P_N^2(x_j)}, \quad 0 \leq j \leq N.$$

(ii) The Chebyshev–Gauss–Lobatto (CGL) points and quadrature weights are

$$(2.7) \quad \begin{aligned} x_j &= -\cos(jh), \quad 0 \leq j \leq N; \\ \omega_0 = \omega_N &= \frac{h}{2}, \quad \omega_j = h, \quad 1 \leq j \leq N-1; \quad h = \frac{\pi}{N}. \end{aligned}$$

Then we have the exactness

$$(2.8) \quad \int_{-1}^1 \phi(x)\omega(x)dx = \sum_{j=0}^N \phi(x_j)\omega_j \quad \forall \phi \in \mathbb{P}_{2N-1},$$

where  $\omega(x) = 1, (1-x^2)^{-1/2}$  for the Legendre and Chebyshev cases, respectively.

Hereafter, let  $\{l_j\}_{j=0}^N$  be the Lagrange interpolation basis polynomials. Denoting  $d_{ij}^{(k)} := l_j^{(k)}(x_i)$ , we introduce the matrices

$$(2.9) \quad \mathbf{D}^{(k)} = (d_{ij}^{(k)})_{0 \leq i, j \leq N}, \quad \mathbf{D}_{\text{in}}^{(k)} = (d_{ij}^{(k)})_{1 \leq i, j \leq N-1}, \quad k \geq 1.$$

In particular, we denote  $\mathbf{D} = \mathbf{D}^{(1)}$  and  $\mathbf{D}_{\text{in}} = \mathbf{D}_{\text{in}}^{(1)}$ . We recall the property (see, e.g., [42, Theorem 3.10])

$$(2.10) \quad \mathbf{D}^{(k)} = \mathbf{D}\mathbf{D} \dots \mathbf{D} = \mathbf{D}^k, \quad k \geq 1,$$

so the higher-order differentiation matrix is a product of the first-order one. Set

$$(2.11) \quad \mathbf{p}^{(k)} := (p^{(k)}(x_0), \dots, p^{(k)}(x_N))^t, \quad \mathbf{p} := \mathbf{p}^{(0)}.$$

The pseudospectral differentiation process is performed via

$$(2.12) \quad \mathbf{D}^{(k)}\mathbf{p} = \mathbf{D}^k\mathbf{p} = \mathbf{p}^{(k)}, \quad k \geq 1.$$

It is noteworthy that differentiation via (2.12) suffers from significant round-off errors for large  $N$ , due to the involvement of ill-conditioned operations (cf. [50]). The matrix  $\mathbf{D}^{(k)}$  is singular (a simple proof:  $\mathbf{D}^{(k)}\mathbf{1} = \mathbf{0}$ , where  $\mathbf{1} = (1, 1, \dots, 1)^t$ , so the rows of  $\mathbf{D}^{(k)}$  are linearly dependent), while  $\mathbf{D}_{\text{in}}^{(k)}$  is nonsingular. In addition, the condition numbers of  $\mathbf{D}_{\text{in}}^{(k)}$  and  $\mathbf{D}^{(k)} - \mathbf{I}_{N+1}$  behave like  $O(N^{2k})$  (see, e.g., [6, section 4.3]).

**2.3. Integration preconditioning.** We briefly examine the essential idea of constructing integration preconditioners in [29, 18] (inspired by [12, 11]). Consider, for example, the Legendre case. By (2.3) and (2.8),

$$(2.13) \quad l_j(x) = \sum_{k=0}^N \frac{\omega_j}{\tilde{\gamma}_k} P_k(x_j) P_k(x), \quad 0 \leq j \leq N, \quad \text{so } l_j''(x) = \sum_{k=2}^N \frac{\omega_j}{\tilde{\gamma}_k} P_k(x_j) P_k''(x),$$

where  $\tilde{\gamma}_k = 2/(2k+1)$  for  $0 \leq k \leq N-1$ , and  $\tilde{\gamma}_N = 2/N$ . The key observation in [29] is that the pseudospectral differentiation process actually involves ill-conditioned operations (see, e.g., [42, (3.176c)]):

$$(2.14) \quad P_k''(x) = \sum_{\substack{0 \leq l \leq k-2 \\ k+l \text{ even}}} (l+1/2)(k(k+1) - l(l+1)) P_l(x),$$

where the coefficients in the summation grow like  $k^2$ . However, the “inverse” operations are stable, thanks to the “compact” formula, derived from (2.4):

$$(2.15) \quad \begin{aligned} P_k(x) &= \alpha_k P_{k-2}''(x) + \beta_k P_k''(x) + \alpha_{k+1} P_{k+2}''(x), \\ \alpha_k &= \frac{1}{(2k-1)(2k+1)}, \quad \beta_k = \frac{-2}{(2k-1)(2k+3)}, \end{aligned}$$

where  $\alpha_k$  and  $\beta_k$  decay like  $k^{-2}$ .

Based on (2.15), [29, 18] attempted to precondition the collocation system by the “inverse” of  $\mathbf{D}^{(2)}$ . However, since  $\mathbf{D}^{(2)}$  is singular, there exist multiple ways to manipulate the involved singular matrices. The boundary conditions were imposed by the penalty method (cf. [22]) in [29] and using auxiliary equations in [18]. The condition number of the preconditioned system for, e.g., the operator  $\frac{d^2}{dx^2} - \mu$  with Dirichlet boundary conditions, behaves like  $O(\sqrt{N})$ .

**2.4. Pseudospectral integration matrix.** We take a quick glance at the idea of the new method to be presented in section 3. Different from (2.12), we consider pseudospectral differentiation merely on interior GL points, for example,

$$(2.16) \quad \tilde{\mathbf{D}}^{(2)} \mathbf{p} = \tilde{\mathbf{p}}^{(2)}, \quad \text{where } \tilde{\mathbf{p}}^{(2)} := (p(-1), p^{(2)}(x_1), \dots, p^{(2)}(x_{N-1}), p(1))^t,$$

and the matrix  $\tilde{\mathbf{D}}^{(2)}$  is obtained by replacing the first and last rows of  $\mathbf{D}^{(2)}$  by  $\mathbf{e}_1 = (1, 0, \dots, 0)$  and  $\mathbf{e}_N = (0, \dots, 0, 1)$ , respectively. Note that the matrix  $\tilde{\mathbf{D}}^{(2)}$  is nonsingular.

Based on a suitable Birkhoff interpolation, we obtain the exact inverse matrix, denoted by  $\mathbf{B}$ , of  $\tilde{\mathbf{D}}^{(2)}$ . This leads to the inverse process of (2.16):

$$(2.17) \quad \mathbf{B} \tilde{\mathbf{p}}^{(2)} = \mathbf{p},$$

which performs twice integration at the interior GL points but leaves the function values at endpoints unchanged. For this reason, we call  $\mathbf{B}$  *the second-order pseudospectral integration matrix*. It is important to point out that the computation of PSIM is stable even for thousands of collocation points, as all operations involve well-conditioned operations (e.g., (2.15) is built-in).

**3. New collocation methods for second-order BVPs.** In this section, we elaborate on the construction of the new approach outlined in section 2.4 for solving second-order BVPs. We start with Dirichlet boundary conditions and then consider general mixed boundary conditions in the latter part of this section.

**3.1. Birkhoff interpolation at GL points.** Let  $\{x_j\}_{j=0}^N$  in (2.1) be a set of GL points as before. Given  $u \in C^2(I)$ , we consider the special case of (2.2):

$$(3.1) \quad \text{Find } p \in \mathbb{P}_N \text{ such that } p''(x_j) = u''(x_j), \quad 1 \leq j \leq N-1; \quad p(\pm 1) = u(\pm 1).$$

The Birkhoff interpolation polynomial  $p$  of  $u$  can be uniquely determined by

$$(3.2) \quad p(x) = u(-1)B_0(x) + \sum_{j=1}^{N-1} u''(x_j)B_j(x) + u(1)B_N(x), \quad x \in [-1, 1],$$

if one can find  $\{B_j\}_{j=0}^N \subseteq \mathbb{P}_N$ , such that

$$(3.3) \quad B_0(-1) = 1, \quad B_0(1) = 0, \quad B_0''(x_i) = 0, \quad 1 \leq i \leq N-1;$$

$$(3.4) \quad B_j(-1) = 0, \quad B_j(1) = 0, \quad B_j''(x_i) = \delta_{ij}, \quad 1 \leq i, j \leq N-1;$$

$$(3.5) \quad B_N(-1) = 0, \quad B_N(1) = 1, \quad B_N''(x_i) = 0, \quad 1 \leq i \leq N-1.$$

We call  $\{B_j\}_{j=0}^N$  the *Birkhoff interpolation basis polynomials* of (3.1), which are the counterpart of the Lagrange basis polynomials  $\{l_j\}_{j=0}^N$ .

THEOREM 3.1. Let  $\{x_j\}_{j=0}^N$  be a set of GL points. The Birkhoff interpolation basis polynomials  $\{B_j\}_{j=0}^N$  defined in (3.3)–(3.5) are given by

$$(3.6) \quad B_0(x) = \frac{1-x}{2}, \quad B_N(x) = \frac{1+x}{2};$$

$$(3.7) \quad B_j(x) = \frac{1+x}{2} \int_{-1}^1 (t-1)\tilde{l}_j(t) dt + \int_{-1}^x (x-t)\tilde{l}_j(t) dt, \quad 1 \leq j \leq N-1,$$

where  $\{\tilde{l}_j\}_{j=1}^{N-1}$  are the Lagrange basis polynomials (of degree  $N-2$ ) associated with  $N-1$  interior GL points  $\{x_j\}_{j=1}^{N-1}$ . Moreover, we have

$$(3.8) \quad \begin{aligned} B'_0(x) &= -B'_N(x) = -\frac{1}{2}; \\ B'_j(x) &= \frac{1}{2} \int_{-1}^1 (t-1)\tilde{l}_j(t) dt + \int_{-1}^x \tilde{l}_j(t) dt, \quad 1 \leq j \leq N-1. \end{aligned}$$

*Proof.* One verifies readily from (3.3) and (3.5) that  $B_0$  and  $B_N$  must be linear polynomials given by (3.6). Using (3.4) and the fact that  $B''_j(x), \tilde{l}_j(x) \in \mathbb{P}_{N-2}$ , we find that  $B''_j(x) = \tilde{l}_j(x)$ , so solving this ordinary differential equation with boundary conditions  $B_j(\pm 1) = 0$  leads to the expression in (3.7). Finally, (3.8) follows from (3.6)–(3.7) directly.  $\square$

Let  $b_{ij}^{(k)} := B_j^{(k)}(x_i)$ , and define the matrices

$$(3.9) \quad \mathbf{B}^{(k)} = (b_{ij}^{(k)})_{0 \leq i, j \leq N}, \quad \mathbf{B}_{\text{in}}^{(k)} = (b_{ij}^{(k)})_{1 \leq i, j \leq N-1}, \quad k \geq 1.$$

In particular, we denote  $b_{ij} := B_j(x_i)$ ,  $\mathbf{B} = \mathbf{B}^{(0)}$ , and  $\mathbf{B}_{\text{in}} = \mathbf{B}_{\text{in}}^{(0)}$ .

Remark 3.2. The integration process (2.17) is a direct consequence of (3.2), as the Birkhoff interpolation polynomial of any  $p \in \mathbb{P}_N$  is itself.

THEOREM 3.3. There hold

$$(3.10) \quad \mathbf{B}^{(k)} = \mathbf{D}^{(k)} \mathbf{B} = \mathbf{D}^k \mathbf{B} = \mathbf{D} \mathbf{B}^{(k-1)}, \quad k \geq 1,$$

$$(3.11) \quad \mathbf{D}_{\text{in}}^{(2)} \mathbf{B}_{\text{in}} = \mathbf{I}_{N-1}, \quad \tilde{\mathbf{D}}^{(2)} \mathbf{B} = \mathbf{I}_{N+1},$$

where  $\mathbf{I}_M$  is an  $M \times M$  identity matrix, and the matrix  $\tilde{\mathbf{D}}^{(2)}$  is defined in (2.16).

To be undistracted from the main results, we postpone the derivation of the formulas to Appendix A. The formula (3.10) can be viewed as an analogue of (2.10), and the matrices  $\mathbf{B}$  and  $\mathbf{B}^{(1)}$  are called the second-order and first-order PSIMs, respectively.

3.2. Computation of PSIMs. Now, we describe stable algorithms for computing the matrices  $\mathbf{B}$  and  $\mathbf{B}^{(1)}$ . For convenience, we introduce the integral operators:

$$(3.12) \quad \partial_x^{-1} u(x) = \int_{-1}^x u(t) dt; \quad \partial_x^{-m} u(x) = \partial_x^{-1} (\partial_x^{-(m-1)} u(x)), \quad m \geq 2.$$

By (2.4), (2.5), and (2.15),

$$(3.13) \quad \partial_x^{-1} P_k(x) = \frac{1}{2k+1} (P_{k+1}(x) - P_{k-1}(x)), \quad k \geq 1; \quad \partial_x^{-1} P_0(x) = 1+x,$$

and

$$(3.14) \quad \begin{aligned} \partial_x^{-2} P_k(x) &= \frac{P_{k+2}(x)}{(2k+1)(2k+3)} - \frac{2P_k(x)}{(2k-1)(2k+3)} + \frac{P_{k-2}(x)}{(2k-1)(2k+1)}, \quad k \geq 2; \\ \partial_x^{-2} P_0(x) &= \frac{(1+x)^2}{2}, \quad \partial_x^{-2} P_1(x) = \frac{(1+x)^2(x-2)}{6}. \end{aligned}$$

Similarly, we have

$$(3.15) \quad \begin{aligned} \partial_x^{-1} T_k(x) &= \frac{T_{k+1}(x)}{2(k+1)} - \frac{T_{k-1}(x)}{2(k-1)} - \frac{(-1)^k}{k^2-1}, \quad k \geq 2; \\ \partial_x^{-1} T_0(x) &= 1+x, \quad \partial_x^{-1} T_1(x) = \frac{x^2-1}{2}. \end{aligned}$$

Using (3.15) recursively yields

$$(3.16) \quad \begin{aligned} \partial_x^{-2} T_k(x) &= \frac{T_{k+2}(x)}{4(k+1)(k+2)} - \frac{T_k(x)}{2(k^2-1)} + \frac{T_{k-2}(x)}{4(k-1)(k-2)} - \frac{(-1)^k(1+x)}{k^2-1} \\ &\quad - \frac{3(-1)^k}{(k^2-1)(k^2-4)}, \quad k \geq 3; \\ \partial_x^{-2} T_0(x) &= \frac{(1+x)^2}{2}, \quad \partial_x^{-2} T_1(x) = \frac{(1+x)^2(x-2)}{6}, \\ \partial_x^{-2} T_2(x) &= \frac{x(1+x)^2(x-2)}{6}. \end{aligned}$$

*Remark 3.4.* Observe that  $\partial_x^{-m} P_k(\pm 1) = 0$  for all  $k \geq m$  with  $m = 1, 2$ , while  $\partial_x^{-m} T_k(1)$  may not vanish. The integrated Legendre and/or Chebyshev polynomials are used to construct well-conditioned spectral-Galerkin methods,  $hp$ -element methods (see [40, 41, 27] and [4] for a review), and spectral integral methods (see, e.g., [9, 17, 25]).

**PROPOSITION 3.5** (Birkhoff interpolation at LGL points). *Let  $\{x_j, \omega_j\}_{j=0}^N$  be the LGL points and weights given in (2.6). Then the Birkhoff interpolation basis polynomials  $\{B_j\}_{j=1}^{N-1}$  in Theorem 3.1 can be computed by*

$$(3.17) \quad B_j(x) = (\beta_{1j} - \beta_{0j}) \frac{x+1}{2} + \sum_{k=0}^{N-2} \beta_{kj} \frac{\partial_x^{-2} P_k(x)}{\gamma_k},$$

where  $\gamma_k = 2/(2k+1)$ ,  $\partial_x^{-2} P_k(x)$  is given in (3.14), and

$$(3.18) \quad \beta_{kj} = \left( P_k(x_j) - \frac{1 - (-1)^{N+k}}{2} P_{N-1}(x_j) - \frac{1 + (-1)^{N+k}}{2} P_N(x_j) \right) \omega_j.$$

Moreover, we have

$$(3.19) \quad B'_j(x) = \frac{\beta_{1j} - \beta_{0j}}{2} + \sum_{k=0}^{N-2} \beta_{kj} \frac{\partial_x^{-1} P_k(x)}{\gamma_k},$$

where  $\partial_x^{-1} P_k(x)$  is given in (3.13).

We provide the proof of this proposition in Appendix B.

PROPOSITION 3.6 (Birkhoff interpolation at CGL points). *The Birkhoff interpolation basis polynomials  $\{B_j\}_{j=1}^{N-1}$  in Theorem 3.1 at  $\{x_j = -\cos(jh)\}_{j=0}^N$  with  $h = \pi/N$  can be computed by*

$$(3.20) \quad B_j(x) = \sum_{k=0}^{N-2} \beta_{kj} \left\{ \partial_x^{-2} T_k(x) - \frac{1+x}{2} \partial_x^{-2} T_k(1) \right\},$$

where  $\partial_x^{-2} T_k(x)$  is given in (3.16), and

$$(3.21) \quad \beta_{kj} = \frac{2}{c_k N} \left\{ T_k(x_j) - \frac{1 - (-1)^{N+k}}{2} T_{N-1}(x_j) - \frac{1 + (-1)^{N+k}}{2} T_N(x_j) \right\}.$$

Moreover, we have

$$(3.22) \quad B'_j(x) = \sum_{k=0}^{N-2} \beta_{kj} \left\{ \partial_x^{-1} T_k(x) - \frac{\partial_x^{-2} T_k(1)}{2} \right\},$$

where  $\partial_x^{-1} T_k(x)$  is computed by (3.15). Here,  $c_0 = 2$  and  $c_k = 1$  for  $k \geq 1$  as in (2.3).

We omit the proof, since it is very similar to that of Proposition 3.5.

Remark 3.7. Like (2.15), the formulas for evaluating integrated Legendre and/or Chebyshev polynomials are sparse and the coefficients decay. This allows for stable computation of PSIM even for thousands of collocation points.

Remark 3.8. In the above, we only provide the Birkhoff basis polynomials for the Legendre and Chebyshev cases, but the method can be extended to Jacobi polynomials straightforwardly.

**3.3. Collocation schemes.** Consider the BVP:

$$(3.23) \quad u''(x) + r(x)u'(x) + s(x)u(x) = f(x), \quad x \in I; \quad u(\pm 1) = u_{\pm},$$

where the given functions  $r, s, f \in C(I)$ . Let  $\{x_j\}_{j=0}^N$  be the set of GL points as in (3.1). Then the collocation scheme for (3.23) is to find  $u_N \in \mathbb{P}_N$  such that

$$(3.24) \quad \begin{aligned} u''_N(x_i) + r(x_i)u'_N(x_i) + s(x_i)u_N(x_i) &= f(x_i), \quad 1 \leq i \leq N-1; \\ u_N(\pm 1) &= u_{\pm}. \end{aligned}$$

- (a) The usual collocation scheme. Let  $\{l_j\}_{j=0}^N$  be the Lagrange basis polynomials. Write

$$u_N(x) = u_- l_0(x) + u_+ l_N(x) + \sum_{j=1}^{N-1} u_N(x_j) l_j(x),$$

and insert it into (3.24), leading to

$$(3.25) \quad (\mathbf{D}_{\text{in}}^{(2)} + \mathbf{\Lambda}_r \mathbf{D}_{\text{in}}^{(1)} + \mathbf{\Lambda}_s) \mathbf{u} = \mathbf{f} - \mathbf{u}_B,$$

where  $\mathbf{f} = (f(x_1), \dots, f(x_{N-1}))^t$ ,  $\mathbf{u}$  is the vector of unknowns  $\{u_N(x_i)\}_{i=1}^{N-1}$ ,  $\mathbf{\Lambda}_r = \text{diag}(r(x_1), \dots, r(x_{N-1}))$ ,  $\mathbf{\Lambda}_s = \text{diag}(s(x_1), \dots, s(x_{N-1}))$ , and  $\mathbf{u}_B$  is the vector of  $\{u_-(d_{i0}^{(2)} + r(x_i)d_{i0}^{(1)}) + u_+(d_{iN}^{(2)} + r(x_i)d_{iN}^{(1)})\}_{i=1}^{N-1}$ . It is known that the condition number of the coefficient matrix in (3.25) grows like  $O(N^4)$ .

- (b) Preconditioning by PSIM. Thanks to the property  $\mathbf{B}_{\text{in}}\mathbf{D}_{\text{in}}^{(2)} = \mathbf{I}_{N-1}$  (see Theorem 3.3), the matrix  $\mathbf{B}_{\text{in}}$  can be used to precondition the ill-conditioned system (3.25), leading to

$$(3.26) \quad (\mathbf{I}_{N-1} + \mathbf{B}_{\text{in}}\mathbf{\Lambda}_r\mathbf{D}_{\text{in}}^{(1)} + \mathbf{B}_{\text{in}}\mathbf{\Lambda}_s)\mathbf{u} = \mathbf{B}_{\text{in}}(\mathbf{f} - \mathbf{u}_B).$$

Note that the matrix of the highest derivative is identity.

*Remark 3.9.* Different from [29, 18], we work with the system involving  $\mathbf{D}_{\text{in}}^{(2)}$ , rather than the singular matrix  $\mathbf{D}^{(2)}$ . On the other hand, the boundary conditions are imposed exactly and are incorporated into the basis polynomials (see section 3.5). Therefore, this requires us to precompute the basis. Note that the boundary conditions in [29] are imposed asymptotically by the penalty method, but this does not require the change of basis for different boundary conditions.

- (c) A modal approach. We have from (3.2) that

$$(3.27) \quad u_N(x) = u_-B_0(x) + u_+B_N(x) + \sum_{j=1}^{N-1} u_N''(x_j)B_j(x).$$

Then the matrix form of (3.24) reads

$$(3.28) \quad (\mathbf{I}_{N-1} + \mathbf{\Lambda}_r\mathbf{B}_{\text{in}}^{(1)} + \mathbf{\Lambda}_s\mathbf{B}_{\text{in}})\mathbf{v} = \mathbf{f} - u_- \mathbf{v}_- - u_+ \mathbf{v}_+,$$

where  $\mathbf{v} = (u_N''(x_1), \dots, u_N''(x_{N-1}))^t$ , and

$$\mathbf{v}_- = \left( -\frac{r(x_1)}{2} + s(x_1)\frac{1-x_1}{2}, \dots, -\frac{r(x_{N-1})}{2} + s(x_{N-1})\frac{1-x_{N-1}}{2} \right)^t,$$

$$\mathbf{v}_+ = \left( \frac{r(x_1)}{2} + s(x_1)\frac{1+x_1}{2}, \dots, \frac{r(x_{N-1})}{2} + s(x_{N-1})\frac{1+x_{N-1}}{2} \right)^t.$$

We take the following steps to solve (3.24):

- (i) Precompute  $\mathbf{B}$  and  $\mathbf{B}^{(1)}$  via the formulas in Propositions 3.5–3.6.
- (ii) Find  $\mathbf{v}$  by solving the system (3.28).
- (iii) Recover  $\mathbf{u} = (u_N(x_1), \dots, u_N(x_{N-1}))^t$  from (3.27):

$$(3.29) \quad \mathbf{u} = \mathbf{B}_{\text{in}}\mathbf{v} + u_- \mathbf{b}_0 + u_+ \mathbf{b}_N,$$

where  $\mathbf{b}_j = (B_j(x_1), \dots, B_j(x_{N-1}))^t$  for  $j = 0, N$ .

*Remark 3.10.* Compared with (3.26), the linear system (3.28) does not involve any differentiation matrix, but an additional step (3.29) is needed for a typical modal basis.

*Remark 3.11.* The unknowns under the new basis in (3.27)–(3.28) are the approximations to  $\{u''(x_j)\}$ . This situation is reminiscent of the spectral integration method [25], which is built upon the orthogonal polynomial expansion of  $u''(x)$ . Thus, approach (iii) can be regarded as the collocation counterpart of the modal approach in [25].

Below, we give some insights into eigenvalues of the new collocation system for the operator  $\frac{d^2}{dx^2} - \mu$  (i.e., Helmholtz (resp., modified Helmholtz) operator for  $\mu < 0$  (resp.,  $\mu \geq 0$ )) with Dirichlet boundary conditions. Its proof is given in Appendix C.

PROPOSITION 3.12. *In the LGL case, the eigenvalues of  $\mathbf{I}_{N-1} - \mu \mathbf{B}_{\text{in}}$  are all real and distinct and are uniformly bounded. More precisely, for any eigenvalue  $\lambda$  of  $\mathbf{I}_{N-1} - \mu \mathbf{B}_{\text{in}}$ , we have*

$$(3.30) \quad 1 + c_N \frac{4\mu\pi^2}{N^4} < \lambda < 1 + \frac{4\mu}{\pi^2} \quad \text{if } \mu \geq 0; \quad 1 + \frac{4\mu}{\pi^2} < \lambda < 1 + c_N \frac{4\mu\pi^2}{N^4} \quad \text{if } \mu < 0,$$

where  $c_N \approx 1$  for large  $N$ .

Remark 3.13. As a consequence of (3.30), the condition number of  $\mathbf{I}_{N-1} - \mu \mathbf{B}_{\text{in}}$  is independent of  $N$ . For example, it is uniformly bounded by  $1 + 4\mu/\pi^2$  for  $\mu \geq 0$ . It is noteworthy that if  $\mu = -k^2$  with  $k \gg 1$  (i.e., Helmholtz equation with high wave-number), then the condition number behaves like  $O(k^2)$ , but independent of  $N$ .

Remark 3.14. We can obtain similar bounds for the CGL case by using the bounds for eigenvalues of  $\mathbf{D}_{\text{in}}^{(2)}$  in, e.g., [51] and [6, section 4.3]. However, it appears open to conduct a similar eigenanalysis for (3.26) and (3.28) with general variable coefficients.

**3.4. Numerical results.** Now, we compare the condition numbers of the linear systems between the Lagrange collocation (LCOL) scheme (3.25), the Birkhoff collocation (BCOL) scheme (3.28), the preconditioned LCOL (P-LCOL) scheme (3.26), and the preconditioned scheme from [18] (which improved that in [29]) (PLCOL), respectively. We also look at the number of iterations for solving the systems via BiCGSTAB in MATLAB and compare their convergence behavior.

We first consider the example

$$(3.31) \quad u''(x) - (1 + \sin x)u'(x) + e^x u(x) = f(x), \quad x \in (-1, 1); \quad u(\pm 1) = u_{\pm},$$

with the exact solution  $u(x) = e^{(x^2-1)/2}$ . Observe from Table 1 that the condition numbers of two new approaches are independent of  $N$  and do not induce round-off errors. As mentioned, the condition number of PLCOL in [18] grows like  $O(\sqrt{N})$ , and that of LCOL behaves like  $O(N^4)$ .

In Figure 1, we depict the distribution of the eigenvalues (in magnitude) of the coefficient matrices of BCOL, PLCOL, and P-LCOL with  $N = 1024$  for both Legendre

TABLE 1  
Comparison of condition numbers, accuracy and iterations for (3.31).

N	LCOL (3.25)			PLCOL [18]			BCOL (3.28)			P-LCOL (3.26)		
	Cond.#	Error	Iters	Cond.#	Error	Iters	Cond.#	Error	Iters	Cond.#	Error	Iters
Legendre												
64	3.97e+05	3.82e-14	286	80.1	1.44e-15	14	6.36	5.55e-16	10	2.86	1.67e-15	8
128	6.23e+06	4.42e-13	1251	156	2.66e-15	13	6.46	1.11e-15	10	2.86	2.44e-15	8
256	9.91e+07	3.95e-13	6988	308	2.33e-15	13	6.51	1.11e-15	11	2.86	2.55e-15	8
512	1.58e+09	1.02e-11	9457	612	3.77e-15	13	6.54	1.89e-15	11	2.86	4.77e-15	8
1024	2.52e+10	6.58e-12	9697	1220	1.03e-14	13	6.55	3.44e-15	11	2.86	1.15e-14	9
Chebyshev												
64	7.23e+05	8.38e-14	285	79.6	1.67e-15	16	6.43	7.77e-16	10	2.86	1.44e-15	8
128	1.16e+07	2.87e-13	1304	156	3.44e-15	16	6.50	7.77e-16	10	2.86	4.22e-15	8
256	1.85e+08	9.74e-13	5868	308	8.44e-15	16	6.53	1.22e-15	11	2.86	6.55e-15	8
512	2.96e+09	4.51e-12	9987	611	4.22e-15	14	6.55	1.78e-15	11	2.86	3.44e-15	8
1024	4.73e+10	1.27e-11	9938	1219	5.22e-15	15	6.56	3.77e-15	11	2.86	6.00e-15	9

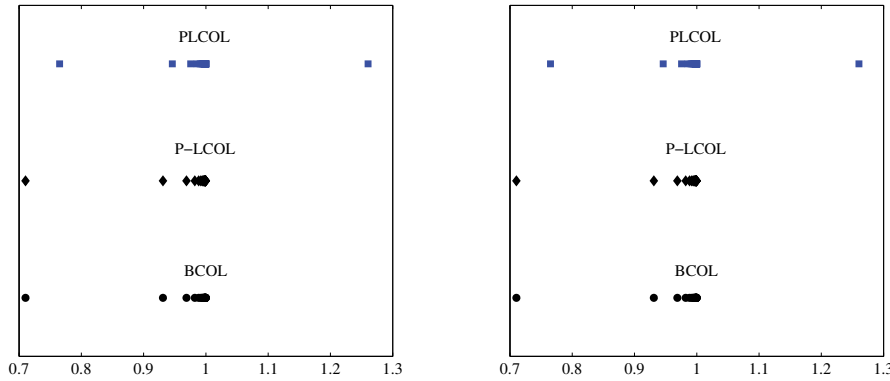


FIG. 1. Distribution of magnitude of eigenvalues for the coefficient matrices of collocation schemes with  $N = 1024$ . Left: LGL; right: CGL.

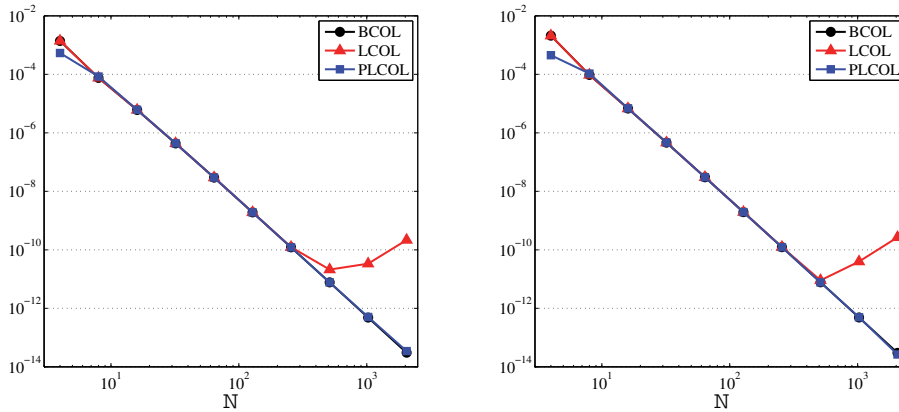


FIG. 2. Comparison of maximum pointwise errors. Left: LGL; right: CGL.

and Chebyshev cases. Observe that almost all of them are concentrated around 1, though it appears nontrivial to show this rigorously as in Proposition 3.12.

We next consider (3.31) with  $f \in C^1(\bar{I})$  and the exact solution  $u \in C^3(\bar{I})$ , given by

$$u(x) = \begin{cases} \cosh(x + 1) - x^2/2 - x, & -1 \leq x < 0, \\ \cosh(x + 1) - \cosh(x) - x + 1, & 0 \leq x \leq 1. \end{cases}$$

Note that  $u$  has a Sobolev-regularity in  $H^{4-\epsilon}(I)$  with  $\epsilon > 0$ . In Figure 2, we graph the maximum pointwise errors for BCOL, LCOL, and PLCOL, where the slope of the lines is approximately  $-4$ . We see that BCOL and PLCOL are free of round-off errors even for thousands of points, though the PLCOL system (in [18]) has a mildly growing condition number.

**3.5. Mixed boundary conditions.** Consider the second-order BVP (3.23) equipped with mixed boundary conditions:

$$(3.32) \quad \mathcal{B}_-[u] := a_-u(-1) + b_-u'(-1) = c_-, \quad \mathcal{B}_+[u] := a_+u(1) + b_+u'(1) = c_+,$$

where  $a_{\pm}, b_{\pm}$ , and  $c_{\pm}$  are given constants. We first assume that

$$(3.33) \quad d := 2a_+a_- - a_+b_- + a_-b_+ \neq 0,$$

which excludes Neumann boundary conditions (i.e.,  $a_- = a_+ = 0$ ) to be considered later.

We associate (3.32) with the Birkhoff-type interpolation:

$$(3.34) \quad \text{Find } p \in \mathbb{P}_N \text{ such that } p''(x_j) = c_j, \quad 1 \leq j \leq N-1, \quad \mathcal{B}_{\pm}[p] = c_{\pm},$$

where  $\{x_j\}_{j=1}^{N-1}$  are interior GL points and  $\{c_{\pm}, c_j\}$  are given data. As before, we look for the interpolation basis polynomials, still denoted by  $\{B_j\}_{j=0}^N$ , satisfying

$$(3.35) \quad \begin{aligned} \mathcal{B}_-[B_0] &= 1, & B_0''(x_i) &= 0, & 1 \leq i \leq N-1, & \mathcal{B}_+[B_0] &= 0; \\ \mathcal{B}_-[B_j] &= 0, & B_j''(x_i) &= \delta_{ij}, & 1 \leq i \leq N-1, & \mathcal{B}_+[B_j] &= 0, & 1 \leq j \leq N-1; \\ \mathcal{B}_-[B_N] &= 0, & B_N''(x_i) &= 0, & 1 \leq i \leq N-1, & \mathcal{B}_+[B_N] &= 1. \end{aligned}$$

Following the same lines as for the proof of Theorem 3.1, we find that if  $d \neq 0$ ,

$$(3.36) \quad B_0(x) = \frac{a_+}{d}(1-x) + \frac{b_+}{d}, \quad B_N(x) = \frac{a_-}{d}(1+x) - \frac{b_-}{d},$$

and for  $1 \leq j \leq N-1$ ,

$$(3.37) \quad B_j(x) = \int_{-1}^x (x-t)\tilde{l}_j(t) dt - \left(\frac{a_-}{d}(1+x) - \frac{b_-}{d}\right) \int_{-1}^1 (a_+(1-t) + b_+)\tilde{l}_j(t) dt,$$

where  $\{\tilde{l}_j\}$  are the Lagrange basis polynomials associated with the interior GL points as defined in Theorem 3.1. Thus, for any  $u \in C^2(I)$ , its interpolation polynomial is given by

$$(3.38) \quad p(x) = (\mathcal{B}_-[u])B_0(x) + \sum_{j=1}^{N-1} u''(x_j)B_j(x) + (\mathcal{B}_+[u])B_N(x).$$

One can find formulas for computing  $\{B_j\}_{j=1}^{N-1}$  on LGL and CGL points by using the same argument as in Proposition 3.5. We leave it to the interested reader.

Armed with the new basis, we can impose mixed boundary conditions exactly, and the linear system resulted from the usual collocation scheme is well-conditioned. Here, we test the method on the second-order equation in (3.23) but with the mixed boundary conditions:  $u(\pm 1) \pm u'(\pm 1) = u_{\pm}$ . In Table 2, we list the condition numbers of the usual collocation method (LCOL, where the boundary conditions are treated by the tau method) and BCOL for both the Legendre and Chebyshev cases. Once again, the new approach is well-conditioned.

**3.6. Neumann boundary conditions.** The previous discussions exclude the Neumann boundary conditions, which need much care. Consider the Poisson equation:

$$(3.39) \quad u''(x) = f(x), \quad x \in I; \quad u'(\pm 1) = 0,$$

where  $f$  is a continuous function such that  $\int_{-1}^1 f(x) dx = 0$ . Its solution is unique up to any additive constant. To ensure the uniqueness, we supply (3.39) with an additional condition:  $u(-1) = u_-$ .

TABLE 2  
Comparison of condition numbers.

N	r = 0 and s = -1				r = s = -1			
	Chebyshev		Legendre		Chebyshev		Legendre	
	BCOL	LCOL	BCOL	LCOL	BCOL	LCOL	BCOL	LCOL
128	2.44	5.88e+07	2.45	3.09e+07	2.64	7.04e+07	2.64	3.70e+07
256	2.44	1.32e+09	2.45	6.88e+08	2.64	1.58e+09	2.64	8.26e+08
512	2.44	2.97e+10	2.44	1.54e+10	2.65	3.57e+10	2.65	1.86e+10
1024	2.44	6.71e+11	2.44	3.48e+11	2.65	8.08e+11	2.65	4.19e+11

Observe that the interpolation problem (3.34) is not well-posed if  $\mathcal{B}_\pm[u] = u'(\pm 1)$ . Here, we consider the following special case of (2.2): Find  $p \in \mathbb{P}_{N+1}$  such that

$$(3.40) \quad p(-1) = y_0^0, \quad p'(-1) = y_0^1, \quad p''(x_j) = y_j^2, \quad 1 \leq j \leq N-1, \quad p'(1) = y_N^1,$$

where  $\{x_j\}_{j=1}^{N-1}$  are interior GL points and the data  $\{y_j^m\}$  are given. However, this interpolation problem is only conditionally well-posed. For example, in the LGL and CGL cases, we have to assume that  $N$  is odd (see Remark 3.15 below). We look for basis polynomials, still denoted by  $\{B_j\}_{j=0}^{N+1}$ , such that for  $1 \leq i, j \leq N-1$ ,

$$\begin{aligned} B'_0(-1) &= 1, \quad B_0(-1) = B''_0(x_i) = B'_0(1) = 0; \\ B'_N(1) &= 1, \quad B_N(-1) = B'_N(-1) = B''_N(x_i) = 0; \\ B_j(-1) &= B'_j(\pm 1) = 0, \quad B''_j(x_i) = \delta_{ij}; \\ B_{N+1}(-1) &= 1, \quad B'_{N+1}(\pm 1) = B''_{N+1}(x_i) = 0. \end{aligned}$$

Let  $Q_N(x) = c_N \prod_{j=1}^{N-1} (x - x_j)$  with  $c_N \neq 0$ . Following the proof of Theorem 3.1, we find that if  $\int_{-1}^1 Q_N(t) dt \neq 0$ , we have

$$(3.41) \quad B_0(x) = 1 + x - \frac{\int_{-1}^x (x-t)Q_N(t) dt}{\int_{-1}^1 Q_N(t) dt}, \quad B_N(x) = \frac{\int_{-1}^x (x-t)Q_N(t) dt}{\int_{-1}^1 Q_N(t) dt},$$

$$B_{N+1}(x) \equiv 1,$$

and for  $1 \leq j \leq N-1$ ,

$$(3.42) \quad B_j(x) = \int_{-1}^x (x-t)\tilde{l}_j(t) dt - \left( \int_{-1}^1 \tilde{l}_j(t) dt \right) B_N(x), \quad \tilde{l}_j(x) = \frac{Q_N(x)}{(x-x_j)Q'_N(x_j)}.$$

*Remark 3.15.* In the Legendre/Chebyshev case, we have  $Q_N(x) = P'_N(x)$  or  $T'_N(x)$ , so by (2.5),

$$\int_{-1}^1 Q_N(t) dt = \int_{-1}^1 P'_N(t) dt = 1 - (-1)^N = \int_{-1}^1 T'_N(t) dt,$$

which is nonzero, if and only if  $N$  is odd.

We plot in Figure 3 the maximum pointwise errors of the usual collocation method (LCOL) and BCOL for (3.39) with the exact solution  $u(x) = \cos(10x) - \cos(10)$ . Note that the condition numbers of systems obtained from BCOL are all 1. We see that BCOL outperforms LCOL as before.

*Remark 3.16.* As noted in [18, section 5.2], how to implement the integration preconditioning technique therein for Neumann boundary conditions remains open.

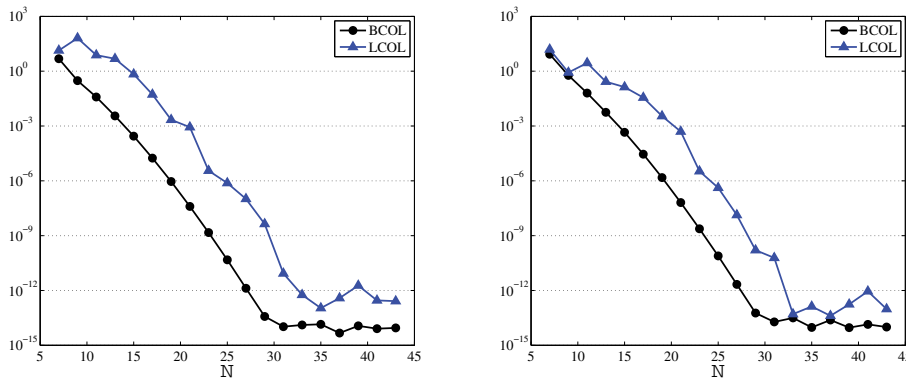


FIG. 3. Comparison of maximum pointwise errors. Left: LGL; right: CGL.

**4. Miscellaneous extensions and discussions.** In this section, we consider various extensions of the Birkhoff interpolation and new collocation methods to numerical solution of first-order IVPs, higher-order equations, and multidimensional problems.

**4.1. First-order IVPs.** To this end, let  $\{x_j\}_{j=0}^N$  in (2.1) be a set of Gauss–Radau interpolation points (with  $x_0 = -1$ ). The counterpart of (3.1) in this context reads as follows: for any  $u \in C^1(I)$ ,

$$(4.1) \quad \text{find } p \in \mathbb{P}_N \text{ such that } p(-1) = u(-1), \quad p'(x_j) = u'(x_j), \quad 1 \leq j \leq N.$$

One verifies readily that  $p(x)$  can be uniquely expressed by

$$(4.2) \quad p(x) = u(-1)B_0(x) + \sum_{j=1}^N u'(x_j)B_j(x), \quad x \in [-1, 1],$$

where the Birkhoff interpolation basis polynomials  $\{B_j\}_{j=0}^N \subseteq \mathbb{P}_N$  satisfy

$$(4.3) \quad \begin{aligned} B_0(-1) &= 1, & B_0'(x_i) &= 0, & 1 \leq i \leq N; \\ B_j(-1) &= 0, & B_j'(x_i) &= \delta_{ij}, & 1 \leq i, j \leq N. \end{aligned}$$

Let  $\{l_j\}_{j=0}^N$  be the Lagrange basis polynomials associated with  $\{x_j\}_{j=0}^N$ . Set  $b_{ij} := B_j(x_i)$  and  $d_{ij} := l_j'(x_i)$ . Define

$$(4.4) \quad \begin{aligned} \mathbf{B} &= (b_{ij})_{0 \leq i, j \leq N}, & \mathbf{B}_{\text{in}} &= (b_{ij})_{1 \leq i, j \leq N}, \\ \mathbf{D} &= (d_{ij})_{0 \leq i, j \leq N}, & \mathbf{D}_{\text{in}} &= (d_{ij})_{1 \leq i, j \leq N}. \end{aligned}$$

Like (3.11), we have the following important properties. Their derivation is essentially the same as that in Theorem 3.3, so we omit it.

**THEOREM 4.1.** *There hold*

$$(4.5) \quad \mathbf{D}_{\text{in}}\mathbf{B}_{\text{in}} = \mathbf{I}_N, \quad \tilde{\mathbf{D}}\mathbf{B} = \mathbf{I}_{N+1},$$

where  $\tilde{\mathbf{D}}$  is obtained by replacing the first row of  $\mathbf{D}$  by  $\mathbf{e}_1 = (1, 0, \dots, 0)$ .

As with Propositions 3.5–3.6, we provide formulas to compute  $\{B_j\}$  for Legendre– and Chebyshev–Gauss–Radau (LGR and CGR) points. To avoid repetition, we omit the proofs.

PROPOSITION 4.2 (Birkhoff interpolation at LGR points). *Let  $\{x_j, \omega_j\}_{j=0}^N$  be the LGR quadrature points (zeros of  $P_N(x) + P_{N+1}(x)$  with  $x_0 = -1$ ) and weights given by*

$$(4.6) \quad \omega_j = \frac{1}{(N+1)^2} \frac{1-x_j}{P_N^2(x_j)}, \quad 0 \leq j \leq N.$$

Then the Birkhoff interpolation basis polynomials  $\{B_j\}_{j=0}^N$  in (4.3) can be computed by

$$(4.7) \quad B_0(x) = 1; \quad B_j(x) = \sum_{k=0}^{N-1} \alpha_{kj} \frac{\partial_x^{-1} P_k(x)}{\gamma_k}, \quad 1 \leq j \leq N,$$

where  $\gamma_k = \frac{2}{2k+1}$ ,  $\partial_x^{-1} P_k(x)$  is given in (3.13), and

$$(4.8) \quad \alpha_{kj} = (P_k(x_j) - (-1)^{N+k} P_N(x_j)) \omega_j.$$

PROPOSITION 4.3 (Birkhoff interpolation at CGR points). *The Birkhoff interpolation basis polynomials  $\{B_j\}_{j=0}^N$  in (4.3) at CGR points  $\{x_j = -\cos(jh)\}_{j=0}^N$ ,  $h = \frac{2\pi}{2N+1}$ , are computed by*

$$(4.9) \quad B_0(x) = 1; \quad B_j(x) = \sum_{k=0}^{N-1} \alpha_{kj} \partial_x^{-1} T_k(x), \quad 1 \leq j \leq N,$$

where  $\partial_x^{-1} T_k(x)$  is defined in (3.15), and

$$(4.10) \quad \alpha_{kj} = \frac{4}{c_k(2N+1)} (T_k(x_j) - (-1)^{N+k} T_N(x_j)),$$

with  $c_0 = 2$  and  $c_k = 1$  for  $k \geq 1$ .

Consider the collocation scheme at GR points for

$$(4.11) \quad u'(x) + \gamma(x)u(x) = f(x), \quad x \in I; \quad u(-1) = u_-,$$

which is to find  $u_N \in \mathbb{P}_N$  such that

$$(4.12) \quad u'_N(x_j) + \gamma(x_j)u_N(x_j) = f(x_j), \quad 1 \leq j \leq N; \quad u_N(-1) = u_-.$$

We intend to compare two collocation approaches based on the Lagrange basis (LCOL), and the new Birkhoff basis (BCOL). The involved linear systems can be formed in the same manner as for the second-order BVPs in section 3.3. We tabulate in Table 3 the condition numbers of LCOL and BCOL with  $\gamma = 1, -\sin x$ , and various  $N$ . As what we have observed from previous section, the condition numbers of BCOL are independent of  $N$ , while those of LCOL grow like  $N^2$ .

We next consider (4.11) with  $\gamma(x) = -\sin x$ ,  $f(x) = 20 \sin(500x^2)$ , and an oscillatory solution:

$$(4.13) \quad u(x) = 20 \exp(-\cos(x)) \int_{-1}^x \exp(\cos(t)) \sin(500t^2) dt.$$

In Figure 4, left, we plot the exact solution (4.13) at 2000 evenly spaced points against the numerical solution obtained by BCOL with  $N = 640$ . In Figure 4, right, we plot the maximum pointwise errors of LCOL and BCOL for the Chebyshev case. It indicates that even for large  $N$ , BCOL is very stable.

TABLE 3  
Comparison of the condition numbers.

N	$\gamma = 1$				$\gamma = -\sin x$			
	Chebyshev		Legendre		Chebyshev		Legendre	
	BCOL	LCOL	BCOL	LCOL	BCOL	LCOL	BCOL	LCOL
128	2.35	5.65e+03	2.34	8.45e+03	2.77	1.35e+04	2.76	2.02e+04
256	2.35	2.25e+04	2.35	3.59e+04	2.77	5.38e+04	2.77	8.58e+04
512	2.35	8.98e+04	2.35	1.52e+05	2.77	2.15e+05	2.77	3.63e+05
1024	2.35	3.59e+05	2.35	6.40e+05	2.77	8.58e+05	2.77	1.53e+06

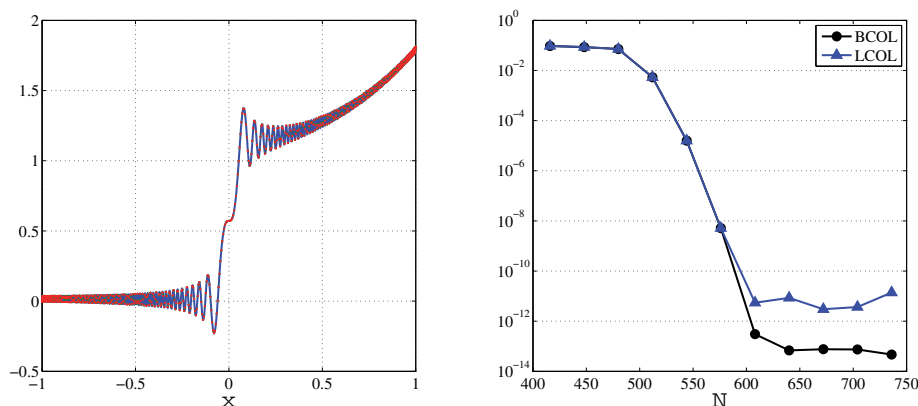


FIG. 4. Left: exact solution versus numerical solution. Right: comparison of numerical errors (Chebyshev).

**4.2. Higher-order equations.** The proposed methods can be directly extended to higher-order BVPs. To illustrate the ideas, we consider fifth-order BVPs and also apply the method in space to solve the time-dependent fifth-order Korteweg–de Vries (KdV) equation.

For example, given the set of the boundary data  $\{u(\pm 1), u'(\pm 1), u''(1)\}$ , we define the associated Birkhoff interpolation problem: Find  $p \in \mathbb{P}_{N+3}$  such that for any  $u \in C^5(-1, 1)$ ,

$$(4.14) \quad \begin{aligned} p^{(5)}(x_j) &= u^{(5)}(x_j), \quad 1 \leq j \leq N-1; \\ p(\pm 1) &= u(\pm 1), \quad p'(\pm 1) = u'(\pm 1), \quad p''(1) = u''(1). \end{aligned}$$

Correspondingly, we can construct the Birkhoff interpolation basis  $\{B_j\}_{j=0}^{N+3}$ , where the basis polynomials associated with the interior GL points  $\{x_j\}_{j=1}^{N-1}$  are defined by

$$B_j(\pm 1) = B_j'(\pm 1) = B_j''(1) = 0, \quad B_j^{(5)}(x_i) = \delta_{ij}, \quad 1 \leq i, j \leq N-1,$$

and the one corresponding to  $u(-1)$  satisfies

$$B_0(-1) = 1, \quad B_0(1) = B_0'(\pm 1) = B_0''(1) = B_0^{(5)}(x_i) = 0, \quad 1 \leq i \leq N-1.$$

Likewise, we can define  $\{B_{N+j}\}_{j=0}^3$ . At the LGL and CGL points, the basis polynomials can be computed stably in terms of integrated Legendre and Chebyshev

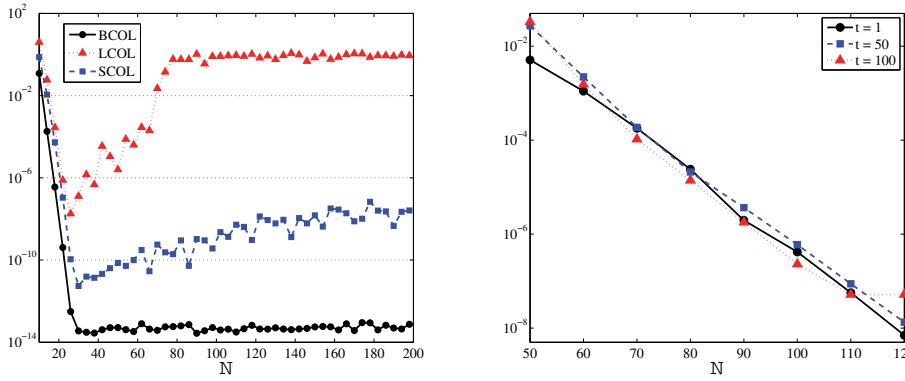


FIG. 5. Comparison of three collocation schemes (left) and maximum pointwise errors of the Crank–Nicolson–leapfrog and BCOL for fifth-order KdV equation (right).

polynomials as in Propositions 3.5–3.6. This leads to the pseudospectral integration matrices for well-conditioned collocation methods. Here, we skip the details and just test the method on the problem:

$$(4.15) \quad \begin{aligned} u^{(5)}(x) + \sin(10x)u'(x) + xu(x) &= f(x), \quad x \in I; \\ u(\pm 1) = u'(\pm 1) = u''(1) &= 0, \end{aligned}$$

with exact solution  $u(x) = \sin^3(\pi x)$ . We compare the usual Lagrange collocation method (LCOL), the new Birkhoff collocation (BCOL) scheme at CGL points, and the special collocation method (SCOL). We refer to the SCOL as in [31] and [42, p. 218], which is based on the following interpolation problem: Find  $p \in \mathbb{P}_{N+3}$  such that

$$p(y_j) = u(y_j), \quad 1 \leq j \leq N - 1; \quad p^{(k)}(\pm 1) = u^{(k)}(\pm 1), \quad k = 0, 1; \quad p''(1) = u''(1),$$

where  $\{y_j\}_{j=1}^{N-1}$  are zeros of the Jacobi polynomial  $P_{N-1}^{(3,2)}(x)$ .

We plot in Figure 5, left, the convergence behavior of three methods, which clearly indicates the new approach is well-conditioned and significantly superior to the other two.

We next apply the new method in space to solve the fifth-order KdV equation:

$$(4.16) \quad \partial_t u + \gamma u \partial_x u + \nu \partial_x^3 u - \mu \partial_x^5 u = 0, \quad u(x, 0) = u_0(x).$$

For  $\gamma \neq 0$  and  $\mu\nu > 0$ , it has the exact soliton solution (cf. [42, p. 233] and the original references therein):

$$(4.17) \quad u(x, t) = \eta_0 + \frac{105\nu^2}{169\mu\gamma} \operatorname{sech}^4 \left( \sqrt{\frac{\nu}{52\mu}} \left[ x - \left( \gamma\eta_0 + \frac{36\nu^2}{169\mu} \right) t - x_0 \right] \right),$$

where  $\eta_0$  and  $x_0$  are any constants. Since the solution decays exponentially, we can approximate the IVPs by imposing homogeneous boundary conditions over  $x \in (-L, L)$  as long as the soliton wave does not reach the boundaries. Let  $\tau$  be the time step size and  $\{\xi_j = Lx_j\}_{j=0}^N$  with  $\{x_j\}_{j=0}^N$  be CGL points. Let  $u^k$  be the finite difference approximation of  $u(\cdot, k\tau)$ . Then we adopt the Crank–Nicolson leap-frog scheme in time and the new collocation method in space, that is, find  $u_N^{k+1} \in \mathbb{P}_{N+3}$  such that for  $1 \leq j \leq N - 1$ ,

$$\begin{aligned}
 (4.18) \quad & \frac{u_N^{k+1}(\xi_j) - u_N^{k-1}(\xi_j)}{2\tau} + \nu \partial_x^3 \left( \frac{u_N^{k+1} + u_N^{k-1}}{2} \right) (\xi_j) - \mu \partial_x^5 \left( \frac{u_N^{k+1} + u_N^{k-1}}{2} \right) (\xi_j) \\
 & = -\gamma \partial_x u_N^k(\xi_j) u_N^k(\xi_j); \\
 & u_N^k(\pm L) = \partial_x u_N^k(\pm L) = \partial_x^2 u_N^k(L) = 0, \quad k \geq 0.
 \end{aligned}$$

In Figure 5, right, we depict the maximum pointwise errors at CGL points for (4.16)–(4.17) with  $\mu = \gamma = 1$ ,  $\nu = 1.1$ ,  $\eta_0 = 0$ ,  $x_0 = -10$ ,  $L = 50$ , and  $\tau = 0.001$  for  $t = 1, 50, 100$ . It indicates that the scheme is stable and accurate, which is comparable to the well-conditioned dual-Petrov–Galerkin scheme in [42, Chapter 6].

**4.3. Multidimensional cases.** For example, we consider the two-dimensional BVP:

$$(4.19) \quad \Delta u - \gamma u = f \quad \text{in } \Omega = (-1, 1)^2; \quad u = 0 \quad \text{on } \partial\Omega,$$

where  $\gamma \geq 0$  and  $f \in C(\Omega)$ . The collocation scheme is on tensorial LGL points: find  $u_N(x, y) \in \mathbb{P}_N^2$  such that

$$(4.20) \quad (\Delta u_N - \gamma u_N)(x_i, y_j) = f(x_i, y_j), \quad 1 \leq i, j \leq N - 1; \quad u_N = 0 \quad \text{on } \partial\Omega,$$

where  $\{x_i\}$  and  $\{y_j\}$  are LGL points. As with the spectral-Galerkin method [40, 43], we use the matrix decomposition (or diagonalization) technique (see [36, 1]). We illustrate the idea by using partial diagonalization (see [42, section 8.1]). Write

$$u_N(x, y) = \sum_{k,l=1}^{N-1} u_{kl} B_k(x) B_l(y),$$

and obtain from (4.20) the system

$$(4.21) \quad \mathbf{U} \mathbf{B}_{\text{in}}^t + \mathbf{B}_{\text{in}} \mathbf{U} - \gamma \mathbf{B}_{\text{in}} \mathbf{U} \mathbf{B}_{\text{in}}^t = \mathbf{F},$$

where  $\mathbf{U} = (u_{kl})_{1 \leq k, l \leq N-1}$  and  $\mathbf{F} = (f_{kl})_{1 \leq k, l \leq N-1}$ . We consider the generalized eigenproblem:

$$(4.22) \quad \mathbf{B}_{\text{in}} \mathbf{x} = \lambda (\mathbf{I}_{N-1} - \gamma \mathbf{B}_{\text{in}}) \mathbf{x}.$$

We know from Proposition 3.12 and Remark 3.14 that the eigenvalues are distinct. Let  $\mathbf{\Lambda}$  be the diagonal matrix of the eigenvalues and  $\mathbf{E}$  be the matrix whose columns are the corresponding eigenvectors. Then we have

$$\mathbf{B}_{\text{in}} \mathbf{E} = (\mathbf{I}_{N-1} - \gamma \mathbf{B}_{\text{in}}) \mathbf{E} \mathbf{\Lambda}.$$

We describe the partial diagonalization (see [42, section 8.1]). Set  $\mathbf{U} = \mathbf{E} \mathbf{V}$ . Then (4.21) becomes

$$\mathbf{V} \mathbf{B}_{\text{in}}^t + \mathbf{\Lambda} \mathbf{V} = \mathbf{G} := \mathbf{E}^{-1} (\mathbf{I}_{N-1} - \gamma \mathbf{B}_{\text{in}})^{-1} \mathbf{F}.$$

Taking the transpose of the above equation leads to

$$\mathbf{B}_{\text{in}} \mathbf{V}^t + \mathbf{V}^t \mathbf{\Lambda} = \mathbf{G}^t.$$

Let  $\mathbf{v}_p$  be the transpose of the  $p$ th row of  $\mathbf{V}$ , and likewise for  $\mathbf{g}_p$ . Then we solve the systems

$$(4.23) \quad (\mathbf{B}_{\text{in}} + \lambda_p \mathbf{I}_{N-1}) \mathbf{v}_p = \mathbf{g}_p, \quad p = 1, 2, \dots, N - 1.$$

As shown in section 2, the coefficient matrix is well-conditioned.

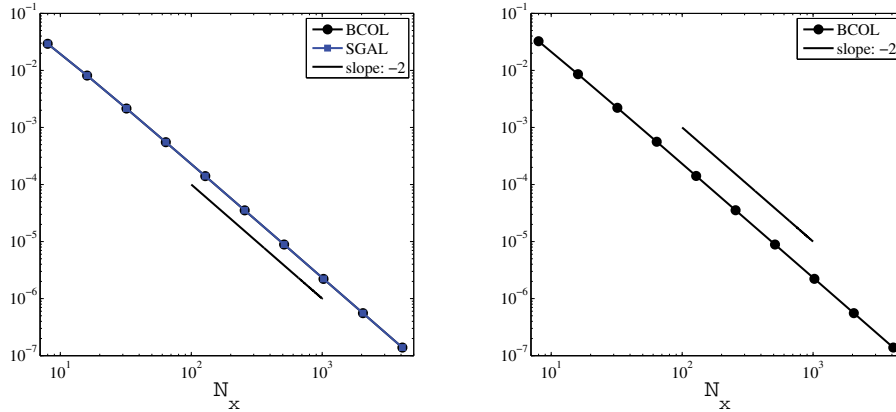


FIG. 6. Maximum pointwise errors. Left: LGL; right: CGL.

*Remark 4.4.* It is seen that the extension to multiple dimensions essentially relies on solving the generalized eigenproblem (4.22). We remark that  $\mathbf{B}_{\text{in}}$  has the same condition number as  $\mathbf{D}_{\text{in}}^{(2)}$ . Nevertheless, this is common for tensor-based approaches, including the spectral-Galerkin method (see, e.g., [42, 1]) and other aforementioned integration preconditioning techniques (see, e.g., [25, 11, 12, 29, 18]).

As a numerical illustration, we consider (4.19) with  $\gamma = 0$  and the exact solution,

$$u = \begin{cases} (\sinh(x+1) - x - 1) \cos(\pi y/2) e^{xy}, & x < 0, \\ (\sinh(x+1) - \sinh(x) - 1 - (\sinh(2) - \sinh(1) - 1)x^3) \cos(\pi y/2) e^{xy}, & x \geq 0, \end{cases}$$

which is first-order differentiable in  $x$  while smooth in  $y$ . We fix  $N_y = 16$  (with negligible errors in  $y$  and requiring solving a generalized eigenproblem) and examine the accuracy for different  $N_x$ . In Figure 6, we plot the maximum pointwise errors against various  $N_x$  of the new approach for more than 1000 points. We see that the new approach is stable with an expected rate of convergence. Moreover, it is comparable to the spectral-Galerkin method in [40], as seen in Figure 6, left, where the errors of two methods are indistinguishable.

**4.4. Concluding remarks.** We conclude the paper with a short summary of the main contributions and make a remark on the Birkhoff interpolation error estimates.

In this paper, we tackled the longstanding ill-conditioning issue of collocation/pseudospectral methods from a new perspective. Based on a suitable Birkhoff interpolation problem, we obtained dual-nature Birkhoff interpolation basis polynomials.

- (i) Such a basis led to optimal integration preconditioners for usual collocation schemes based on Lagrange interpolation. For the first time, we introduced in this paper the notion of pseudospectral integration matrix.
- (ii) The collocation linear system under the new basis is well-conditioned, and the matrix corresponding to the highest derivative of the equation is diagonal or identity. The new approach could be viewed as the collocation analogue of the well-conditioned Galerkin method in [40].

We considered in the paper the new collocation method based on Legendre and Chebyshev polynomials. One can extend the method to general Jacobi polynomials, and orthogonal systems in unbounded domains.

We make a final remark on the error estimates of the Birkhoff interpolation. We revisit the interpolation problem (4.1) at LGR points. For any  $u \in C^1(-1, 1)$ , we denote its Birkhoff interpolant by  $I_N^B u$ , which satisfies the interpolation conditions:

$$(4.24) \quad (I_N^B u)'(x_j) = u'(x_j), \quad 1 \leq j \leq N; \quad (I_N^B u)(-1) = u(-1).$$

Let  $I_{N-1}^G$  be the Lagrange–Gauss interpolation operator at the interior LGR points  $\{x_j\}_{j=1}^N$  such that for any  $v \in C(-1, 1)$ ,  $(I_{N-1}^G v)(x_j) = v(x_j)$ ,  $1 \leq j \leq N$ . Then we find from (4.24) that

$$(4.25) \quad (I_N^B u)'(x) = (I_{N-1}^G u')(x) \in \mathbb{P}_{N-1} \quad \forall x \in [-1, 1].$$

Note that  $\{x_j\}_{j=1}^N$  are zeros of the Jacobi polynomial  $P_N^{(0,1)}(x)$ . Define the weighted  $L_\omega^2$ -space with  $\omega = 1 - x$  with the norm  $\|\cdot\|_\omega$ . Using (4.25) and [42, Theorem 3.41], we obtain that for  $2 \leq m \leq N + 1$ ,

$$(4.26) \quad \begin{aligned} \|(I_N^B u - u)'\|_\omega &= \|I_{N-1}^G u' - u'\|_\omega \\ &\leq c \sqrt{\frac{(N - m + 2)!}{N!}} (N + m)^{-\frac{m}{2}} \|(1 - x^2)^{(m-1)/2} \partial_x^m u\|_\omega, \end{aligned}$$

where  $c$  is a positive constant independent of  $m, N$ , and  $u$ . Note that if  $m$  is fixed, the order of convergence is  $O(N^{1-m})$ .

*Remark 4.5.* By (4.24) and (4.25),

$$(I_N^B u - u)(x) = \int_{-1}^x [(I_{N-1}^G u')(t) - u'(t)] dt.$$

We expect the convergence  $\|I_N^B u - u\|_{L^2} = O(N^{-m})$ . However, it appears challenging to obtain this optimal order, though we observed such a convergence in computation. We wish to report this and error estimates for other related Birkhoff interpolations e.g., (3.1) in a future work.

**Appendix A. Proof of Theorem 3.3.** We first prove (3.10). For any  $\phi \in \mathbb{P}_N$ , we write  $\phi(x) = \sum_{p=0}^N \phi(x_p) l_p(x)$ , so we have  $\phi^{(k)}(x) = \sum_{p=0}^N \phi(x_p) l_p^{(k)}(x)$ ,  $k \geq 1$ . Taking  $\phi = B_j \in \mathbb{P}_N$  and  $x = x_i$ , we obtain

$$(A.1) \quad b_{ij}^{(k)} = \sum_{p=0}^N d_{ip}^{(k)} b_{pj}, \quad k \geq 1,$$

which implies  $\mathbf{B}^{(k)} = \mathbf{D}^{(k)} \mathbf{B}$ . The second equality follows from (2.10), and the last identity in (3.10) is due to the recursive relation  $\mathbf{B}^{(k-1)} = \mathbf{D}^{k-1} \mathbf{B}$ .

We now turn to the proof of (3.11). It is clear that by (3.5),  $b_{0j} = b_{Nj} = 0$  for  $1 \leq j \leq N - 1$  and  $b_{ij}^{(2)} = \delta_{ij}$  for  $1 \leq i, j \leq N - 1$ . Taking  $k = 2$  in (A.1) leads to

$$\delta_{ij} = \sum_{p=1}^{N-1} d_{ip}^{(2)} b_{pj}, \quad 1 \leq i, j \leq N - 1.$$

This yields  $\mathbf{D}_{\text{in}}^{(2)} \mathbf{B}_{\text{in}} = \mathbf{I}_{N-1}$ , from which the second statement follows directly.

**Appendix B. Proof of Proposition 3.5.** Since  $B_j'' \in \mathbb{P}_{N-2}$ , we expand it in terms of Legendre polynomials:

$$(B.1) \quad B_j''(x) = \sum_{k=0}^{N-2} \beta_{kj} \frac{P_k(x)}{\gamma_k}, \quad \text{where } \beta_{kj} = \int_{-1}^1 B_j''(x) P_k(x) dx.$$

Using (2.8), (2.5), and (3.4) leads to

(B.2)

$$\beta_{kj} = \int_{-1}^1 B_j''(x)P_k(x)dx = ((-1)^k B_j''(-1) + B_j''(1))\omega_0 + P_k(x_j)\omega_j, \quad 1 \leq j \leq N-1.$$

Notice that the last identity of (B.2) is valid for all  $k \leq N+1$ . Taking  $k = N-1, N$ , we obtain from (2.3) that the resulted integrals vanish, so we have the linear system of  $B_j''(\pm 1)$ :

$$\begin{aligned} ((-1)^{N-1} B_j''(-1) + B_j''(1))\omega_0 + P_{N-1}(x_j)\omega_j &= 0, \\ ((-1)^N B_j''(-1) + B_j''(1))\omega_0 + P_N(x_j)\omega_j &= 0. \end{aligned}$$

Therefore, we solve it and find that

$$(B.3) \quad B_j''(\pm 1) = -(\pm 1)^N \frac{\omega_j}{2\omega_0} (P_N(x_j) \pm P_{N-1}(x_j)), \quad 1 \leq j \leq N-1.$$

Inserting (B.3) into (B.2) yields the expression for  $\beta_{kj}$  in (3.18).

Next, it follows from (B.1) that

$$(B.4) \quad B_j(x) = \sum_{k=0}^{N-2} \beta_{kj} \frac{\partial_x^{-2} P_k(x)}{\gamma_k} + C_1 + C_2(x+1),$$

where  $C_1$  and  $C_2$  are constants to be determined by  $B_j(\pm 1) = 0$ . Observe from (3.14) that  $\partial_x^{-2} P_k(-1) = 0$  for  $k \geq 0$  and  $\partial_x^{-2} P_k(1) = 0$  for  $k \geq 2$ . This implies  $C_1 = 0$  and

$$2C_2 = -\frac{\beta_{0j}}{\gamma_0} \partial_x^{-2} P_0(1) - \frac{\beta_{1j}}{\gamma_1} \partial_x^{-2} P_1(1) = \beta_{1j} - \beta_{0j}.$$

Thus, (3.17) follows. Finally, differentiating (3.17) leads to (3.19).

**Appendix C. Proof of Proposition 3.12.** From [52, Theorem 7], we know that all eigenvalues of  $\mathbf{D}_{\text{in}}^{(2)}$ , denoted by  $\{\lambda_{N,l}\}_{l=1}^{N-1}$ , are real, distinct, and negative. We arrange them as  $\lambda_{N,N-1} < \dots < \lambda_{N,1} < 0$ . We diagonalize  $\mathbf{D}_{\text{in}}^{(2)}$  and write it as  $\mathbf{D}_{\text{in}}^{(2)} = \mathbf{Q}\mathbf{\Lambda}_\lambda\mathbf{Q}^{-1}$ , where  $\mathbf{Q}$  is formed by the eigenvectors and  $\mathbf{\Lambda}_\lambda$  is the diagonal matrix of all eigenvalues. Since  $\mathbf{B}_{\text{in}} = (\mathbf{D}_{\text{in}}^{(2)})^{-1}$  (cf. Theorem 3.3), we have  $\mathbf{I}_{N-1} - \mu\mathbf{B}_{\text{in}} = \mathbf{Q}(\mathbf{I}_{N-1} - \mu\mathbf{\Lambda}_\lambda^{-1})\mathbf{Q}^{-1}$ . Therefore, the eigenvalues of  $\mathbf{I}_{N-1} - \mu\mathbf{B}_{\text{in}}$  are  $\{1 - \mu\lambda_{N,l}^{-1}\}_{l=1}^{N-1}$ , which are real and distinct. Then the bounds in (3.30) can be obtained from the properties  $-\lambda_{N,1} > \pi^2/4$  (see [52, p. 286] and [2, Theorem 2.1]) and  $-\lambda_{N,N-1} = c_N N^4/(4\pi^2)$  (see [52, Proposition 9]).

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