

INTEGRATION PRECONDITIONING OF PSEUDOSPECTRAL OPERATORS. I. BASIC LINEAR OPERATORS*

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Abstract. This paper develops a family of preconditioners for pseudospectral approximations of p th-order linear differential operators subject to various types of boundary conditions. The approximations are based on ultraspherical polynomials with special attention being paid to Legendre and Chebyshev polynomial methods based on Gauss–Lobatto quadrature points.

The eigenvalue spectrum of the preconditioned operators are obtained in closed analytic form and the weakly enforced boundary conditions are shown to result in a rank $2p$ perturbation of the identity operator, i.e., the majority of the preconditioned eigenvalues are unity. The spectrum of the preconditioned advective operator is shown to be bounded independent of the order of the approximation, N . However, the preconditioned diffusive operator is, in general, indefinite with four real eigenvalues. For Dirichlet boundary conditions the spectral radius grows as \sqrt{N} , while it scales as N for the case of Neumann boundary conditions. These results are shown to be asymptotically optimal within the present framework. Generalizations to higher-order differential operators, general boundary conditions, and arbitrary polynomial basis and quadrature nodes are discussed.

Key words. pseudospectral methods, preconditioning, penalty methods

AMS subject classifications. 65M70, 65N35, 15A12, 65F10

1. Introduction. In recent decades, pseudospectral methods have proven efficient for obtaining accurate solutions to partial differential equations, the basic idea being to replace the exact derivatives with derivatives of interpolating polynomials at the collocation points [1, 2]. For boundary value problems, this approach involves the solution of very ill-conditioned linear systems of equations, e.g., the condition number of the pseudospectral first-order operator grows like N^2 , while the condition number for the second-order operator typically scales like N^4 . Thus, to apply iterative methods like GMRES, see, e.g., [3], for solving such systems, it becomes crucial to develop efficient preconditioners.

Previous work on preconditioners for pseudospectral operators includes the use of finite difference preconditioners for the advective operator [4] as well as for the diffusive operator [5]. More recently, the use of finite element preconditioners has been advocated [6] and applied with significant success to a large variety of operators. However, a general property of previously proposed preconditioners is their reliance on a low-order approximation of the inverse operator. In this work we take a different route and develop a family of preconditioners of the same order as the polynomial approximation itself. This results in the preconditioners being full matrices which, however, is only a natural consequence of using global methods. On the other hand, utilizing the properties of the polynomial basis itself allows for the development of efficient preconditioners for approximations based on any of the classical orthogonal polynomials and for general p th order linear one-dimensional differential operators. Moreover, the general framework applies directly to pseudospectral methods based on any of the Gauss quadrature points.

*Received by the editors March 31, 1997; accepted for publication (in revised form) October 25, 1997; published electronically May 21, 1998. This work was supported by NSF grant ASC-9504002 and by DOE grant DE-FG02-95ER25239.

<http://www.siam.org/journals/sinum/35-4/31918.html>

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The pseudospectral preconditioners presented here are closely related to previous work on preconditioning of spectral differentiation operators as they appear in spectral τ -methods [7, 8]. However, the extension to pseudospectral methods requires renewed attention to the boundary conditions and how these affect the efficiency of the preconditioners. We propose to enforce the boundary conditions only weakly, using a penalty term [9, 10]. This allows for a fairly complete analysis of the preconditioned operators and we can, in most cases, obtain the complete eigenvalue spectrum of the preconditioned operator in analytic form. Moreover, enforcing the boundary conditions through the penalty term allows for a direct generalization to situations with arbitrary boundary conditions.

The remaining part of this paper is organized as follows. In section 2 we introduce the ultraspherical polynomials and discuss their properties, with special attention being given to the Legendre and Chebyshev polynomials. We continue by introducing spectral as well as pseudospectral methods, as the connection between these two approaches lies at the heart of the motivation leading to the integration preconditioners, being developed in section 3. Section 4 addresses the performance of the preconditioners for the advective operator, with special attention being given to the effect of the boundary conditions. The analysis is carried out in detail for Gauss–Lobatto–Legendre and –Chebyshev pseudospectral methods. In section 5 we present a similar analysis for the diffusion operator, i.e., the Poisson equation, subject to Dirichlet as well as Neumann boundary conditions. Section 6 contains a few concluding remarks and discusses generalizations to problems involving general boundary conditions and methods based on general orthogonal polynomials as well as general Gauss quadrature nodal sets.

2. Ultraspherical polynomials and spectral methods. In this section we review several topics central to the subsequent analysis. In particular, we introduce the ultraspherical polynomials and discuss in some detail the theory underlying spectral as well as pseudospectral methods for the solution of partial differential equations.

2.1. Ultraspherical polynomials. The ultraspherical polynomials, $P_n^{(\alpha)}(x)$, appear as eigensolutions to the singular Sturm–Liouville problem in the finite domain $x \in [-1, 1]$ [11, 12], with the first two being

$$P_0^{(\alpha)}(x) = 1, \quad P_1^{(\alpha)}(x) = (2\alpha + 1)x,$$

while the remaining polynomials are given through the recursion formula

$$(1) \quad xP_n^{(\alpha)}(x) = a_{n-1,n}P_{n-1}^{(\alpha)}(x) + a_{n+1,n}P_{n+1}^{(\alpha)}(x),$$

with the recurrence coefficients

$$(2) \quad a_{n-1,n} = \frac{n + 2\alpha}{2n + 2\alpha + 1}, \quad a_{n+1,n} = \frac{n + 1}{2n + 2\alpha + 1}.$$

The polynomials, $P_n^{(\alpha)}(x)$, are normalized such that

$$(3) \quad P_n^{(\alpha)}(\pm 1) = (\pm 1)^n \binom{n + 2\alpha}{n},$$

$$(4) \quad \frac{dP_n^{(\alpha)}(\pm 1)}{dx} = (2\alpha + 1)(\pm 1)^{n+1} \binom{n + 2\alpha + 1}{n - 1}.$$

To simplify the subsequent notation, the recursion, (1)–(2), is written as

$$x\mathbf{P} = \mathbf{P}\mathbf{A},$$

where

$$\mathbf{A} = \begin{bmatrix} 0 & a_{0,1} & 0 & 0 & 0 & \cdots \\ a_{1,0} & 0 & a_{1,2} & 0 & 0 & \cdots \\ 0 & a_{2,1} & 0 & a_{2,3} & 0 & \cdots \\ 0 & 0 & a_{3,2} & 0 & a_{3,4} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix},$$

while the row vector, \mathbf{P} , is

$$\mathbf{P} = [P_0^{(\alpha)}(x), \dots, P_N^{(\alpha)}(x)].$$

A relation between the polynomials and their derivatives appears on the form

$$(5) \quad P_n^{(\alpha)}(x) = b_{n-1,n}^{(1)} \frac{dP_{n-1}^{(\alpha)}(x)}{dx} + b_{n+1,n}^{(1)} \frac{dP_{n+1}^{(\alpha)}(x)}{dx},$$

with the coefficients

$$(6) \quad b_{n-1,n}^{(1)} = -\frac{1}{2n + 2\alpha + 1}, \quad b_{n+1,n}^{(1)} = \frac{1}{2n + 2\alpha + 1}.$$

Equations (5)–(6) may likewise be expressed in matrix form as

$$\mathbf{P} = \mathbf{P}_x \mathbf{B}^{(-1)},$$

where

$$\mathbf{B}^{(-1)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ b_{1,0}^{(1)} & 0 & b_{1,2}^{(1)} & 0 & 0 & \cdots \\ 0 & b_{2,1}^{(1)} & 0 & b_{2,3}^{(1)} & 0 & \cdots \\ 0 & 0 & b_{3,2}^{(1)} & 0 & b_{3,4}^{(1)} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix},$$

while \mathbf{P}_x refers to the derivative of the row vector, \mathbf{P} . We have chosen the notation $\mathbf{B}^{(-1)}$ since this matrix operator essentially plays the role of integration of the polynomial basis. Observe that since $P_0^{(\alpha)}(x) = 1$, its first derivative vanishes and the entries of the first row of $\mathbf{B}^{(-1)}$ can be set to zero, thus reflecting its singular nature.

We shall also need the less well-known recurrence formula

$$(7) \quad P_n^{(\alpha)}(x) = b_{n-2,n}^{(2)} \frac{d^2 P_{n-2}^{(\alpha)}(x)}{dx^2} + b_{n,n}^{(2)} \frac{d^2 P_n^{(\alpha)}(x)}{dx^2} + b_{n+2,n}^{(2)} \frac{d^2 P_{n+2}^{(\alpha)}(x)}{dx^2},$$

with the coefficients

$$(8) \quad b_{n-2,n}^{(2)} = \frac{1}{(2n + 2\alpha + 1)(2n + 2\alpha - 1)}, \quad b_{n+2,n}^{(2)} = \frac{1}{(2n + 2\alpha + 1)(2n + 2\alpha + 3)},$$

$$b_{n,n}^{(2)} = -\frac{2}{(2n + 2\alpha - 1)(2n + 2\alpha + 3)}.$$

In matrix form this yields

$$\mathbf{P} = \mathbf{P}_{xx}\mathbf{B}^{(-2)},$$

with

$$\mathbf{B}^{(-2)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ b_{2,0}^{(2)} & 0 & b_{2,2}^{(2)} & 0 & b_{2,4}^{(2)} & 0 & \dots \\ 0 & b_{3,1}^{(2)} & 0 & b_{3,3}^{(2)} & 0 & b_{3,5}^{(2)} & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

As for $\mathbf{B}^{(-1)}$, we take the two first rows of the second-order integration operator, $\mathbf{B}^{(-2)}$, to be zero since the two first elements of \mathbf{P}_{xx} are identically zero. Recurrence relations for higher-order derivatives may likewise be obtained by repeatedly combining the relations, (5)–(8).

The general part of the subsequent analysis will be concerned with methods based on the ultraspherical polynomials, although we shall pay particular attention to schemes based on Legendre polynomials, $L_n(x)$, and Chebyshev polynomials, $T_n(x)$. We shall, therefore, briefly recall the most important properties of these two families of polynomials.

2.1.1. Legendre polynomials. The Legendre polynomials, $L_n(x)$, relate to the ultraspherical polynomial as

$$L_n(x) = P_n^{(0)}(x),$$

such that

$$L_0(x) = 1, \quad L_1(x) = x,$$

while the subsequent polynomials appear from (1) with

$$a_{n-1,n} = \frac{n}{2n + 1}, \quad a_{n+1,n} = \frac{n + 1}{2n + 1}.$$

The boundary values are given as

$$(9) \quad L_n(\pm 1) = (\pm 1)^n, \quad \frac{dL_n(\pm 1)}{dx} = \frac{1}{2}(\pm 1)^{n+1}n(n + 1).$$

The recurrence coefficients of (5), providing the entries of $\mathbf{B}^{(-1)}$, become

$$(10) \quad b_{n-1,n}^{(1)} = -\frac{1}{2n + 1}, \quad b_{n+1,n}^{(1)} = \frac{1}{2n + 1},$$

while the entries of $\mathbf{B}^{(-2)}$, being the coefficients of (7), are

$$(11) \quad b_{n-2,n}^{(2)} = \frac{1}{(2n + 1)(2n - 1)}, \quad b_{n+2,n}^{(2)} = \frac{1}{(2n + 1)(2n + 3)},$$

$$b_{n,n}^{(2)} = -\frac{2}{(2n - 1)(2n + 3)}.$$

Further details on Legendre polynomials can be found in, e.g., [11, 12].

2.1.2. Chebyshev polynomials. The Chebyshev polynomials, $T_n(x)$, appear as the special case of the ultraspherical polynomials with

$$T_n(x) = n \lim_{\alpha \rightarrow -\frac{1}{2}} \Gamma(2\alpha + 1) P_n^{(\alpha)}(x) = \cos(n \arccos x).$$

Here $\Gamma(x)$ is the gamma function and the limit is taken since $\Gamma(2\alpha + 1)$ has a simple pole for $\alpha = -1/2$. However, the limit exists and the Chebyshev polynomials are recovered [11].

Although there exists a closed form expression for the Chebyshev polynomials, it remains illustrative to recall that

$$T_0(x) = 1, \quad T_1(x) = x,$$

while the higher-order Chebyshev polynomials are recovered from (1) with

$$a_{n-1,n} = \frac{1}{2}, \quad a_{n+1,n} = \frac{c_n}{2},$$

where $c_0 = 2$ and $c_n = 1$ otherwise. The Chebyshev polynomials take the values

$$(12) \quad T_n(\pm 1) = (\pm 1)^n, \quad \frac{dT_n(\pm 1)}{dx} = (\pm 1)^{n+1} n^2,$$

and the entries of $B^{(-1)}$, establishing a connection between $T_n(x)$ and its derivatives, become

$$(13) \quad b_{n-1,n}^{(1)} = -\frac{1}{2(n-1)}, \quad b_{n+1,n}^{(1)} = \frac{c_n}{2(n+1)}.$$

The recurrence coefficients for (7), providing the entries of $B^{(-2)}$, are

$$(14) \quad b_{n-2,n}^{(2)} = \frac{1}{4(n-1)(n-2)}, \quad b_{n+2,n}^{(2)} = \frac{c_n}{4(n+1)(n+2)},$$

$$b_{n,n}^{(2)} = -\frac{1}{2(n^2-1)},$$

Much more on the properties of Chebyshev polynomials can be found in, e.g., [11, 12].

2.2. Spectral methods. When applying spectral methods for the solution of partial differential equations, one seeks polynomial solutions

$$\mathcal{P}_N u(x) \in \mathbb{Q}_0^N, \quad \mathbb{Q}_0^N = \text{span} \left\{ P_n^{(\alpha)} \right\}_{n=0}^N$$

of the form

$$(15) \quad \mathcal{P}_N u(x) = \sum_{n=0}^N \hat{u}_n P_n^{(\alpha)}(x),$$

where \hat{u}_n represents the continuous expansion coefficients. Utilizing the orthogonality of the ultraspherical polynomials in $L_w^2[-1, 1]$, we have

$$\gamma_n \delta_{nm} = \int_{-1}^1 P_n^{(\alpha)}(x) P_m^{(\alpha)}(x) (1-x^2)^\alpha dx,$$

where the continuous normalization factor, γ_n , is

$$(16) \quad \gamma_n = 2^{2\alpha+1} \frac{\Gamma^2(\alpha + 1)\Gamma(n + 2\alpha + 1)}{n!(2n + 2\alpha + 1)\Gamma^2(2\alpha + 1)},$$

and the continuous expansion coefficients appear as

$$\hat{u}_n = \frac{1}{\gamma_n} \int_{-1}^1 u(x)P_n^{(\alpha)}(x)(1 - x^2)^\alpha dx.$$

The exact evaluation of this integral naturally poses a problem in most situations and approximations of the expansion coefficients are computed using a Gauss quadrature. For boundary value problems the Gauss–Lobatto quadrature appear as the natural choice as it involves the grid

$$\{x_i\}_{i=0}^N = \left\{ x \in [-1, 1] \mid (1 - x^2) \frac{dP_N^{(\alpha)}(x)}{dx} = 0 \right\},$$

assumed ordered as

$$-1 = x_0 < x_1 < \dots < x_{N-1} < x_N = 1.$$

Using this grid we obtain the discrete expansion coefficients, \tilde{u}_n , through the sum

$$\tilde{u}_n = \frac{1}{\tilde{\gamma}_n} \sum_{i=0}^N u(x_i)P_n^{(\alpha)}(x_i)w_i,$$

where the discrete normalization, $\tilde{\gamma}_n = \gamma_n$, for $n < N$, while

$$(17) \quad \tilde{\gamma}_N = 2^{2\alpha+1} \frac{\Gamma^2(\alpha + 1)\Gamma(N + 2\alpha + 1)}{NN!\Gamma^2(2\alpha + 1)}.$$

The Gauss–Lobatto weights, w_i , are

$$(18) \quad w_i = \begin{cases} 2^{2\alpha+1} \frac{(N - 1)!\Gamma(\alpha + 1)\Gamma(\alpha + 2)}{\Gamma(N + 2\alpha + 2)} & i = 0, N, \\ -2^{2\alpha+1} \frac{\Gamma^2(\alpha + 1)\Gamma(N + 2\alpha + 1)}{N!(N + 2\alpha + 1)\Gamma^2(2\alpha + 1)} \left[P_N^{(\alpha)}(x_i) \frac{d}{dx} P_{N-1}^{(\alpha)}(x_i) \right]^{-1} & i \in [1, N - 1]. \end{cases}$$

To simplify the notation we introduce the two vectors

$$\mathbf{u} = (u(-1), u(x_1), \dots, u(x_{N-1}), u(1))^T, \quad \tilde{\mathbf{u}} = (\tilde{u}_0, \dots, \tilde{u}_N)^T,$$

being related through the transformations

$$\mathbf{u} = \mathbf{T}^{-1}\tilde{\mathbf{u}}, \quad \tilde{\mathbf{u}} = \mathbf{T}\mathbf{u},$$

where the entries of the $(N + 1) \times (N + 1)$ matrices, \mathbf{T}^{-1} and \mathbf{T} , are given as

$$\mathbf{T}_{ij}^{-1} = P_j^{(\alpha)}(x_i), \quad \mathbf{T}_{ij} = \frac{1}{\tilde{\gamma}_i} P_i^{(\alpha)}(x_j)w_j.$$

We observe that T^{-1} and T are real orthogonal matrices since $T^{-1}T = I$ and, with appropriate normalization being possible since $\tilde{\gamma}_n$ and w_j are strictly positive, we have that $T^T = T^{-1}$. Hence, T^{-1} and T provide a similarity transform.

We shall devote the subsequent analysis to schemes based on the discrete expansion coefficients, \tilde{u}_n , as this in practice is the only feasible approach. The error incurred by this choice, recognized as the aliasing error, is discussed in, e.g., [1, 2].

Solving partial differential equations involves the need for computing derivatives. Hence, given the approximation

$$\mathbf{u} = T^{-1}\tilde{\mathbf{u}},$$

we need to compute the vector of expansion coefficients, $\tilde{\mathbf{u}}^{(1)}$, such that

$$\frac{d}{dx}\mathbf{u} = T^{-1}\tilde{\mathbf{u}}^{(1)}.$$

Utilizing the properties of the polynomials, this relation is obtained as

$$\frac{d}{dx}\mathbf{u} = T^{-1}\tilde{\mathbf{u}}^{(1)} = T_x^{-1}B^{(-1)}\tilde{\mathbf{u}}^{(1)} = T_x^{-1}\tilde{\mathbf{u}},$$

by using equations (5)–(6), such that

$$\tilde{\mathbf{u}} = B^{(-1)}\tilde{\mathbf{u}}^{(1)},$$

where $\tilde{\mathbf{u}}^{(1)}$ is computed directly by backward recursion, with the exception of $\tilde{u}_N^{(1)}$ which must, however, take the value zero for any finite order expansion. We note that $B^{(-1)}$ plays the role of integration since one recovers $\tilde{\mathbf{u}}$ up to a constant only.

To directly obtain $\tilde{\mathbf{u}}^{(1)}$ from $\tilde{\mathbf{u}}$ we need to invert $B^{(-1)}$, which, however, requires some care since $B^{(-1)}$ is singular. Nevertheless, by realizing that

$$B^{(-1)} : \mathbb{Q}_0^{N-1} \rightarrow \mathbb{Q}_1^N,$$

the inverse of $B^{(-1)}$, which we shall denote by $B^{(1)}$, is given uniquely in the restricted space as

$$B^{(1)} : \mathbb{Q}_1^N \rightarrow \mathbb{Q}_0^{N-1},$$

implying that the first column and the last row of $B^{(1)}$ must be identically zero. It is well known that $B^{(1)}$ takes the form of a strictly upper triangular matrix when considering expansions based on ultraspherical polynomials and that $B^{(1)}$ has a condition number that grows like N^2 [1, 13].

Likewise, we obtain

$$\tilde{\mathbf{u}} = B^{(-2)}\tilde{\mathbf{u}}^{(2)},$$

where $\tilde{\mathbf{u}}^{(2)}$ refers to the vector of expansions coefficients for the second-order derivative of \mathbf{u} at the collocation points. The inverse relation involves

$$B^{(2)} : \mathbb{Q}_2^N \rightarrow \mathbb{Q}_0^{N-2},$$

i.e., the first two columns and the last two rows of $B^{(2)}$ must be identically zero. We recall that such second-order spectral differentiation matrices are strictly upper triangular with a condition number proportional to N^4 [1, 13].

Although we only consider first- and second-order operators, the same sequence of arguments can be applied to derive spectral differentiation operators of arbitrary order utilizing (5)–(8).

2.3. Pseudospectral methods. Let us now turn our attention towards the issue of pseudospectral methods and their relation to the spectral methods based on the use of the discrete expansion coefficients. If we introduce the projection

$$\mathcal{I}_N u(x) = \sum_{n=0}^N \tilde{u}_n P_n^{(\alpha)}(x),$$

the key observation is that

$$\forall x_i : \mathcal{I}_N u(x_i) = u(x_i),$$

where x_i represents the Gauss–Lobatto quadrature points used to compute the discrete expansion coefficients, \tilde{u}_n . Thus, the discrete projection is exact at the collocation points, and, therefore, $\mathcal{I}_N u(x)$ is identical to the interpolating polynomial based on these nodal points. This result appears by using the Christoffel–Darboux identity [11] for orthogonal polynomials together with (3)–(4) and the expression for the Gauss–Lobatto weights, w_i , given in (18). We may express the approximating polynomial as

$$\mathcal{I}_N u(x) = \sum_{n=0}^N \tilde{u}_n P_n^{(\alpha)}(x) = \sum_{i=0}^N u(x_i) l_i(x),$$

where the interpolating Lagrange polynomials, $l_i(x)$, take the form

$$l_i(x) = w_i \sum_{n=0}^N \frac{1}{\tilde{\gamma}_n} P_n^{(\alpha)}(x_i) P_n^{(\alpha)}(x).$$

Note that we need only consider the grid point values of the approximated function, while the discrete expansion coefficients, so vital in the spectral formulation, never appear.

Let us again return to the computation of derivatives of the approximation. Indeed, since $\mathcal{I}_N u(x)$ is nothing else than a polynomial, we may simply differentiate these polynomials so that

$$\mathbf{u}^{(1)} = \mathbf{D}^{(1)} \mathbf{u}$$

yields the derivative of $u(x)$ at the grid points with

$$\mathbf{u}^{(1)} = (u^{(1)}(x_0), \dots, u^{(1)}(x_N))^T, \quad \mathbf{u} = (u(x_0), \dots, u(x_N))^T,$$

and the entries of the differentiation matrix, $\mathbf{D}^{(1)}$, become

$$(19) \quad \mathbf{D}_{ij}^{(1)} = \frac{dl_j(x_i)}{dx} = w_j \sum_{n=0}^N \frac{1}{\tilde{\gamma}_n} P_n^{(\alpha)}(x_j) \frac{dP_n^{(\alpha)}(x_i)}{dx}.$$

It is well known that $\mathbf{D}^{(1)}$ is a centro-antisymmetric full matrix [14] with a condition number proportional to N^2 , much like the spectral first-order differentiation operator, $\mathbf{B}^{(1)}$.

Likewise, we obtain the second-order derivatives of $u(x)$ at the grid points as

$$\mathbf{u}^{(2)} = \mathbf{D}^{(2)} \mathbf{u},$$

with the entries of the second-order differentiation matrix, $D^{(2)}$, being

$$(20) \quad D_{ij}^{(2)} = \frac{d^2 l_j(x_i)}{dx^2} = w_j \sum_{n=0}^N \frac{1}{\tilde{\gamma}_n} P_n^{(\alpha)}(x_j) \frac{d^2 P_n^{(\alpha)}(x_i)}{dx^2}.$$

The second-order differentiation matrix is known to be a full centro-symmetric matrix [14] with a condition number proportional to N^4 , as for the second-order spectral differentiation operator, $B^{(2)}$.

3. Integration preconditioning. The development of the integration preconditioners for the pseudospectral differentiation matrices is centered around the following result.

THEOREM 3.1. *Given the spectral differentiation matrices, $B^{(1)}$ and $B^{(2)}$, the similarity transformation, T and T^{-1} , and the pseudospectral differentiation matrices, $D^{(1)}$ and $D^{(2)}$, the following relation holds*

$$D^{(1)} = T^{-1}B^{(1)}T, \quad D^{(2)} = T^{-1}B^{(2)}T.$$

Proof. The theorem is established by expressing the pseudospectral differentiation matrices, (19) and (20), as

$$D^{(1)} = T_x^{-1}T, \quad D^{(2)} = T_{xx}^{-1}T,$$

where the entries of the two matrices, T_x^{-1} and T_{xx}^{-1} , are given as

$$(T_x^{-1})_{ij} = \frac{dP_j^{(\alpha)}(x_i)}{dx}, \quad (T_{xx}^{-1})_{ij} = \frac{d^2 P_j^{(\alpha)}(x_i)}{dx^2}.$$

However, since

$$T^{-1} = T_x^{-1}B^{(-1)}, \quad T^{-1} = T_{xx}^{-1}B^{(-2)},$$

the result follows. \square

Theorem 3.1 suggests using

$$(21) \quad \tilde{P}^{(-1)} = T^{-1}B^{(-1)}T, \quad \tilde{P}^{(-2)} = T^{-1}B^{(-2)}T,$$

for preconditioning of the first- and second-order pseudospectral differentiation matrices, respectively, since we immediately obtain

$$(22) \quad \tilde{P}^{(-1)}D^{(1)} = I_1^N, \quad \tilde{P}^{(-2)}D^{(2)} = I_2^N.$$

Here I_a^b denotes the matrix with unity along the diagonal for $i \in [a, b]$, while the remaining elements are identically zero, e.g., I_0^N equals the identity matrix.

However, the preconditioners defined in (21) are singular. Fortunately, we may overcome this problem while maintaining the essence of (22). Indeed, if we define the

modified spectral integration operator, $\tilde{B}^{(-1)}$, as

$$\tilde{B}^{(-1)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \alpha_1^{(1)} \\ b_{1,0}^{(1)} & 0 & b_{1,2}^{(1)} & 0 & 0 & \cdots & 0 & 0 \\ 0 & b_{2,1}^{(1)} & 0 & b_{2,3}^{(1)} & 0 & \cdots & 0 & 0 \\ 0 & 0 & b_{3,2}^{(1)} & 0 & b_{3,4}^{(1)} & \ddots & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & b_{N-1,N-2}^{(1)} & 0 & b_{N-1,N}^{(1)} \\ 0 & 0 & 0 & \cdots & \cdots & 0 & b_{N,N-1}^{(1)} & 0 \end{bmatrix},$$

we maintain that $\tilde{B}^{(-1)}B^{(1)} = I_1^N$ since $B^{(1)} : \mathbb{Q}_1^N \rightarrow \mathbb{Q}_0^{N-1}$, while $\tilde{B}^{(-1)}$ is made nonsingular by properly choosing the parameter, $\alpha_1^{(1)}$, a choice that allows for optimizing the preconditioner. Hence, the pseudospectral integration preconditioner for the first-order pseudospectral differentiation matrix becomes

$$(23) \quad P^{(-1)} = T^{-1}\tilde{B}^{(-1)}T,$$

while we return to the exact specification of $\alpha_1^{(1)}$ shortly.

Similarly, we define the modified spectral second-order integration operator, $\tilde{B}^{(-2)}$, as

$$\tilde{B}^{(-2)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \alpha_{11}^{(2)} & \alpha_{12}^{(2)} \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \alpha_{21}^{(2)} & \alpha_{22}^{(2)} \\ b_{2,0}^{(2)} & 0 & b_{2,2}^{(2)} & 0 & b_{2,4}^{(2)} & 0 & \cdots & 0 & 0 \\ 0 & b_{3,1}^{(2)} & 0 & b_{3,3}^{(2)} & 0 & b_{3,5}^{(2)} & \cdots & 0 & 0 \\ 0 & 0 & b_{4,2}^{(2)} & 0 & b_{4,4}^{(2)} & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & 0 & b_{N-2,N}^{(2)} \\ 0 & 0 & 0 & \cdots & 0 & \ddots & 0 & b_{N-1,N-1}^{(2)} & 0 \\ 0 & 0 & 0 & \cdots & \cdots & 0 & b_{N,N-2}^{(2)} & 0 & b_{N,N}^{(2)} \end{bmatrix},$$

where we introduce the four parameters, $\alpha_{11}^{(2)}$, $\alpha_{12}^{(2)}$, $\alpha_{21}^{(2)}$, and $\alpha_{22}^{(2)}$ to avoid the singularity of $B^{(-2)}$ and define the pseudospectral integration preconditioner as

$$(24) \quad P^{(-2)} = T^{-1}\tilde{B}^{(-2)}T.$$

As a direct consequence of (23)–(24) the eigenvalue spectrum of the preconditioned differentiation matrices,

$$P^{(-1)}D^{(1)} = T^{-1}I_1^N T, \quad P^{(-2)}D^{(2)} = T^{-1}I_2^N T,$$

are known in explicit form as are the pseudospectral integration preconditioners themselves.

Enforcing boundary conditions in pseudospectral methods is traditionally done by directly modifying the differentiation matrices, e.g., by deleting the appropriate rows and columns in the matrices in case of Dirichlet boundary conditions [1, 2]. Unfortunately, this procedure destroys the delicate symmetries leading to Theorem 3.1, i.e., the development of the pseudospectral integration preconditioners fails. In [9], Funaro and Gottlieb introduced a penalty method which enforces the boundary condition only weakly through a boundary correction rather than modifying the matrix operators. Such penalty methods have been studied thoroughly for a number of problems in [10] and we shall rely heavily on these results in the subsequent analysis.

4. Preconditioning of the advective operator. Let us consider the first-order problem

$$(25) \quad \frac{du(x)}{dx} = f(x), \quad u(1) = 0,$$

and seek solutions of polynomial form using the discrete approximation

$$(26) \quad D^{(1)}\mathbf{u} = \mathbf{f}, \quad u(1) = 0.$$

Here \mathbf{u} and \mathbf{f} refer to the grid vectors of the two functions, $u(x)$ and $f(x)$, at the Gauss–Lobatto collocation points associated with the polynomial basis, $P_n^{(\alpha)}(x)$.

Imposing the boundary conditions strongly would amount to deleting the last row and column and solving the resulting matrix problem. However, since the condition number of $D^{(1)}$ is proportional to N^2 , this may well be nontrivial for N large. Unfortunately, since we have destroyed the structure of $D^{(1)}$, we can no longer rely on $P^{(-1)}$ for preconditioning.

To proceed, we, therefore, propose to impose the boundary conditions weakly as

$$(27) \quad \left[D^{(1)} - \tau I_N^N \right] \mathbf{u} = \mathbf{f},$$

following the development of the penalty method in [9, 10]. The penalty parameter, τ , is chosen such that

$$D^{(1)} - \tau I_N^N,$$

is nonpositive definite. Such choices are discussed in depth in [10] for specific choices of the polynomial basis, and we shall return to this issue shortly. For now, we simply assume that τ is given and consider preconditioning of (27). Since $D^{(1)}$ is now unaltered, it seems only natural to use $P^{(-1)}$ for preconditioning

$$\left[T^{-1} I_1^N T - \tau P^{(-1)} I_N^N \right] \mathbf{u} = P^{(-1)} \mathbf{f}.$$

Estimating the spectral radius of the preconditioned operator

$$T^{-1} I_1^N T - \tau P^{(-1)} I_N^N = T^{-1} \left[I_1^N - \tau \tilde{B}^{(-1)} T I_N^N T^{-1} \right] T$$

thus becomes the crucial point. Since T and T^{-1} are orthogonal and the eigenvalues of I_1^N are obvious, we shall focus on the contribution appearing from the penalty term. The operator, $R^+ = T I_N^N T^{-1}$, has the entries

$$(28) \quad R_{ij}^+ = \frac{1}{\tilde{\gamma}_i} P_i^{(\alpha)}(1) P_j^{(\alpha)}(1) \omega_N,$$

and the entries of $S = \tilde{B}^{(-1)}R^+$ become

$$S_{ij} = \begin{cases} \alpha_1^{(1)}R_{N,j}^+ & i = 0, \\ b_{i,i-1}^{(1)}R_{i-1,j}^+ + b_{i,i+1}^{(1)}R_{i+1,j}^+ & i \in [1, N - 1], \\ b_{N,N-1}^{(1)}R_{N-1,j}^+ & i = N. \end{cases}$$

To continue beyond this point of the analysis we shall rely on the remarkable symmetries of the polynomial expansions. Indeed, for $i \in [1, N - 2]$, we utilize that

$$i \in [1, N - 2] : b_{i,i-1}^{(1)}R_{i-1,j}^+ + b_{i,i+1}^{(1)}R_{i+1,j}^+ = 0,$$

which appears as a result of the identity

$$(29) \quad b_{i,i-1}^{(1)} \frac{1}{\gamma_{i-1}} P_{i-1}^{(\alpha)}(\pm 1) + b_{i,i+1}^{(1)} \frac{1}{\gamma_{i+1}} P_{i+1}^{(\alpha)}(\pm 1) = 0,$$

as derived by combining (3), (6), and (16). Since, $\tilde{\gamma}_N \neq \gamma_N$ (equation (17)), we obtain a special row for $i = N - 1$ as

$$S_{ij} = \begin{cases} \alpha_1^{(1)}R_{N,j}^+ & i = 0, \\ 0 & i \in [1, N - 1], \\ b_{N-1,N-2}^{(1)}R_{N-2,j}^+ + b_{N-1,N}^{(1)}R_{N,j}^+ & i = N - 1, \\ b_{N,N-1}^{(1)}R_{N-1,j}^+ & i = N. \end{cases}$$

Considering the eigenvalues of the operator, $I_1^N - \tau S$, it is clear that at least $N - 2$ of the $N + 1$ eigenvalues are unity irrespective of the actual ultraspherical polynomial basis. Moreover, using a permutation matrix, the remaining three eigenvalues are recovered as the eigenvalues of a 3×3 matrix, $W^{(1)}$, with the entries

$$(30) \quad W^{(1)} = \begin{bmatrix} -\tau S_{0,0} & -\tau S_{0,N-1} & -\tau S_{0,N} \\ -\tau S_{N-1,0} & 1 - \tau S_{N-1,N-1} & -\tau S_{N-1,N} \\ -\tau S_{N,0} & -\tau S_{N,N-1} & 1 - \tau S_{N,N} \end{bmatrix}.$$

To arrive at a more complete understanding of these remaining three eigenvalues, let us consider the shifted operator, $W^{(1)} - I$, which is singular since the last two rows are linearly dependent as seen by introducing (28). Moreover, after bringing $W^{(1)} - I$ into block form using a similarity transform that eliminates row 3, the final two complex conjugate eigenvalues appear from a 2×2 matrix, $\tilde{W}^{(1)}$, the determinant of which is given as

$$|\tilde{W}^{(1)}| = \tau(\alpha + 1) \left[\frac{1}{(N + 2\alpha)(2N + 2\alpha + 1)} + \frac{1}{N(N + 2\alpha + 1)} \right].$$

The first thing to note is that the unknown factor, $\alpha_1^{(1)}$, does not appear in the determinant which we recall is equivalent to the product of the eigenvalues. Also, provided τ scales as N^2 , the determinant is asymptotically bounded and, consequently, the spectrum might also be bounded. Naturally, the actual value of the bound depends on the choice of τ and thus on the particular scheme, but the possibility of boundedness of the spectrum is a general result.

Making the quite reasonable choice of a purely real spectrum, we obtain that

$$\lambda_{1,2}(\tilde{W}^{(1)}) = \pm \sqrt{|\tilde{W}^{(1)}|},$$

while the actual value of $\alpha_1^{(1)}$ is obtained by using the trace of $\tilde{W}^{(1)}$ as

$$\alpha_1^{(1)} = -\frac{\tilde{\gamma}_N}{\tau P_N^{(\alpha)}(1)\omega_N} \left(|\tilde{W}^{(1)}|^2 + 1 \pm 2\sqrt{|\tilde{W}^{(1)}|} \right),$$

hence completing the specification of the preconditioner for the advective operator.

Due to their extensive use, let us consider the results of the general analysis for the case of Legendre- and Chebyshev-based approximations.

4.1. Analysis of the Legendre method. We first consider the Legendre–Gauss–Lobatto approximation, i.e., the weights at the endpoints, ω_0 and ω_N , are

$$(31) \quad \omega_0 = \omega_N = \frac{2}{N(N+1)}, \quad \tilde{\gamma}_i = \begin{cases} \frac{2}{2i+1} & i < N, \\ \frac{2}{N} & i = N, \end{cases}$$

while $\tilde{\gamma}_i$ refers to the discrete normalization factor, equation (17).

Following [10], we take

$$\tau = \frac{1}{2\omega_N} = \frac{N(N+1)}{4}$$

for stability and note that τ does indeed scale like N^2 , i.e., there is a possibility that the spectrum of the preconditioned advective operator is bounded in N .

Utilizing the general results derived above in the special case of $\alpha = 0$, yields a spectrum with $N - 1$ unit eigenvalues while the remaining two take the value of

$$(32) \quad \lambda_{1,2} = 1 + \sqrt{\frac{3N+2}{4(2N+1)}},$$

assuming that the free parameter, $\alpha_1^{(1)}$, in the preconditioner is specified as

$$\alpha_1^{(1)} = -\frac{1}{N(2N+1)} \left[11N + 6 + \sqrt{16(2N+1)(3N+2)} \right].$$

The spectral radius is uniformly bounded as

$$\lim_{N \rightarrow 1} \lambda_{1,2} = 1 + \sqrt{\frac{5}{12}}, \quad \lim_{N \rightarrow \infty} \lambda_{1,2} = 1 + \sqrt{\frac{3}{8}}$$

and decays monotonically in N . Thus, the spectrum of the preconditioned operator is uniformly bounded as

$$\lambda \left(P^{(-1)} \left[D^{(1)} - \tau I_N^N \right] \right) \in \left[1, 1 + \sqrt{\frac{5}{12}} \right].$$

Moreover, $N - 1$ of the $N + 1$ eigenvalues are unity while the remaining two eigenvalues are real, equal, and given by (32).

4.2. Analysis of the Chebyshev method. The analysis for the Chebyshev–Gauss–Lobatto approximation follow the same route as the aforementioned. The weights at the endpoints, ω_0 and ω_N , and the normalizing constant, $\tilde{\gamma}_i$, are given by

$$(33) \quad \omega_0 = \omega_N = \frac{\pi}{2N}, \quad \tilde{\gamma}_i = \bar{c}_i \frac{\pi}{2},$$

where $\bar{c}_0 = \bar{c}_N = 2$ and $\bar{c}_i = 1$, otherwise.

Following [10], the penalty parameter is taken as

$$\tau = \frac{N^2}{2},$$

for stability, implying that the spectrum contains $N - 1$ unit eigenvalues while the remaining two eigenvalues are

$$(34) \quad \lambda_{1,2} = 1 + \sqrt{\frac{3N - 2}{8(N - 1)}},$$

provided only that the free parameter, $\alpha_1^{(1)}$, in the preconditioner is taken to be

$$\alpha_1^{(1)} = -\frac{1}{2N(N - 1)} \left[11N - 10 + \sqrt{32(N - 1)(3N - 2)} \right].$$

Note that these expressions are only valid for $N > 1$, the reason being that the entries of $W^{(1)}$ would be slightly changed for $N = 1$ as a result of (13). However, the case of $N = 1$ hardly deserves a special analysis as no preconditioning is needed in this case.

Indeed, we recover a spectrum with asymptotic bounds as in the case of Legendre methods since

$$\lim_{N \rightarrow 2} \lambda_{1,2} = 1 + \frac{1}{\sqrt{2}}, \quad \lim_{N \rightarrow \infty} \lambda_{1,2} = 1 + \sqrt{\frac{3}{8}}.$$

Hence, the spectrum of the preconditioned operator is uniformly bounded as

$$\lambda \left(P^{(-1)} \left[D^{(1)} - \tau I_N^N \right] \right) \in \left[1, 1 + \frac{1}{\sqrt{2}} \right],$$

with $N - 1$ of the $N + 1$ eigenvalues being unity while the remaining two eigenvalues are equal, real and given by (34).

5. Preconditioning of the diffusive operator. Contrary to the situation for the advective operator, we shall need to discuss the effect of a number of different types of boundary conditions, e.g., Dirichlet, Neumann, or combinations thereof, when considering preconditioning of the second-order operator. We shall, however, restrict the subsequent analysis to Dirichlet and Neumann boundary conditions only as they represent the most frequently appearing cases. The general framework may likewise be applied to develop and analyze integration preconditioners for problems involving Robin boundary conditions.

5.1. The Dirichlet problem. Let us consider the homogeneous elliptic problem

$$(35) \quad \frac{d^2 u(x)}{dx^2} = f(x), \quad u(\pm 1) = 0,$$

and seek solutions of polynomial form leading to a discrete form of (35) as

$$(36) \quad D^{(2)}\mathbf{u} = \mathbf{f}, \quad u(\pm 1) = 0,$$

where \mathbf{u} and \mathbf{f} refer to the vectors of $u(x)$ and $f(x)$ at the Gauss-Lobatto quadrature points.

Following the development of the preconditioner for the advection operator, we impose boundary conditions weakly through a penalty term as

$$(37) \quad \left[D^{(2)} - \tau^- I_0^0 - \tau^+ I_N^N \right] \mathbf{u} = \mathbf{f},$$

where τ^- and τ^+ refer to the penalty parameters at -1 and 1 , respectively, and are chosen such that the resulting operator is negative definite [10].

Applying the preconditioner, $P^{(-2)}$, yields

$$\left[T^{-1} I_2^N T - \tau^- P^{(-2)} I_0^0 - \tau^+ P^{(-2)} I_N^N \right] \mathbf{u} = P^{(-2)} \mathbf{f},$$

implying that the spectrum of the preconditioned operator is similar to that of

$$I_2^N - \tau^- \tilde{B}^{(-2)} T I_0^0 T^{-1} - \tau^+ \tilde{B}^{(-2)} T I_N^N T^{-1} = I_2^N - \tau^- \tilde{B}^{(-2)} R^- - \tau^+ \tilde{B}^{(-2)} R^+.$$

Here we have introduced the matrix $R^- = T I_0^0 T^{-1}$ with the entries

$$(38) \quad R_{ij}^- = \frac{1}{\tilde{\gamma}_i} P_i^{(\alpha)}(-1) P_j^{(\alpha)}(-1) \omega_0,$$

while R^+ is defined in equation (28).

Let us now for simplicity take $\tau^- = \tau^+ = \tau$, which is indeed a valid assumption as we shall see shortly, and introduce the operator $S = \tilde{B}^{(-2)}(R^- + R^+) = \tilde{B}^{(-2)}R$, having the entries

$$(39) \quad S_{ij} = \begin{cases} \alpha_{11}^{(2)} R_{N-1,j} + \alpha_{12}^{(2)} R_{N,j} & i = 0, \\ \alpha_{21}^{(2)} R_{N-1,j} + \alpha_{22}^{(2)} R_{N,j} & i = 1, \\ 0 & i \in [2, N-3], \\ b_{i,i-2}^{(2)} R_{i-2,j} + b_{i,i}^{(2)} R_{i,j} + b_{i,i+2}^{(2)} R_{i+2,j} & i = N-2, \\ b_{i,i-2}^{(2)} R_{i-2,j} + b_{i,i}^{(2)} R_{-i,j} & i = N-1, N, \end{cases}$$

where

$$(40) \quad R_{ij} = \frac{1}{\tilde{\gamma}_i} P_i^{(\alpha)}(1) P_j^{(\alpha)}(1) \omega \times \begin{cases} 2 & i + j \text{ even,} \\ 0 & i + j \text{ odd,} \end{cases}$$

with $\omega = \omega_0 = \omega_N$ in (18). The remarkable reduction in S follows from utilizing the definition of R along with (8), (3), and (16).

The spectrum of the preconditioned matrix,

$$(41) \quad I_2^N - \tau S,$$

consequently consists of at least $N - 4$ eigenvalues taking the exact value of unity. However, as for the advective operator we can rearrange the rows and columns of (41) to arrive at a 5×5 matrix of the form

$$W^{(2)} = \begin{bmatrix} -\tau S_{0,0} & -\tau S_{0,1} & -\tau S_{0,N-2} & -\tau S_{0,N-1} & -\tau S_{0,N} \\ -\tau S_{1,0} & -\tau S_{1,1} & -\tau S_{1,N-2} & -\tau S_{1,N-1} & -\tau S_{1,N} \\ -\tau S_{N-2,0} & -\tau S_{N-2,1} & 1 - \tau S_{N-2,N-2} & 0 & -\tau S_{N-2,N} \\ -\tau S_{N-1,0} & -\tau S_{N-1,1} & 0 & 1 - \tau S_{N-1,N-1} & 0 \\ -\tau S_{N,0} & -\tau S_{N,1} & -\tau S_{N,N-2} & 0 & 1 - \tau S_{N,N} \end{bmatrix},$$

the eigenvalues of which determine the remaining five eigenvalues. We note that due to the definition of R , equation (40), the details of the analysis depends on whether N is even or odd.

As for the advective operator we continue the analysis by shifting the spectrum as $W^{(2)} - I$ and find that the third and fifth rows are linearly dependent, i.e., $N - 3$ of the $N + 1$ eigenvalues are unity, while the remaining four eigenvalues appear as the spectrum of the 4×4 matrix, $\tilde{W}^{(2)}$, appearing as the upper block of the block-diagonalized operator $W^{(2)} - I$.

Computing the determinant, $|\tilde{W}^{(2)}|$, yields

$$(42) \quad \frac{4\tau^2(\alpha + 1)^2[N^2(N - 1) - 2\alpha(2\alpha + 3)(2N + 2\alpha + 1)]}{N(N + 2\alpha)^2(N + 2\alpha + 1)^2(N + 2\alpha - 1)(2N + 2\alpha + 1)^2(2N + 2\alpha + 3)},$$

with the asymptotic behavior

$$\lim_{N \rightarrow \infty} |\tilde{W}^{(2)}| = \tau^2 \frac{(\alpha + 1)^2}{2N^6}.$$

Hence, only for τ scaling at most like N^3 , can we hope to have a bounded spectrum. Note that this result is entirely independent of the choices of the free parameters, $\alpha_{ij}^{(2)}$, that enter the specification of the preconditioner, equation (24).

Let us consider the details of the eigenvalue spectrum for a few special choices of α , e.g., for Legendre- and Chebyshev-based schemes.

5.1.1. Analysis of the Legendre method. First consider the Legendre–Gauss–Lobatto approximation for which we recover that

$$(43) \quad S_{0,j} = \frac{2}{N(N + 1)} \left[\frac{\alpha_{11}^{(2)}}{\tilde{\gamma}_{N-1}} (1 - (-1)^{N+j}) + \frac{\alpha_{12}^{(2)}}{\tilde{\gamma}_N} (1 + (-1)^{N+j}) \right],$$

using (39), (31), and (9). Hence, the effect of $\alpha_{11}^{(2)}$ and $\alpha_{12}^{(2)}$ are decoupled and their individual action depends on whether N is even or odd. The same holds for $S_{1,j}$ since

$$(44) \quad S_{1,j} = \frac{2}{N(N + 1)} \left[\frac{\alpha_{21}^{(2)}}{\tilde{\gamma}_{N-1}} (1 - (-1)^{N+j}) + \frac{\alpha_{22}^{(2)}}{\tilde{\gamma}_N} (1 + (-1)^{N+j}) \right].$$

We shall exploit this decoupling of the unknown coefficients, $\alpha_{ij}^{(2)}$, by always taking two of the four coefficients to be zero. Indeed, we shall assume that $\alpha_{11}^{(2)} = \alpha_{22}^{(2)} = 0$ for N , even while we take $\alpha_{21}^{(2)} = \alpha_{12}^{(2)} = 0$ for N odd. The reason for this particular

choice lies in the ease by which we may obtain the eigenvalues of $W^{(2)}$ in analytic form. With this particular choice of $\alpha_{ij}^{(2)}$, $W^{(2)}$ reduces to a sparse matrix with a checkerboard structure. This allows for restructuring, using permutation operators, into block-diagonal form, consisting of a 3×3 block and a 2×2 block, a scenario that can be dealt with in a simple fashion. While the assumption that two of the four parameters, $\alpha_{ij}^{(2)}$, take the value zero may seem restrictive, it does not pose any restrictions on the performance of the preconditioners as we shall see shortly.

Following [10] we choose the penalty parameter, $\tau = \tau^+ = \tau^-$, as

$$\tau = \frac{1}{4c\omega^2} = \frac{N^2(N+1)^2}{16c},$$

where $c > 0$ is a constant. According to [10] we should use $c = 1$. However, extensive computational results showed that $c = 4$ guarantees that the spectrum remains in the negative half-plane. The actual value, however, is less important at this point of the analysis.

Let us now analyze the spectrum of the preconditioned operator for N even, i.e., we seek $\alpha_{12}^{(2)}$ and $\alpha_{21}^{(2)}$ such as to minimize the spectral radius of $\tilde{W}^{(2)}$ and, hence, (41). The spectrum of $\tilde{W}^{(2)}$ consists of two pairs of complex conjugate eigenvalues, $\lambda_{1,2}(\tilde{W}^{(2)})$ and $\lambda_{3,4}(\tilde{W}^{(2)})$, where the former is a function of $\alpha_{21}^{(2)}$ only, while the latter depends on $\alpha_{12}^{(2)}$ only.

If we attempt to identify $\alpha_{21}^{(2)}$ and $\alpha_{12}^{(2)}$ such that $\lambda_{1,2}(\tilde{W}^{(2)})$ and $\lambda_{3,4}(\tilde{W}^{(2)})$ cluster pairwise, we find

$$\alpha_{12}^{(2)} = \frac{N^3 - (32c - 1)N^2 - 8c(8N + 3)}{N^2(N + 1)(2N + 1)(2N + 3)} \pm i\sqrt{\frac{32c}{N^2(N + 1)(2N + 1)(2N + 3)}},$$

and

$$\alpha_{21}^{(2)} = \frac{N^2 - (16c - 1)N - 8c}{N(N + 1)(2N + 1)(2N - 1)} \pm i\sqrt{\frac{32c(2N + 1)}{N(N + 1)(4N^2 - 1)^2}}.$$

At first, this seems a rather discouraging result as the optimal values of both parameters are complex, i.e., the preconditioner, $P^{(-2)}$, becomes complex, which certainly is undesirable. To avoid this complication we rely on the observation that the imaginary part of $\alpha_{ij}^{(2)}$ is about \sqrt{N} smaller than the real part, i.e., using only the real part yields a good asymptotic approximation. Thus, for N even we choose the parameters in $P^{(-2)}$ as

$$\alpha_{11}^{(2)} = 0, \quad \alpha_{12}^{(2)} = \frac{1}{(2N + 1)(2N + 3)} - \frac{8c}{N^2(N + 1)},$$

$$\alpha_{21}^{(2)} = \frac{1}{(2N - 1)(2N + 1)} - \frac{8c}{N(N + 1)(2N - 1)}, \quad \alpha_{22}^{(2)} = 0.$$

This yields the remaining four purely real eigenvalues of (41) on the form

$$(45) \quad \lambda_{1,2} = 1 \pm \sqrt{\frac{N(N + 1)}{8c(2N + 1)}}, \quad \lambda_{3,4} = 1 \pm \sqrt{\frac{N^2(N + 1)}{8c(2N + 1)(2N + 3)}}.$$

We observe that the spectrum no longer remains bounded in N , as we saw in section 4, but grows with \sqrt{N} and becomes indefinite for some value of N depending on the

actual value of c , e.g., for $c = 4$ the maximum eigenvalue crosses 0 for $N \simeq 64$. One could naturally speculate whether the particular pattern of $\alpha_{ij}^{(2)}$ chosen here is at fault and if a more general analysis would yield a bounded spectrum. However, computing

$$|\tilde{W}^{(2)}| = \frac{N^3(N+1)^2}{64c^2(2N+1)^2(2N+3)}$$

helps us settle this point. We find that the determinant scales as N^2 , i.e., the optimal asymptotic behavior of the spectrum we can hope for is indeed \sqrt{N} . Moreover, the optimal behavior within the present framework appears for a spectrum scaling as

$$\lim_{N \rightarrow \infty} \lambda = 1 \pm \frac{1}{4} \sqrt{\frac{N}{\sqrt{2c}}},$$

which is very close to the behavior of $\lambda_{1,2}$ and confirms the asymptotic optimality of the preconditioners.

For N odd we recover the exact same spectrum, (45), when $\alpha_{ij}^{(2)}$ is given as

$$(46) \quad \alpha_{11}^{(2)} = \frac{1}{(2N-1)(2N+1)} - \frac{8c}{N(N+1)(2N-1)}, \quad \alpha_{12}^{(2)} = 0,$$

$$(47) \quad \alpha_{21}^{(2)} = 0, \quad \alpha_{22}^{(2)} = \frac{1}{(2N+1)(2N+3)} - \frac{8c}{N^2(N+1)}.$$

5.1.2. Analysis of the Chebyshev method. Let us also consider the behavior of the preconditioned second-order differentiation matrix, (41), based on the Chebyshev–Gauss–Lobatto grid. Using (39), (33), and (12), we realize that the entries of $S_{0,j}$ and $S_{1,j}$ share the properties discussed in regard to equations (43)–(44).

Following [10] we choose the penalty parameter, $\tau = \tau^+ = \tau^-$, as

$$\tau = \frac{N^4}{4c},$$

where $c > 0$ is a constant. According to [10] we should use $c = 1$. However, extensive computational results have shown that even for $c = 12.5$ does the spectrum remain in the negative half-plane. The actual value, however, is less important at this point of the analysis.

As was the case for the Legendre-based approximation, choosing $\alpha_{ij}^{(2)}$ in order to minimize the spectral radius results in generally complex results, however, with an imaginary part that is \sqrt{N} smaller than the real part. Thus, neglecting the imaginary part yields a purely real preconditioner.

Hence, for N even the parameters, $\alpha_{ij}^{(2)}$, entering $P^{(-2)}$ should be

$$\alpha_{11}^{(2)} = 0, \quad \alpha_{12}^{(2)} = \frac{N^2 - N + 4}{4N(N^2 - 1)(N - 2)} - \frac{4c}{N^3},$$

$$\alpha_{21}^{(2)} = \frac{1}{4N(N - 1)} - \frac{2c}{N^3}, \quad \alpha_{22}^{(2)} = 0.$$

This yields the remaining four real eigenvalues of the preconditioned operators as

$$\lambda_{1,2} = 1 \pm \sqrt{\frac{N^2}{8c(N-1)}}, \quad \lambda_{3,4} = 1 \pm \sqrt{\frac{N^2(N^2 - N + 4)}{16c(N+1)(N-1)(N-2)}}.$$

As for the preconditioned Legendre operator, the spectral radius grows like \sqrt{N} , at some point making the preconditioned operator indefinite, e.g., for $c = 12.5$ as advocated in [10] the matrix becomes indefinite for $N \simeq 100$. However, from (42) we obtain

$$|\tilde{W}^{(2)}| = \frac{N^4(N^2 - N + 4)}{128c^2(N + 1)(N - 1)^2(N - 2)},$$

confirming that the \sqrt{N} -behavior is the best asymptotic behavior we can hope for within the present framework.

For N odd, we recover the same spectrum by choosing $\alpha_{ij}^{(2)}$ as

$$\alpha_{11}^{(2)} = \frac{1}{4N(N - 1)} - \frac{2c}{N^3}, \quad \alpha_{12}^{(2)} = 0,$$

$$\alpha_{21}^{(2)} = 0, \quad \alpha_{22}^{(2)} = \frac{N^2 - N + 4}{4N(N^2 - 1)(N - 2)} - \frac{4c}{N^3}.$$

5.2. The Neumann problem. Consider finally the problem of preconditioning of the Poisson problem subject to Neumann conditions as

$$(48) \quad \frac{d^2u(x)}{dx^2} = f(x), \quad \left. \frac{du}{dx} \right|_{\pm 1} = 0.$$

We seek solutions of polynomial form as

$$(49) \quad D^{(2)}\mathbf{u} = \mathbf{f}, \quad D^{(1)}\mathbf{u}(\pm 1) = 0,$$

where \mathbf{u} and \mathbf{f} represent the vectors of $u(x)$ and $f(x)$ at the Gauss–Lobatto points.

Enforcing the boundary conditions only weakly yields

$$(50) \quad \left[D^{(2)} + \tau^- I_0^0 D^{(1)} - \tau^+ I_N^N D^{(1)} \right] \mathbf{u} = \mathbf{f},$$

where τ^- and τ^+ refer to the penalty parameters at -1 and 1 , respectively, and are chosen to ensure that the discrete operator is negative semidefinite [10]. Note the sign difference in the penalty term as compared to the case of Dirichlet boundary conditions, equation (37). For simplicity we shall assume that $\tau^- = \tau^+ = \tau$ in the subsequent analysis. As we shall see shortly, this is a reasonable choice.

Applying the preconditioner, $P^{(-2)}$, we obtain

$$\left[T^{-1} I_2^N T - \tau P^{(-2)} (-I_0^0 + I_N^N) D^{(1)} \right] \mathbf{u} = P^{(-2)} \mathbf{f},$$

with a spectrum being similar to that of

$$(51) \quad I_2^N - \tau \tilde{B}^{(-2)} \tilde{R} = I_2^N - \tau \tilde{S}.$$

Here we have introduced $\tilde{R} = T (-I_0^0 + I_N^N) D^{(1)} T^{-1}$ with the entries

$$(52) \quad \tilde{R}_{ij} = \frac{1}{\gamma_i} P_i^{(\alpha)}(1) \frac{dP_j^{(\alpha)}(1)}{dx} \omega \times \begin{cases} 2 & i + j \text{ even,} \\ 0 & i + j \text{ odd,} \end{cases}$$

where $\omega = \omega_0 = \omega_N$ in (18). These simple expressions appear as a result of

$$\begin{aligned} \left(D^{(1)}T^{-1}\right)_{ij} &= \sum_{k=0}^N \left(D^{(1)}\right)_{ik} \left(T^{-1}\right)_{kj} = \sum_{k=0}^N P_j^{(\alpha)}(x_k)\omega_k \sum_{n=0}^N \frac{1}{\tilde{\gamma}_n} P_n^{(\alpha)}(x_k) \frac{dP_n^{(\alpha)}(x_i)}{dx} \\ &= \sum_{n=0}^N \frac{dP_k^{(\alpha)}(x_i)}{dx} \left(\frac{1}{\tilde{\gamma}_n} \sum_{k=0}^N P_j^{(\alpha)}(x_k)P_n^{(\alpha)}(x_k)\omega_k\right) \\ &= \sum_{n=0}^N \frac{dP_n^{(\alpha)}(x_i)}{dx} \delta_{jn} = \frac{dP_j^{(\alpha)}(x_i)}{dx}, \end{aligned}$$

as quadrature is exact for the orthogonal polynomials.

Consequently, the definition of \tilde{S} is exactly as given in equation (39) with R being replaced with \tilde{R} and we immediately recover that the preconditioned Neumann problem has $N - 3$ of the $N + 1$ eigenvalues being exact unity. Moreover, since $\tilde{R}_{i0} = 0$, the first column of \tilde{S} is zero, thereby introducing a zero eigenvalue. This, however, is only natural as Neumann boundary conditions leave a constant undetermined when solving the Poisson equation. This zero column also implies that the value of the parameters $\alpha_{1j}^{(2)}$ has no influence on the spectrum and can be taken to be unity.

As in the previous cases the remaining three eigenvalues appear from $\tilde{W}^{(2)}$, the determinant of which is

$$(53) \quad |\tilde{W}^{(2)}| = \tau^2 \frac{(N - 1)(N^2 - 4N - 2\alpha N - 2(\alpha + 1)(2\alpha + 3))}{(N + 2\alpha)(N + 2\alpha + 1)(2N + 2\alpha + 1)^2(2N + 2\alpha + 3)}.$$

Hence, to hope for a bounded spectrum, we must have that τ scales as N . Unfortunately, this is, in general, not the case as we shall see in the following analysis.

5.2.1. Analysis of the Legendre method. Following [10] we choose τ as

$$\tau^- = \tau^+ = \frac{N(N + 1)}{2c},$$

where c may take values in the interval $[1 - 4]$.

Contrary to the case of Dirichlet boundary conditions, the details of the analysis are different depending on whether N is even or odd, although the general picture remains the same. For N even we find an optimal value for $\alpha_{21}^{(2)}$ as

$$\alpha_{21}^{(2)} = \frac{N(N - 1)}{2(4N^2 - 1)} - c \frac{2N + 1}{4N^2 - 1} \pm i \sqrt{\frac{2cN(N - 1)(2N + 1)}{(4N^2 - 1)^2}},$$

while $\alpha_{22}^{(2)}$ has no effect on the spectrum due to the structure of $\tilde{W}^{(2)}$ and can be taken to be zero. As in the case of Dirichlet boundary conditions the optimal value is complex. However, since the imaginary part is significantly smaller than the real part, we use the latter as the value of $\alpha_{21}^{(2)}$ to be included in $P^{(-2)}$. The final three eigenvalues of the preconditioned Neumann operator appear as

$$\lambda_1 = 1 + \frac{(N + 1)(N^2 - 4N - 6)}{2c(2N + 1)(2N + 3)}, \quad \lambda_{2,3} = 1 \pm \sqrt{\frac{N(N - 1)}{2c(2N + 1)}}.$$

Hence, $N - 3$ of the $N + 1$ eigenvalues are exactly unity, and two eigenvalues, $\lambda_{2,3}$, grow like \sqrt{N} , one eigenvalue takes the value of zero while the spectral radius of the preconditioned operator, at least asymptotically, is dominated by one eigenvalue, λ_1 , growing like N . However, for moderate values of N , the three unbounded eigenvalues are of comparable value.

Computing the determinant, (53), as

$$|\tilde{W}^{(2)}| = \frac{N(N^2 - 1)(N^2 - 4N - 6)}{8c^2(2N + 1)^2(2N + 3)} \sim \frac{N^2}{64c^2},$$

confirms that we cannot expect to have a bounded spectrum. Moreover, since λ_1 is unaffected by the choice of $\alpha_{21}^{(2)}$, the spectrum given above is asymptotically optimal.

The situation for N odd is slightly more complicated, this being an effect of $\gamma_N \neq \tilde{\gamma}_N$. Nevertheless, proceeding as previously stated we obtain a value

$$\alpha_{22}^{(2)} = \frac{(N + 1)(2N + 1)(2N + 3)}{2N(2N + 1)(2N + 3)} - \frac{c}{N},$$

while $\alpha_{21}^{(2)}$ has no effect on the spectrum and is set to zero. This results in the remaining three eigenvalues being

$$\lambda_1 = 1 + \frac{N(N - 1)}{2c(2N + 1)}, \quad \lambda_{2,3} = 1 \pm \sqrt{\frac{(N + 1)(N^2 - 4N - 6)}{2c(2N + 1)(2N + 3)}},$$

i.e., a spectrum which shares the characteristics of the one obtained for N being even.

5.2.2. Analysis for the Chebyshev method. Let us finally consider the details of the preconditioner in the case of a Chebyshev–Gauss–Lobatto approximation of the Poisson equation subject to Neumann conditions. From [10] we recover that τ should be

$$\tau^- = \tau^+ = \frac{N^2}{c},$$

where c may take values in the interval $[1 - 12.5]$.

Following the above analysis we obtain for N even that the proper choice of $\alpha_{21}^{(2)}$ is given as

$$\alpha_{21}^{(2)} = \frac{N - 1}{4N} - \frac{c}{2N},$$

when neglecting the imaginary part, while $\alpha_{22}^{(2)} = 0$. This yields the remaining three eigenvalues as

$$\lambda_1 = 1 + \frac{N(N^2 - 3N - 2)}{4c(N^2 - 1)}, \quad \lambda_{2,3} = 1 \pm \sqrt{\frac{N - 1}{2c}},$$

i.e., a spectrum with characteristics very similar to Legendre–Gauss–Lobatto approximation. Also, computing the determinant, (53), confirms the asymptotic optimality of the preconditioner.

In the case of N odd, we find the optimal value of $\alpha_{22}^{(2)}$ to be

$$\alpha_{22}^{(2)} = \frac{N^2 - 3N - 2}{4(N^2 - 1)} - \frac{c}{N},$$

and $\alpha_{21}^{(2)} = 0$, completing the specification of the spectrum as

$$\lambda_1 = 1 + \frac{N-1}{2c}, \quad \lambda_{2,3} = 1 \pm \sqrt{\frac{N(N^2 - 3N - 2)}{4c(N^2 - 1)}}.$$

6. Concluding remarks and generalizations. The pseudospectral integration preconditioners presented in this paper are different from previously developed preconditioners for the pseudospectral differentiation operators in a number of ways. Rather than approximating the process of integration by inverting a low-order approximation to the operator, the integration operators are based on the properties of the polynomial basis itself. This generally makes the preconditioners full, which, however, is only natural as we are considering global methods. Moreover, imposing the boundary conditions weakly through a penalty term allows for a complete analysis of the preconditioner, revealing a highly clustered eigenvalue spectrum appearing from a very low rank modification of the identity operator. We were also able to show the asymptotic optimality of the proposed family of preconditioners.

The most appealing feature of the basic approach, however, is its degree of generality. Our framework relies on the use of ultraspherical polynomials, including such prominent members as the Legendre and Chebyshev polynomials, for constructing the approximate solutions at the Gauss–Lobatto quadrature points.

The general framework, however, remains valid within a much wider context. Recall that the integration preconditioners are a consequence of the three-term recurrence relations, (5). Hence, integration preconditioners may be defined for any of the classical orthogonal polynomials, e.g., Jacobi, Laguerre, and Hermite polynomials. Moreover, the choice of Gauss–Lobatto quadrature points may be relaxed to include approximations based on Gauss or Gauss–Radau quadrature points. If we again return to the heart of the development of the preconditioner, (5), and the second-order recurrence, (7), it is clear that similar recurrence formulas, e.g., the relation between the polynomials and their fourth-order derivatives, can be established to arrive at the integration preconditioner for the bi-harmonic operator. Certainly, this process can be repeated for any order operator under consideration. Also, the spectrum of the preconditioned p th-order operator appears as a rank $2p$ perturbation of the identity operator, independent of N and irrespective of the type of boundary condition, which can be of arbitrary form as the enforcement through the penalty term is straightforward.

Nevertheless, several important issues require further study in order to establish the usefulness of the pseudospectral integration preconditioners within a more general context. Issues like the analysis and performance of the integration preconditioners for mixed operators, e.g., the advection-diffusion operator, and time-dependent problems leading to preconditioning of the Helmholtz-operator, remains open. However, based on the results quoted in [7] for the spectral case, we expect that the development of integration preconditioners can be successfully extended to deal with these important cases also. The same can be said for multidimensional extensions where the combination of a tensor product formulation with the penalty method supplies the proper framework in which one can expect the one-dimensional results to carry over. We hope to pursue these important questions in the very near future.

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