

1                                   **A GENERIC AND STRICTLY BANDED SPECTRAL**  
2                                   **PETROV-GALERKIN METHOD FOR DIFFERENTIAL EQUATIONS**  
3                                   **WITH POLYNOMIAL COEFFICIENTS**

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5                   **Abstract.** In this paper we describe a generic spectral Petrov-Galerkin method that is sparse and  
6 strictly banded for any linear ordinary differential equation with polynomial coefficients. The method applies  
7 to all subdivisions of Jacobi polynomials (e.g., Chebyshev and Legendre), utilises well-known recurrence  
8 relations of orthogonal polynomials and leads to almost exactly the same discretized system of equations  
9 as the integration preconditioners (IP) [Coutsias et al., Math Comp, 65 (1996), 611–635], if this method  
10 was redesigned to make use of trial functions that satisfy a given problems boundary conditions. A link  
11 between the new Petrov-Galerkin method and IP is revealed through a new recursion relation for Jacobi  
12 polynomials. Because of the strictly banded nature of all coefficient matrices, the new method extends easily  
13 and efficiently to multiple dimensions though the use of tensor product methods.

14                   **1. Introduction.** Spectral methods are widespread in most branches of natural sci-  
15 ences, with several books dedicated entirely to the subject [3, 35, 16, 5, 22, 19]. Spectral  
16 methods are favoured by scientists aiming at ultimate accuracy in as few degrees of freedom  
17 as possible, making them particularly successful in fields such as meteorology, turbulence,  
18 hydrodynamic stability, geophysical flows, stochastic differential equations and uncertainty  
19 quantifications. Common for these fields is that physical processes can be studied with high  
20 precision in simple Cartesian product domains, which is a requirement since global spectral  
21 methods can be difficult, or impossible, to apply to irregular domains. This disadvantage can  
22 sometimes be overcome by mapping a complex domain into a regular through an explicit,  
23 smooth [30], or a Gordon-Hall mapping [15], or, alternatively, by embedding the complex  
24 domain into a larger regular domain [18]. Still, the possibility of studying physical processes  
25 with extreme accuracy in very few degrees of freedom has always been attractive to scien-  
26 tists, and it has recently inspired the development of several spectral software frameworks  
27 [10, 28, 4, 26, 25].

28                   We will in this paper be interested in the global spectral methods that are referred  
29 to as spectral Galerkin, and more specifically spectral Petrov-Galerkin methods. These  
30 methods solve equations in spectral space, as opposed to collocation (or pseudospectral)  
31 methods [13] that solve equations in physical space. The Galerkin methods have a clean  
32 and elegant design, using variational principles and function spaces with built-in boundary  
33 conditions, that can be easily analysed. The Galerkin method is also easily implemented  
34 and automated, evidenced, e.g., by the large number of generic finite element software  
35 frameworks that have emerged in later years [1]. The Tau [24] method is quite closely  
36 related to spectral Galerkin, also solving equations in spectral space, but with a primary  
37 focus on finding spectral differentiation matrices in the orthogonal basis. The Tau and  
38 Galerkin methods differ the most in how the boundary conditions are specified. The Tau  
39 method enforces boundary conditions by modifying rows of the coefficient matrix, whereas  
40 Galerkin builds homogeneous boundary conditions into the basis functions, and adds non-  
41 homogeneous boundary conditions through additional lifting functions [2]. The Galerkin  
42 approach has the advantage that the coefficient matrices remain strictly banded regardless  
43 of boundary condition, whereas the Tau-matrices become *almost-banded*, see, e.g., [27].

44                   We will in this work limit ourselves to global spectral methods that make use of or-

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45 thogonal Jacobi polynomials  $P_n^{(\alpha,\beta)}(x)$  as basis functions. This includes both Chebyshev,  
 46 Legendre and all ultraspherical polynomials, but excludes Fourier exponentials and Her-  
 47 mite/Laguerre polynomials. Many efficient global methods for the Jacobi polynomials have  
 48 already been described, and most of these methods are based on ideas that date back to  
 49 Clenshaw [6] and Orzag [29], taking advantage of several recurrence relations that exist for  
 50 orthogonal polynomials. Of particular importance is the recurrence relation

$$51 \quad (1.1) \quad Q_n^{(\alpha)}(x) = b_{n-1,n} \frac{d}{dx} Q_{n-1}^{(\alpha)}(x) + b_{n+1,n} \frac{d}{dx} Q_{n+1}^{(\alpha)}(x),$$

52 for the ultraspherical polynomial  $Q_n^{(\alpha)}(x) \sim P_n^{(\alpha,\alpha)}(x)$ , where  $B = (b_{ij})$  is a matrix oper-  
 53 ator. The best global methods that are known to take advantage of recursions like (1.1),  
 54 are probably those based on integration reformulation [17, 36, 11], the related integration  
 55 preconditioner [8, 7, 23] or the ultraspherical approach [27, 4, 14]. With integration refor-  
 56 mulation the  $n$ 'th order differential equation is first integrated  $n$  times, before an integral  
 57 version of (1.1) is used on all lower order terms in the equation, leading to a banded lin-  
 58 ear system of equations (see, e.g., [36]). With integration preconditioners the matrix  $B$  of  
 59 the recurrence (1.1) is used explicitly as a preconditioner on the otherwise poorly condi-  
 60 tioned and full algebraic equations that are assembled for the Tau-method. The integration  
 61 preconditioners also make use of other recurrence relations and obtain sparse systems of  
 62 equations for linear differential equations with rational functions as coefficients, see [7]. The  
 63 ultraspherical approach [27] makes use of recurrence (1.1), but is somewhat camouflaged  
 64 into a correlation between Chebyshev polynomials of first  $T_k(x)$  and second  $U_k(x)$  kind,  
 65 see relation (2.8) given in [27]. Numerous other methods (e.g., [17, 14, 12]) rely on the  
 66 same recurrence relations, in one form or another. However, there has to the author's best  
 67 knowledge never been described a generic spectral Galerkin, or Petrov-Galerkin, method  
 68 for Jacobi polynomials that take systematic advantage of recurrence relations, and that can  
 69 match the sparsity of for example the integration preconditioners for variable coefficient  
 70 equations. For specific equations, boundary conditions and bases there are of course excep-  
 71 tions. Shen has suggested a sparse and efficient method with compact Legendre polynomials  
 72 [31], whereas Guo et al. [20] obtain sparse and efficient methods using generalized Jacobians.  
 73 Elbarbary [12] describe a sparse Petrov-Galerkin method with Chebyshev polynomials for  
 74 constant coefficient second-order equations subject to either Dirichlet or Neumann boundary  
 75 conditions.

76 In his seminal paper series on efficient direct solvers for the spectral-Galerkin method  
 77 [31, 32, 33, 34] Shen notes that *it is surprising that virtually no effort has been made to*  
 78 *construct appropriate bases for the spectral Galerkin method.* His recommended approach  
 79 is to use the most compact combinations of orthogonal basis functions that satisfy a given  
 80 problems boundary conditions, for both the identical test and trial spaces. However, this  
 81 does not always lead to sparse matrices, and in general it leads to algebraic problems that  
 82 require tailored solvers for efficiency. In this paper we intend to show that a  $k$ 'th order  
 83 linear differential equation with polynomial coefficients simply can use a basis with the very  
 84 specific test function

$$85 \quad (1.2) \quad \phi_n^{(k)}(x) = (1-x^2)^k \frac{d^k}{dx^k} P_{n+k}^{(\alpha,\beta)}(x), \quad n \geq 0, k > 0,$$

86 regardless of boundary conditions for the problem under investigation. We will then auto-  
 87 matically get a sparse and strictly banded Petrov-Galerkin method in the natural  $L_{\omega^{(\alpha,\beta)}}^2$

88 space, as long as the trial function is chosen compactly (basis recombination) from the nat-  
 89 ural basis  $\{P_n^{(\alpha,\beta)}\}$ . Furthermore, through a new recurrence relation we will show that such  
 90 a Petrov-Galerkin method will have a lot in common with the integration preconditioners  
 91 [8, 7], or the quasi-inverse [23] approach if restricted to constant coefficient equations and  
 92 Chebyshev polynomials.

93 This paper is outlined as follows: in Sec. 2 we present the necessary theory for Jacobi  
 94 and ultraspherical polynomials and a new recursion relation. In Sec. 3 we consider spectral  
 95 differentiation in the frequency space and show how a test function like (1.2) can simplify the  
 96 description considerably through a Petrov-Galerkin formulation. In Sec. 4 we present the  
 97 new and sparse Petrov-Galerkin method for linear differential equations with either constant  
 98 or polynomial coefficients. The extension to multiple dimensions is described briefly, and  
 99 some numerical examples are presented. Conclusions are drawn in Sec. 5

100 **2. Preliminaries.** In this section we introduce some necessary identities and recur-  
 101 rence relations for Jacobi polynomials. We will mainly be interested in ultraspherical poly-  
 102 nomials, like Legendre or Chebyshev, but the main results are applicable for any Jacobi  
 103 basis, which is why we find it natural to start here.

104 **2.1. Jacobi polynomials.** The Jacobi polynomials,  $P_n^{(\alpha,\beta)}(x)$ , are found as eigenso-  
 105 lutions to the Sturm-Liouville problem in the domain  $x \in [-1, 1]$ . The first two polynomials  
 106 are

$$107 \quad (2.1) \quad P_0^{(\alpha,\beta)} = 1, \quad P_1^{(\alpha,\beta)} = \frac{1}{2}(\alpha + \beta + 2)x + \frac{1}{2}(\alpha - \beta),$$

108 and the remaining can be found through the recurrence relation

$$109 \quad (2.2) \quad xP_n^{(\alpha,\beta)} = a_{n-1,n}^{(\alpha,\beta)}P_{n-1}^{(\alpha,\beta)} + a_{n,n}^{(\alpha,\beta)}P_n^{(\alpha,\beta)} + a_{n+1,n}^{(\alpha,\beta)}P_{n+1}^{(\alpha,\beta)},$$

110 where

$$111 \quad a_{n-1,n}^{(\alpha,\beta)} = \frac{2(n+\alpha)(n+\beta)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta)},$$

$$112 \quad (2.3) \quad a_{n,n}^{(\alpha,\beta)} = -\frac{\alpha^2 - \beta^2}{(2n+\alpha+\beta+2)(2n+\alpha+\beta)},$$

$$113 \quad a_{n+1,n}^{(\alpha,\beta)} = \frac{2(n+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+2)(2n+\alpha+\beta+1)}.$$

115 The two parameters  $\alpha$  and  $\beta$  are both real numbers  $> -1$ , and the boundary values of the  
 116 Jacobi polynomials can be found as

$$117 \quad (2.4) \quad P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}, \quad P_n^{(\alpha,\beta)}(-1) = (-1)^n \binom{n+\beta}{n}.$$

118 In matrix form we will write

$$119 \quad (2.5) \quad x\mathbf{P} = A^T\mathbf{P},$$

120 for the infinite-dimensional matrix operator  $A^{(\alpha,\beta)} = (a_{mn}^{(\alpha,\beta)})_{m,n=0}^\infty$  and the column vector  
 121  $\mathbf{P}^{(\alpha,\beta)} = (P_0^{(\alpha,\beta)}, P_1^{(\alpha,\beta)}, \dots)^T$ . Note that if the parameters are simply  $(\alpha, \beta)$ , and it is

122 possible to avoid confusion, then we will simply omit the superscript from the matrix and  
 123 vector operators, like in Eq. (2.5).

124 If we multiply (2.5) by  $x^{q-1}$ , for integer  $q > 0$ , and then use the original (2.5)  $q - 1$   
 125 times on the right hand side, we get a nested recursion

$$126 \quad (2.6) \quad x^q \mathbf{P} = (A^q)^T \mathbf{P},$$

127 where  $A^q = (a_{mn}^{(q)})_{m,n=0}^\infty$  is the  $q$ 'th matrix power of  $A$ .

128 For integer  $k > 0$  the  $k$ 'th derivative of  $P_n^{(\alpha,\beta)}$  with respect to  $x$  is known to be [35]

$$129 \quad (2.7) \quad \partial^k P_n^{(\alpha,\beta)} = \psi_n^{(k,\alpha,\beta)} P_{n-k}^{(\alpha+k,\beta+k)}, \quad n \geq k,$$

130 where  $\partial^k$  is conveniently used to represent the ordinary derivative  $\frac{d^k}{dx^k}$ , and

$$131 \quad (2.8) \quad \psi_n^{(k,\alpha,\beta)} = \frac{(n + \alpha + \beta + 1)_k}{2^k},$$

132 using the Pochhammer symbol  $(\alpha)_k = \Gamma(\alpha + k)/\Gamma(\alpha)$ .

133 The Jacobi polynomials also satisfy a recurrence relation of the form

$$134 \quad (2.9) \quad P_n^{(\alpha,\beta)} = b_{n-1,n}^{(\alpha,\beta)} \partial P_{n-1}^{(\alpha,\beta)} + b_{n,n}^{(\alpha,\beta)} \partial P_n^{(\alpha,\beta)} + b_{n+1,n}^{(\alpha,\beta)} \partial P_{n+1}^{(\alpha,\beta)},$$

135 or

$$136 \quad (2.10) \quad \mathbf{P} = B^T \partial \mathbf{P},$$

137 where the matrix operator  $B = (b_{mn}^{(\alpha,\beta)})_{m,n=0}^\infty$ ,  $\partial \mathbf{P} = (0, \partial P_1^{(\alpha,\beta)}, \partial P_2^{(\alpha,\beta)}, \dots)^T$  and

$$138 \quad (2.11) \quad b_{n-1,n}^{(\alpha,\beta)} = -\frac{a_{n-1,n}^{(\alpha,\beta)}}{n + \alpha + \beta}, \quad b_{n,n}^{(\alpha,\beta)} = -\frac{2a_{n,n}^{(\alpha,\beta)}}{\alpha + \beta}, \quad b_{n+1,n}^{(\alpha,\beta)} = \frac{a_{n+1,n}^{(\alpha,\beta)}}{n + 1}.$$

139 Note that negative indices into the matrix components are here and throughout treated by  
 140 setting the component to zero.

141 Higher order derivatives satisfy (see Eq. (11) [7])

$$142 \quad (2.12) \quad \partial^{k-l} \mathbf{P} = (B^l)^T \partial^k \mathbf{P},$$

143 where  $0 < l \leq k$ , and the first  $k$  items of the vector  $\partial^k \mathbf{P}$  are 0. Note that the bandwidth of  
 144 the matrix  $B^l$  is  $\leq 1 + 2l$ , see [7].

145 The Jacobi polynomials  $\mathbf{P}_N^{(\alpha,\beta)} = (P_0^{(\alpha,\beta)}, P_1^{(\alpha,\beta)}, \dots, P_N^{(\alpha,\beta)})^T$  form an orthogonal basis  
 146 in  $L^2_{\omega^{(\alpha,\beta)}}[-1, 1]$  for  $P_N$ , which is the set of polynomials of degree less than or equal to  $N$ .

147 The weight  $\omega^{(\alpha,\beta)} = (1 - x)^\alpha (1 + x)^\beta$ , and we have

$$148 \quad \left( P_n^{(\alpha,\beta)}, P_m^{(\alpha,\beta)} \right)_{\omega^{(\alpha,\beta)}} = \int_{-1}^1 P_n^{(\alpha,\beta)} P_m^{(\alpha,\beta)} \omega^{(\alpha,\beta)} dx,$$

$$149 \quad (2.13) \quad = h_m^{(\alpha,\beta)} \delta_{mn},$$

151 where  $\delta_{mn}$  is the Kronecker delta-function and

$$152 \quad (2.14) \quad h_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}}{(2n + \alpha + \beta + 1)n!} \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)}{\Gamma(n + \alpha + \beta + 1)}.$$

153 Using (2.7) in (2.13) we find that the  $k$ 'th derivatives of the Jacobi polynomials are orthog-  
154 onal with respect to  $\omega^{(\alpha+k, \beta+k)}$

$$155 \quad (2.15) \quad \left( \partial^k P_{n+k}^{(\alpha, \beta)}, \partial^k P_{m+k}^{(\alpha, \beta)} \right)_{\omega^{(\alpha+k, \beta+k)}} = h_{m+k}^{(k, \alpha, \beta)} \delta_{m+k, n+k}, \quad \text{for } m, n \geq 0,$$

156 where

$$157 \quad (2.16) \quad h_n^{(k, \alpha, \beta)} = h_{n-k}^{(\alpha+k, \beta+k)} \left( \psi_n^{(k, \alpha, \beta)} \right)^2.$$

158 This result is also derived in [35], and it is the key to the sparse spectral Galerkin methods  
159 discussed in the current paper. Note that  $h_n^{(k, \alpha, \beta)} = 0$  for  $n < k$ , and for simplicity we  
160 use  $h_n^{(\alpha, \beta)} = h_n^{(0, \alpha, \beta)}$ . In matrix form we will use the diagonal matrix operators  $H =$   
161  $\text{diag}(h_0^{(\alpha, \beta)}, h_1^{(\alpha, \beta)}, \dots)$  and  $H^{(k)} = \text{diag}(h_0^{(k, \alpha, \beta)}, h_1^{(k, \alpha, \beta)}, \dots)$ , where the first  $k$  rows and  
162 columns of the matrix  $H^{(k)}$  are 0.

163 Since  $\partial^k \mathbf{P}$  are orthogonal polynomials they will also satisfy a three-term recurrence  
164 relation like (2.5), when multiplied by  $x$ . The relation is easily obtained by inserting for  
165 (2.7) in (2.5)

$$166 \quad (2.17) \quad x \partial^k P_n^{(\alpha, \beta)} = \sum_{m=n-1}^{n+1} \underline{a}_{mn}^{(k, \alpha, \beta)} \partial^k P_m^{(\alpha, \beta)},$$

167 where the nonzero components of the tri-diagonal matrix operator  $\underline{a}_{mn}^{(k, \alpha, \beta)}$  are

$$168 \quad (2.18) \quad \underline{a}_{m+k, n+k}^{(k, \alpha, \beta)} = \left( \psi_{m+k}^{(k, \alpha, \beta)} \right)^{-1} a_{mn}^{(\alpha+k, \beta+k)} \psi_{n+k}^{(k, \alpha, \beta)}, \quad \forall m, n \geq 0.$$

169 In matrix form we get

$$170 \quad (2.19) \quad x \partial^k \mathbf{P} = \underline{\mathbf{A}}^T \partial^k \mathbf{P},$$

171 where  $\underline{\mathbf{A}}^{(k, \alpha, \beta)} = (\underline{a}_{mn}^{(k, \alpha, \beta)})_{m, n=0}^{\infty}$  has both the first  $k$  columns and rows equal to 0. Multi-  
172 plying (2.19) by  $x^{q-1}$ , for integer  $q > 0$ , and recursively using (2.19) on the right hand side  
173 leads to

$$174 \quad (2.20) \quad x^q \partial^k P_n^{(\alpha, \beta)} = \sum_{m=n-q}^{n+q} \underline{a}_{mn}^{(k, q, \alpha, \beta)} \partial^k P_m^{(\alpha, \beta)},$$

175 where  $\underline{a}_{mn}^{(k, q, \alpha, \beta)}$  is a component of the  $q$ 'th matrix power of  $\underline{\mathbf{A}}^{(k, \alpha, \beta)}$ . Note that  $\mathbf{A}^{(\alpha, \beta)} =$   
176  $\underline{\mathbf{A}}^{(0, \alpha, \beta)}$ .

177 Using the recursion relations above together with the orthogonality (2.15) we can obtain  
178 three important inner products in  $L^2_{\omega^{(\alpha+k, \beta+k)}}[-1, 1]$  for the Jacobi polynomials

$$179 \quad (2.21) \quad \left( \partial^{k-l} P_n, \partial^k P_m \right)_{\omega^{(\alpha+k, \beta+k)}} = h_m^{(k)} b_{mn}^{(l)},$$

$$180 \quad (2.22) \quad \left( \partial^k P_n, x^q \partial^k P_m \right)_{\omega^{(\alpha+k, \beta+k)}} = h_m^{(k)} \underline{a}_{mn}^{(k, q)},$$

$$181 \quad (2.23) \quad \left( \partial^{k-l} P_n, x^q \partial^k P_m \right)_{\omega^{(\alpha+k, \beta+k)}} = \sum_{s=m-q}^{m+q} h_m^{(k)} \underline{a}_{ms}^{(k, q)} b_{sn}^{(l)},$$

182

183 where the  $(\alpha, \beta)$  superscript has been dropped for simplicity. Also, we have used the trans-  
184 pose equality

$$185 \quad (2.24) \quad h_n^{(k)} \underline{a}_{nm}^{(k,q)} = h_m^{(k)} \underline{a}_{mn}^{(k,q)},$$

186 which follows since  $(\partial^k P_n, x^q \partial^k P_m)_{\omega(\alpha+k, \beta+k)} = (x^q \partial^k P_n, \partial^k P_m)_{\omega(\alpha+k, \beta+k)}$ . Equation (2.21)  
187 follows by inserting for  $\partial^{k-l} P_n$  on the left hand side using (2.12), and then forming the right  
188 hand side using (2.15). Equation (2.22) follows by combining (2.20) and (2.15), whereas  
189 (2.23) follows by using (2.20) and (2.21). The bandwidth of (2.21) is  $1+2l$ , of (2.22)  $1+2q$ ,  
190 and of (2.23) it is  $1+2(q+l)$ . Note that Eq. (2.23) is a generic form that simplifies to Eq.  
191 (2.22) for  $l=0$ , Eq. (2.21) for  $q=0$ , Eq. (2.15) for  $l=q=0$ , and (2.13) for  $k=l=q=0$ .  
192 The matrix components on the right hand side are then simplified by using that the zeroth  
193 matrix power equals the identity matrix.

194 Finally, we introduce in Lemma (2.1) a new recursion relation that will be heavily  
195 utilized in this paper.<sup>1</sup>

196 LEMMA 2.1. *The Jacobi polynomials satisfy the recursion relation*

$$197 \quad (2.25) \quad (1-x^2)^k \partial^k \mathbf{P} = (C^{(k)})^T \mathbf{P},$$

198 where  $(C^{(k)})^T = H^{(k)} B^k H^{-1}$  for integer  $k > 0$ .

199 *Proof.* We first write the relation in index form as

$$200 \quad (2.26) \quad (1-x^2)^k \partial^k P_m = \sum_{s=m-k}^{m+k} h_m^{(k)} b_{ms}^{(k)} h_s^{-1} P_s, \quad m \geq 0.$$

201 The relation is obviously true for  $0 \leq m < k$  since both sides are then zero. It is also obvious  
202 that both sides of the equation have the same polynomial order  $m+k$  for any given  $m \geq k$ .  
203 Hence we can write the left hand side as an expansion in Jacobi polynomials

$$204 \quad (2.27) \quad (1-x^2)^k \partial^k P_m = \sum_{s=0}^{m+k} c_{sm}^{(k)} P_s, \quad m \geq k,$$

205 for some matrix  $C^{(k)}$  with upper bandwidth  $k$ . In order to show that  $c_{sm}^{(k)} = h_m^{(k)} b_{ms}^{(k)} h_s^{-1}$  we  
206 take the weighted inner product of (2.27) with  $P_n$ , for  $n \geq 0$

$$207 \quad (P_n, (1-x^2)^k \partial^k P_m)_{\omega(\alpha, \beta)} = \sum_{s=0}^{m+k} (P_n, c_{sm}^{(k)} P_s)_{\omega(\alpha, \beta)}.$$

208 The inner product on the left is given by (2.21) with  $k=l$ , and the right hand side can be  
209 simplified using (2.15)

$$210 \quad h_m^{(k)} b_{mn}^{(k)} = \sum_{s=0}^{m+k} c_{sm}^{(k)} h_s \delta_{ns}.$$

212 A final step sets necessarily  $s=n$  and hence  $c_{nm}^{(k)} = h_m^{(k)} b_{mn}^{(k)} h_n^{-1}$  for all  $m \geq k$  and  $n > 0$ ,  
213 which concludes the proof.  $\square$

<sup>1</sup>The relation in Lemma 2.1 is well-known for  $k=1$ , but Lemma 2.1 for  $k > 1$  is not simply a recursive (or nested) version of this relation.

214 **2.2. Special instances of the Jacobi polynomials.** The Jacobi polynomials are  
 215 commonly used with specific combinations of the parameters  $\alpha$  and  $\beta$ , and often with differ-  
 216 ent standardizations. For simplicity we will use the following form for a special orthogonal  
 217 polynomial

$$218 \quad (2.28) \quad Q_n^{(\alpha,\beta)}(x) = g_n^{(\alpha,\beta)} P_n^{(\alpha,\beta)}(x),$$

219 where  $g_n^{(\alpha,\beta)}$  is a scaling function. The boundary values of  $Q_n$  will depend on  $g_n$ , and the  
 220 basis  $\{Q_n\}$  is obviously orthogonal with weight  $\omega^{(\alpha,\beta)}$ , which will normally be abbreviated  
 221 as simply  $\omega$  if it is possible to avoid confusion. We will also normally drop the  $(\alpha,\beta)$   
 222 superscript on the special polynomials.

223 The orthogonal polynomials  $\mathbf{Q} = (Q_0, Q_1, \dots)^T$  need to take the function  $g_n$  into ac-  
 224 count when forming the recursion relations from Sec. 2.1. For example, for (2.5) we get

$$225 \quad (2.29) \quad x\mathbf{Q} = A^T \mathbf{Q},$$

226 where the matrix operator  $A$  with components  $a_{mn} = (g_m^{(\alpha,\beta)})^{-1} a_{mn}^{(\alpha,\beta)} g_n^{(\alpha,\beta)}$  now has been  
 227 defined to include the scaling function. All the other recursion relations and inner product  
 228 equalities in Sec. 2.1, like (2.10), (2.12), (2.20), (2.25), (2.15), (2.21), (2.22) and (2.23) are  
 229 used exactly as they stand simply by replacing the components  $P_m$  with  $Q_m$  and using scaled  
 230 matrices and normalization factor  $h_m^{(k)} = (g_m^{(\alpha,\beta)})^2 h_m^{(k,\alpha,\beta)}$ . All the matrix operators that  
 231 belong to a specific family  $\{Q_n\}$  are in what follows written without the  $(\alpha,\beta)$  superscript,  
 232 whereas the Jacobi operators maintain theirs. Hence  $A = (a_{mn})$  and  $B = (b_{mn})$  will refer  
 233 to the specific operators for a basis family that include  $g_n$ .

234 The basis functions  $\mathbf{Q}_N = (Q_0, Q_1, \dots, Q_N)^T$  form a discrete function space  $\mathbf{Q}_N =$   
 235  $\text{span}\{Q_n\}_{n=0}^N$ , and a function  $u(x) \in \mathbf{Q}_N$  will be approximated as the truncated

$$236 \quad (2.30) \quad u(x) = \sum_{n=0}^N \hat{u}_n Q_n(x),$$

237 where  $\hat{u}_n = (u, Q_n)_w / h_n$  for  $n = 0, 1, \dots, N$ .

238 **2.3. Ultraspherical polynomials.** The ultraspherical polynomials are defined as Ja-  
 239 cobi polynomials with only one parameter  $\alpha = \beta$  (see, e.g., Sec. 4.2.3 of [22])

$$240 \quad (2.31) \quad Q_n^{(\alpha)}(x) = g_n^{(\alpha)} P_n^{(\alpha,\alpha)}(x), \quad \alpha > -1,$$

241 and normally (see [22]) the scaling factor in use is  $g_n^{(\alpha)} = \frac{(2\alpha+1)_n}{(\alpha+1)_n}$ . However, the regular  
 242 ultraspherical polynomials have boundary values that make them slightly awkward to use  
 243 with spectral Galerkin methods, and we will here follow Doha [9] and scale the ultraspherical  
 244 polynomials as

$$245 \quad (2.32) \quad Q_n^{(\alpha)}(x) = \frac{\Gamma(n+1)}{(\alpha+1)_n} P_n^{(\alpha,\alpha)}(x),$$

246 where the scaling factor corresponds to  $g_n^{(\alpha)} = 1/P_n^{(\alpha,\alpha)}(1)$ , such that

$$247 \quad (2.33) \quad Q_n^{(\alpha)}(\pm 1) = (\pm 1)^n.$$

248 Legendre and Chebyshev polynomials of the first kind are ultraspherical polynomials  
 249 with the scaling used in (2.32) and  $\alpha = 0$  and  $-1/2$ , respectively. Chebyshev polynomials

Family	Ultraspherical $Q_n^{(\alpha)}$	Legendre $L_n = Q_n^{(0)}$	Cheb. 1st $T_n = Q_n^{(-1/2)}$	Cheb. 2nd $U_n = (n+1)Q_n^{(1/2)}$
$g_n$	$\frac{\Gamma(n+1)}{(\alpha+1)_n}$	1	$\frac{\Gamma(n+1)}{(1/2)_n}$	$\frac{\Gamma(n+2)}{(3/2)_n}$
$a_{n-1,n}$	$\frac{n}{2n+2\alpha+1}$	$\frac{n}{2n+1}$	$\frac{1}{2}$	$\frac{1}{2}$
$a_{n+1,n}$	$\frac{(n+2\alpha+1)}{(2n+2\alpha+1)}$	$\frac{n+1}{2n+1}$	$\frac{c_n}{2}$	$\frac{1}{2}$
$b_{n-1,n}$	$-\frac{n}{(n+2\alpha)(2n+2\alpha+1)}$	$-\frac{1}{2n+1}$	$-\frac{1}{2(n-1)}$	$-\frac{1}{2(n+1)}$
$b_{n+1,n}$	$\frac{(n+2\alpha+1)}{2n+2\alpha+1(n+1)}$	$\frac{1}{2n+1}$	$\frac{c_n}{2(n+1)}$	$\frac{1}{2(n+1)}$
$h_n^{(k)}$	$\frac{2^{2\alpha+1}(n!)^2\Gamma^2(\alpha+1)(n+2\alpha+k)!}{(2n+2\alpha+1)(n-k)!\Gamma^2(n+2\alpha+1)}$	$\frac{2(n+k)!}{(n-k)!(2n+1)}$	$\frac{c_{n+k}\pi n\Gamma(n+k)}{2(n-k)!}$	$\frac{\pi\Gamma(n+k+2)}{2(n+1)(n-k)!}$

TABLE 1

Recursion matrices and normalization factors for ultraspherical polynomials. The Pochhammer symbol is represented as  $(a)_n = \Gamma(a+n)/\Gamma(a)$ .

of the second kind are defined with  $\alpha = 1/2$  and a slightly different scaling  $g_n^{(1/2)} = (n+1)/P_n^{(1/2,1/2)}(1)$ , such that  $U_n(x) = (n+1)Q_n^{(1/2)}(x)$ . A summary of the recursion matrices and normalization factors for these important families of ultraspherical polynomials is given in Table 1.

**3. Spectral differentiation.** For  $u(x) \in P_N$  and  $u'(x) \in P_{N-1}$  we have the expansions

$$(3.1) \quad u(x) = \sum_{n=0}^N \hat{u}_n Q_n(x) \in P_N, \quad \text{and} \quad u'(x) = \sum_{n=0}^N \hat{u}_n^{(1)} Q_n(x) \in P_{N-1},$$

with  $\hat{u}_N^{(1)} = 0$ . The process of finding  $\hat{\mathbf{u}}^{(1)} = \{\hat{u}_n^{(1)}\}_{n=0}^N \in \mathbb{R}^{N+1}$  in terms of  $\hat{\mathbf{u}} = \{\hat{u}_n\}_{n=0}^N \in \mathbb{R}^{N+1}$  is usually termed spectral differentiation in the frequency space. In this section we will use spectral differentiation to introduce the idea of the new Petrov-Galerkin method, which we arrive at in Sec. 3.4.

**3.1. Recursive approach.** The most common approach for spectral differentiation in the frequency space is to assume

$$(3.2) \quad \sum_{n=0}^N \hat{u}_n^{(1)} Q_n = \sum_{n=0}^N \hat{u}_n \partial Q_n,$$

and then invoke (2.10) on the left hand side to get

$$(3.3) \quad \sum_{n=0}^N \sum_{s=n-1}^{n+1} \hat{u}_n^{(1)} b_{sn} \partial Q_s = \sum_{n=0}^N \hat{u}_n \partial Q_n.$$

The method is now usually described through equating coefficients, but we can also take the  $L^2_{\omega_{\alpha+1,\beta+1}}[-1,1]$  inner product of (3.3) with  $\{\partial Q_m\}_{m=1}^N$  and use orthogonality (2.15) to obtain

$$(3.4) \quad \sum_{n=0}^N b_{mn} \hat{u}_n^{(1)} = \hat{u}_m, \quad \text{for } m = 1, 2, \dots, N.$$



270 This linear system of equations is not square. However, we can use  $\hat{u}_N^{(1)} = 0$  and then solve  
 271 (3.4) with back substitution (see, e.g., Ch. (3.2.6) of [35]) such that  $\hat{u}_{N-1}^{(1)} = \hat{u}_N/b_{N,N-1}$   
 272 and

$$273 \quad (3.5) \quad \hat{u}_n^{(1)} = \frac{1}{b_{n+1,n}} \left( \hat{u}_{n+1} - b_{n+1,n+1} \hat{u}_{n+1}^{(1)} - b_{n+1,n+2} \hat{u}_{n+2}^{(1)} \right), \quad \text{for } n = N-2, N-3, \dots, 0.$$

274 Note that the first row of the singular matrix  $B \in \mathbb{R}^{N+1 \times N+1}$  is never being used.

275 **3.2. A Galerkin approach.** The most obvious Galerkin method for finding  $\hat{\mathbf{u}}^{(1)}$  is  
 276 to take the  $L_\omega^2[-1, 1]$  inner product of (3.2) by  $\{Q_m\}_{m=0}^N$

$$277 \quad (3.6) \quad \sum_{n=0}^N (Q_n, Q_m)_\omega \hat{u}_n^{(1)} = \sum_{n=0}^N (\partial Q_n, Q_m)_\omega \hat{u}_n, \quad \forall m = 0, 1, \dots, N,$$

278 using orthogonality (2.13) on the left hand side and inverting

$$279 \quad (3.7) \quad \hat{u}_m^{(1)} = \frac{1}{h_m} \sum_{n=0}^N (\partial Q_n, Q_m)_\omega \hat{u}_n, \quad \forall m = 0, 1, \dots, N,$$

280 which automatically finds also  $\hat{u}_N^{(1)} = 0$ . The outcome is the same as with the recursive  
 281 approach, but the differentiation matrix  $d_{mn}^{(1)} = (\partial Q_n, Q_m)_\omega$  is badly conditioned, upper  
 282 triangular and full, and the matrix vector product is costly unless the structure of the  
 283 matrix is accounted for. In matrix form we can write

$$284 \quad (3.8) \quad \hat{\mathbf{u}}^{(1)} = \underline{D}^{(1)} \hat{\mathbf{u}},$$

285 where  $\underline{d}_{mn}^{(1)} = (\partial Q_n, h_m^{-1} Q_m)_\omega$ ,  $\underline{D}^{(1)} = (\underline{d}_{mn}^{(1)})_{n,m=0}^N \in \mathbb{R}^{N+1 \times N+1}$  is the spectral differentia-  
 286 tion matrix, and  $D^{(1)} = (d_{mn}^{(1)})_{n,m=0}^N \in \mathbb{R}^{N+1 \times N+1}$ .

287 **3.3. The Integration Preconditioner (IP) approach.** The IP approach [8, 7] is  
 288 to invoke the recursion (2.10) directly on (3.8), which is achieved by multiplying (3.8) from  
 289 the left by the square matrix  $B_{[1]} \in \mathbb{R}^{N+1 \times N+1}$  to get

$$290 \quad (3.9) \quad B_{[1]} \hat{\mathbf{u}}^{(1)} = I_{[1]} \hat{\mathbf{u}},$$

291 where  $B_{[1]} \underline{D}^{(1)} = I_{[1]}$ ,  $I$  is the identity matrix, and the square bracket notation on  $B_{[k]}$   
 292 and  $I_{[k]}$  (which we get from [8]) is used to indicate that the first  $k$  rows of the matrix are  
 293 set to zero. If the first row of (3.9) is ignored, the matrix equation can be solved with  
 294 back substitution for the first  $N$  components of  $\hat{\mathbf{u}}^{(1)}$ , and the solution algorithm becomes  
 295 identical to Eq. (3.5). Like for  $B$ , the fact that  $B_{[1]}$  is singular demands special attention  
 296 and complicates the description of the method, see [8, 7, 21].

297 From a Galerkin perspective, we can get a further understanding of the IP method if  
 298 we first rewrite (3.6) by dividing each row of both sides by the normalization factor  $h_m$

$$299 \quad (3.10) \quad \sum_{n=0}^N (Q_n, h_m^{-1} Q_m)_\omega \hat{u}_n^{(1)} = \sum_{n=0}^N (\partial Q_n, h_m^{-1} Q_m)_\omega \hat{u}_n,$$

300 and then apply the preconditioner  $B_{[1]}$  from the left. The action of the preconditioner is then  
 301 simply to invoke (2.10) and to replace a scaled test function  $\tilde{Q}_m = h_m^{-1}Q_m$  by component  
 302  $m$  of the matrix vector product  $B_{[1]}\tilde{Q}_N$ . With notation  $\rho_{N,m} = (B_{[1]}\tilde{Q}_N)_m$ , we get that

$$303 \quad (3.11) \quad \sum_{n=0}^N (Q_n, \rho_{N,m})_{\omega} \hat{u}_n^{(1)} = \sum_{n=0}^N (\partial Q_n, \rho_{N,m})_{\omega} \hat{u}_n,$$

304 where the matrix on the right hand side is the diagonal  $I_{[1]}$  and the matrix on the left is  
 305  $(B_{[1]})_{mn} = (Q_n, \rho_{N,m})_{\omega}$ . As such the IP method can be interpreted as a variational method  
 306 that is using the test function basis  $\{\rho_{N,m}\}_{m=1}^N$  for the  $N$  unknowns  $\{\hat{u}_n\}_{n=0}^{N-1}$  of the trial  
 307 basis  $\{Q_n\}_{n=0}^{N-1}$ . Again, the mapping of indices  $1, 2, \dots, N$  for the rows of  $B$  to indices  
 308  $0, 1, \dots, N-1$  of  $\hat{\mathbf{u}}^{(1)}$  requires special attention.

309 **3.4. A new Petrov Galerkin approach.** We will now consider an alternative Petrov-  
 310 Galerkin approach for finding specifically  $\hat{\mathbf{u}}^{(1)}$ , and in general  $\hat{\mathbf{u}}^{(k)}$ , from  $\hat{\mathbf{u}}$ . To set the stage  
 311 we consider the specific version of the orthogonality equation (2.15) after dividing both sides  
 312 by the normalization factor, shifting the  $m$ -index to nonzero values and rearranging

$$313 \quad (3.12) \quad \left( \partial^k Q_n, \frac{(1-x^2)^k}{h_{m+k}^{(k)}} \partial^k Q_{m+k} \right)_{\omega^{(\alpha,\beta)}} = \delta_{m+k,n}, \quad \text{for } m, n \geq 0.$$

314 From (3.12) we realise that a test function defined as

$$315 \quad (3.13) \quad \phi_m^{(k)} = \frac{(1-x^2)^k}{h_{m+k}^{(k)}} \partial^k Q_{m+k} \in \mathbb{P}_{m+2k}, \quad \text{for } m \geq 0,$$

316 would, for the corresponding (the same parameters  $\alpha, \beta$ ) orthogonal trial basis  $\{Q_n\}$ , lead  
 317 to a  $k$ 'th order differentiation matrix with one single constant upper diagonal

$$318 \quad (3.14) \quad (\partial^k Q_n, \phi_m^{(k)})_{\omega^{(\alpha,\beta)}} = \delta_{m+k,n}.$$

319 This will now be utilized for finding  $\hat{\mathbf{u}}^{(k)}$  from  $\hat{\mathbf{u}}$ .

320 For simplicity we will first consider  $\hat{\mathbf{u}}^{(1)}$ , and start by multiplying (3.2) with the test  
 321 function  $\phi_m^{(1)}$  and the weight  $\omega^{(\alpha,\beta)}$ , and then integrate over the domain to obtain

$$322 \quad (3.15) \quad \frac{1}{h_{m+1}^{(1)}} \sum_{n=0}^N (Q_n, \partial Q_{m+1})_{\omega^{(\alpha+1,\beta+1)}} \hat{u}_n^{(1)} = \sum_{n=0}^N (\partial Q_n, \phi_m^{(1)})_{\omega^{(\alpha,\beta)}} \hat{u}_n.$$

323 In order for this to be a square and well defined system of equations, we let  $m = 0, 1, \dots, N$ .  
 324 The right hand side matrix is already known from (3.14). Furthermore, the inner product  
 325 matrix on the left  $(Q_n, \partial Q_{m+1})_{\omega^{(\alpha+1,\beta+1)}} = h_{m+1}^{(1)} b_{m+1,n}$ , which we get from (2.21) (using  
 326  $k = l = 1$ ). The common factor  $h_{m+1}^{(1)}$  falls out and Eq. (3.15) becomes

$$327 \quad (3.16) \quad \sum_{n=0}^N b_{m+1,n} \hat{u}_n^{(1)} = \sum_{n=0}^N \delta_{m+1,n} \hat{u}_n.$$

328 In matrix form we get

$$329 \quad (3.17) \quad B_{(1)} \hat{\mathbf{u}}^{(1)} = I_{(1)} \hat{\mathbf{u}},$$

330 where the upper shift matrix  $I_{(1)} = (\delta_{m+1,n})_{m,n=0}^N \in \mathbb{R}^{N+1 \times N+1}$ , and the mass matrix  
 331  $B_{(1)} = (b_{m+1,n})_{m,n=0}^N \in \mathbb{R}^{N+1 \times N+1}$  is the upper triangular

$$332 \quad (3.18) \quad B_{(1)} = \begin{bmatrix} b_{1,0} & b_{1,1} & b_{1,2} & 0 & 0 & \cdots & 0 \\ 0 & b_{2,1} & b_{2,2} & b_{2,3} & 0 & \cdots & 0 \\ 0 & 0 & b_{3,2} & b_{3,3} & b_{3,4} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & b_{N-1,N-2} & b_{N-1,N-1} & b_{N-1,N} \\ 0 & 0 & \cdots & \cdots & 0 & b_{N,N-1} & b_{N,N} \\ 0 & 0 & \cdots & \cdots & \cdots & 0 & b_{N+1,N} \end{bmatrix}.$$

333 *Remark 3.1.* For index shifted matrices, like  $B_{(1)}$  and  $I_{(1)}$ , we will in this paper use a  
 334 special subscript notation with parenthesis to indicate the shift:  $A_{(p,q)} = (a_{m+p,n+q})_{m,n=0}^\infty$ .  
 335 If only the row is shifted, we will use only one number:  $A_{(p)} = (a_{m+p,n})_{m,n=0}^\infty$ . The notation  
 336 applies both to infinite-dimensional matrix operators and finite-dimensional matrices.

337 We note that the mass matrix  $B_{(1)}$  is just a shifted version of  $B$ , where row 0 has been  
 338 excluded. Hence we are back at more or less exactly the same solution as obtained with  
 339 explicit use of an integration preconditioner, which was also found to be exactly the same  
 340 as the recursive approach. Apparently, nothing has been gained, and nothing has been  
 341 lost. However, the Petrov-Galerkin approach suggested here has a slight advantage. The  
 342 mass matrix  $B_{(1)}$  is invertible and the condition  $\hat{u}_N^{(1)} = 0$  is naturally part of the solution.  
 343 Another advantage is that we can describe this Petrov Galerkin approach very compactly:  
 344 with  $u_N \in \mathbb{Q}_N$  find  $u \in \mathbb{Q}_N$  such that

$$345 \quad (3.19) \quad (u - u'_N, v)_\omega = 0, \quad \forall v \in \text{span}\{\phi_n^{(1)}\}_{n=0}^N,$$

346 and the recursive solution from back substitution then falls out naturally, with no tweaking  
 347 or mapping of indices whatsoever. Regarding the function space used for the test function  
 348 in (3.19), we note that  $\phi_n^{(1)}(x)$  satisfies homogeneous Dirichlet boundary conditions on both  
 349 sides of the domain. An appropriate test space is thus  $V_N^{(1)} = \{v \in P_N \mid v(\pm 1) = 0\}$  of  
 350 dimension  $N - 1$ , which is spanned by the basis  $\{\phi_n^{(1)}\}_{n=0}^{N-2}$ . To get the correct dimension,  
 351 the space used in (3.19) is thus  $V_{N+2}^{(1)} = \text{span}\{\phi_n^{(1)}\}_{n=0}^N$ .

352 We can proceed exactly the same way for higher order spectral differentiation. For  
 353 second order differentiation we use the basis function  $\phi_m^{(2)}$ , which satisfies the four conditions  
 354  $\phi_m^{(2)}(\pm 1) = \partial \phi_m^{(2)}(\pm 1) = 0$ . An appropriate space for  $\phi_m^{(2)}$  is thus the biharmonic  $V_N^{(2)} =$   
 355  $\{v \in P_N \mid v(\pm 1) = v'(\pm 1) = 0\}$  of dimension  $N - 3$ . In general, the basis function  $\phi_m^{(k)}$  will  
 356 satisfy  $2k$  boundary conditions, and for  $k$ 'th order an appropriate space is thus

$$357 \quad (3.20) \quad V_N^{(k)} = \{v \in P_N \mid \partial^n v(\pm 1) = 0, \forall n = 0, 1, \dots, k - 1\},$$

358 of dimension  $N - 2k + 1$ . For  $k$ 'th order spectral differentiation the problem becomes: with  
 359  $u_N \in \mathbb{Q}_N$  find  $u \in \mathbb{Q}_N$  such that

$$360 \quad (3.21) \quad (u - \partial^k u_N, v)_{\omega(\alpha,\beta)} = 0, \quad \forall v \in V_{N+2k}^{(k)} = \text{span}\{\phi_n^{(k)}\}_{n=0}^N.$$

361 Following the same approach as above for  $k = 1$  we get that

$$362 \quad (3.22) \quad \frac{1}{h_{m+k}^{(k)}} \sum_{n=0}^N (Q_n, \partial^k Q_{m+k})_{\omega^{(\alpha+k, \beta+k)}} \hat{u}_n^{(k)} = \sum_{n=0}^N \delta_{m+k, n} \hat{u}_n,$$

363 or

$$364 \quad (3.23) \quad B_{(k)}^{(k)} \hat{\mathbf{u}}^{(k)} = I_{(k)} \hat{\mathbf{u}}.$$

365 Here  $I_{(k)} \in \mathbb{R}^{N+1 \times N+1}$  and the mass matrix defined as  $B_{(k)}^{(l)} = (b_{m+k, n}^{(l)})_{m, n=0}^N \in \mathbb{R}^{N+1 \times N+1}$   
 366 with  $k = l$  (which we get from (2.21)), is upper triangular, and not to be confused with the  
 367  $l$ 'th matrix power of  $B_{(k)}$ . Similarly, the IP method for  $k$ 'th order spectral differentiation is

$$368 \quad (3.24) \quad B_{[k]}^k \hat{\mathbf{u}}^{(k)} = I_{[k]} \hat{\mathbf{u}},$$

369 which is basically the same linear algebra system as (3.23). In fact, we can get back to  
 370 (3.23), except from the last  $k$  rows that will be zero, by multiplying (3.24) from the left by  
 371  $I_{(k)}$ .

372 *Remark 3.2.* With the new recursion (2.25) and index shifting it is evident that we can  
 373 also write the new test function  $\phi_m^{(k)}$  as

$$374 \quad (3.25) \quad \phi_m^{(k)} = (B^k \tilde{\mathbf{Q}})_{m+k} = (B_{(k)}^{(k)} \tilde{\mathbf{Q}})_m \in \mathbb{P}_{m+2k} \quad \text{for } m \geq 0,$$

375 which highlights a link to the other methods described in this section, through the recursive  
 376 matrix operator  $B$ .

377 There is a minor technical difference between the Petrov-Galerkin method described  
 378 in this section and the IP method, even though they here lead to exactly the same result.  
 379 For finite-dimensional systems IP corresponds to using a test function  $\rho_{N, m}^{(k)} = (B^k \tilde{\mathbf{Q}}_N)_m \in$   
 380  $\mathbb{P}_{\min(m+k, N)}$ , with the finite matrix  $B^k$  and vector  $\tilde{\mathbf{Q}}_N$ , instead of the non-truncated  $\phi_m^{(k)} =$   
 381  $(B^k \tilde{\mathbf{Q}})_m \in \mathbb{P}_{m+k}$ . This leads for IP to *test functions that are not all in the same space*,  
 382 and there will be a difference from the PG method in the  $k$  highest wavenumbers. However,  
 383 since spectral differentiation and thus (3.21) assumes  $u_N \in \mathbb{Q}_N$ , orthogonality makes all  
 384 terms involving  $Q_{N+k}$  for  $k > 0$  disappear and this minor detail is thus not significant for  
 385 spectral differentiation, where  $\{\hat{u}_n^{(k)}\}_{n=N-k+1}^N = 0$ . However, the difference will matter for  
 386 regular differential equations, as we will see in Sec. 4.

387 **3.5. Spectral differentiation with ultraspherical polynomials.** For ultraspheri-  
 388 cal polynomials the basis function used for  $V_{N+2k}^{(k)}$  is

$$389 \quad (3.26) \quad \phi_n^{(k, \alpha)} = \frac{(1-x^2)^k \partial^k Q_{n+k}^{(\alpha)}}{h_{n+k}^{(k)}} = (B^k \tilde{\mathbf{Q}}^{(\alpha)})_{n+k}.$$

390 For ultraspherical polynomials defined as (2.32) it can be shown that

$$391 \quad (3.27) \quad \frac{b_{n+1, n}}{h_n} = -\frac{b_{n+1, n+2}}{h_{n+2}} = -\frac{\Gamma(n+2\alpha+2)}{2^{2\alpha+1} \Gamma^2(\alpha+1) \Gamma(n+2)},$$

Family	$\phi_n^{(1)}$	$\phi_n^{(2)}$
Legendre	$\frac{1}{2}(L_n - L_{n+2})$	$\frac{1}{2(2n+3)} \left( L_n - \frac{2(2n+5)}{2n+7} L_{n+2} + \frac{2n+3}{2n+7} L_{n+4} \right)$
Cheb. 1st	$\frac{1}{\pi(n+1)}(T_n - T_{n+2})$	$\frac{1}{2\pi(n+1)(n+2)} \left( T_n - \frac{2(n+2)}{n+3} T_{n+2} + \frac{n+1}{n+3} T_{n+4} \right)$
Cheb. 2nd	$\frac{1}{\pi} \left( \frac{U_n}{n+1} - \frac{U_{n+2}}{n+3} \right)$	$\frac{1}{2\pi(n+1)(n+2)} \left( U_n - \frac{2(n+1)}{n+4} U_{n+2} + \frac{(n+1)(n+2)}{(n+3)(n+4)} U_{n+4} \right)$

TABLE 2

Basis functions  $\phi_n^{(1)}$  and  $\phi_n^{(2)}$  on expanded form for Legendre and Chebyshev polynomials.

392 and the basis functions for  $k = 1$  and 2 can be written as

393 (3.28) 
$$\phi_n^{(1)} = \frac{b_{n+1,n}}{h_n} \left( Q_n^{(\alpha)} - Q_{n+2}^{(\alpha)} \right),$$

394 (3.29) 
$$\phi_n^{(2)} = \frac{b_{n+2,n}^{(2)}}{h_n} \left( Q_n^{(\alpha)} - (1 + c_n)Q_{n+2}^{(\alpha)} + c_n Q_{n+4}^{(\alpha)} \right),$$
  
395

396 where  $c_n = \frac{2n+2\alpha+3}{2n+2\alpha+7}$ . For the Legendre and Chebyshev families the basis functions of lowest  
397 order are given in Table 2. It is interesting to note that, for both Legendre and Chebyshev  
398 of the first kind,  $\phi_n^{(1)}$  and  $\phi_n^{(2)}$  correspond to scaled versions of the well known Dirichlet  
399 and biharmonic basis functions of Shen [31, 32]. Also, the basis function (3.28) is a scaled  
400 version of the function used by Doha [9].

401 **4. Sparse methods for differential equations.** For spectral Galerkin methods the  
402 trial functions are constructed as linear combinations of orthogonal polynomials, in order  
403 to satisfy a given problems boundary conditions. Since we now know that the test function  
404  $\phi_n^{(k)}$  turns the  $k$ 'th order differentiation matrix  $(\partial^k Q_n, \phi_m^{(k)})_\omega$  into a matrix with one single  
405 upper diagonal, this means that  $\phi_m^{(k)}$  will make the differentiation matrix of any spectral  
406 Galerkin problem sparse and banded. Because of (2.23) we also know that  $\phi_n^{(k)}$  will make  
407 any lower order differentiation matrix with polynomial coefficients  $(\partial^{k-l} Q_n, x^q \phi_m^{(k)})_\omega$  sparse  
408 and banded.

409 **4.1. The new sparse method.** We consider a linear differential equation of the form

410 (4.1) 
$$\sum_{l=0}^k p_l(x) \partial^{k-l} u = f, \quad \text{for } x \in [-1, 1],$$

411 subject to the  $k$  homogeneous boundary conditions

412 (4.2) 
$$\mathcal{T}^{(l)} u = 0, \quad l = 0, 1, \dots, k-1.$$

413 The coefficients  $\{p_l(x)\}_{l=0}^k$  are polynomials of different degree, and there are  $k$  boundary  
414 conditions (Dirichlet, Neumann, etc), specified at either side of the domain. If required,  
415 inhomogeneous boundary conditions can easily be incorporated using a lifting technique [2],  
416 which does not affect any of the coefficient matrices derived below.

417 We choose a trial space  $S_N^{(k)} = \{v \in P_N \mid \mathcal{T}^{(l)} v = 0, l = 0, 1, \dots, k-1\}$  of dimension  
418  $M+1 = N - k + 1$ . The new Petrov-Galerkin method is to find  $u \in S_N^{(k)}$  such that

419 (4.3) 
$$\sum_{l=0}^k (p_l \partial^{k-l} u, v)_\omega = (f, v)_\omega, \quad \forall v \in V_{N+k}^{(k)},$$

420 using basis  $\phi^{(k)} = \{\phi_m^{(k)}\}_{m=0}^M$  for the test space  $V_{N+k}^{(k)}$  (see (3.20)). A basis for  $S_N^{(k)}$  is  
 421  $\psi = \{\psi_n\}_{n=0}^M$ , where  $\psi_n$  is constructed from a small number of neighbouring orthogonal  
 422 basis functions. For simplicity we will write the trial functions as

$$423 \quad (4.4) \quad \psi = K\mathbf{Q}_N, \quad \text{and thus} \quad u(x) = \sum_{n=0}^M \hat{u}_n (K\mathbf{Q}_N)_n \in P_N,$$

424 where  $K = (\kappa_{ij}) \in \mathbb{R}^{M+1 \times N+1}$  is a strictly banded stencil matrix, normally with lower  
 425 bandwidth 0 and upper  $k$ . The stencil matrix is used in order to derive one set of algebraic  
 426 equations to be used for different problems and trial functions, satisfying different boundary  
 427 conditions.

428 *Remark 4.1.* An uncommon feature of (4.3) is that there is a discrepancy in polynomial  
 429 order between the  $m$ 'th trial function  $\psi_m \in P_{m+k}$  and the test function  $\phi_m^{(k)} \in P_{m+2k}$ , and  
 430 we search for a solution in  $P_N$ , using the slightly larger test space  $P_{N+k}$ . The feature stems  
 431 from the different number of boundary conditions used in test and trial spaces.

432 *Remark 4.2.* For the basis  $\phi^{(k)}$  the matrix  $K_s = B_{(k)}^{(k)} H^{-1} \in \mathbb{R}^{M+1 \times N+k+1}$  can be  
 433 interpreted as a stencil matrix, since

$$434 \quad (4.5) \quad \phi^{(k)} = K_s \mathbf{Q}_{N+k}.$$

435 **4.1.1. Constant coefficients.** Assume that all the coefficients  $p_l$  are constant, and  
 436 that  $p_0 = 1$ . Insert for test and trial functions in the bilinear part of (4.3)

$$437 \quad (4.6) \quad (\partial^{k-l} u, v)_\omega = \sum_{n=0}^M \sum_{s=0}^N (\partial^{k-l} Q_s, \phi_m^{(k)})_\omega \kappa_{ns} \hat{u}_n, \quad \text{for } m = 0, 1, \dots, M,$$

438 and use the inner products from Eqs. (2.21) and (2.13). Equation (4.3) on matrix form thus  
 439 becomes

$$440 \quad (4.7) \quad \left( I_{(k)} + \sum_{l=1}^k p_l B_{(k)}^{(l)} \right) K^T \hat{\mathbf{u}} = \tilde{\mathbf{f}},$$

441 where the matrices  $I_{(k)}$  and  $B_{(k)}^{(l)}$  are of shape  $\mathbb{R}^{M+1 \times N+1}$ . The right hand side  $\tilde{\mathbf{f}} =$   
 442  $\{(f, \phi_m^{(k)})_\omega\}_{m=0}^M \in \mathbb{R}^{M+1}$ . However, using (3.25) we can also write

$$443 \quad (4.8) \quad \tilde{\mathbf{f}} = B_{(k)}^{(k)} \hat{\mathbf{f}},$$

444 where  $\hat{\mathbf{f}} = \{\hat{f}_m\}_{m=0}^{N+k}$ ,  $\hat{f}_m = (f, \tilde{Q}_m)_\omega$  and  $B_{(k)}^{(k)} \in \mathbb{R}^{M+1 \times N+k+1}$ , which is of different shape  
 445 from  $B_{(k)}^{(k)}$  on the left hand side of (4.7). Simply restricting the right hand side as  $f \in P_N$   
 446 (like the trial function), we get  $\hat{\mathbf{f}} = \{\hat{f}_m\}_{m=0}^N$  and can use the same  $B_{(k)}^{(k)} \in \mathbb{R}^{M+1 \times N+1}$  on  
 447 the right hand side as on the left. With this restriction we get for Chebyshev polynomials  
 448 and constant coefficients more or less the same method that is defined as the "quasi-inverse"  
 449 method with Galerkin trial functions by Julien and Watson [23]. But here generalised to all  
 450 Jacobi polynomials and wrapped up in a Petrov-Galerkin formulation.

451 **4.1.2. Variable coefficients.** Assume now that  $p_l(x) = x^q$ , with integer  $q > 0$ , such  
 452 that we need to compute  $(\partial^{k-l}u, x^q v)_\omega$  for some  $l \leq k$ . Inserting for test and trial function  
 453 we get

$$454 \quad (4.9) \quad (\partial^{k-l}u, x^q v)_\omega = \sum_{n=0}^M \sum_{s=0}^N (\partial^{k-l}Q_s, x^q \phi_m^{(k)})_\omega \kappa_{ns} \hat{u}_n, \quad \text{for } m = 0, 1, \dots, M,$$

455 where the inner product matrix is computed using (2.23) as

$$456 \quad (4.10) \quad (\partial^{k-l}Q_s, x^q \phi_m^{(k)})_\omega = \sum_{p=m-q}^{m+q} \underline{a}_{m+k, p+k}^{(k,q)} b_{p+k, s}^{(l)}.$$

457 In matrix form we get

$$458 \quad (4.11) \quad (\partial^{k-l}u, x^q v)_\omega = L^{(k,q,l)} K^T \hat{\mathbf{u}},$$

459 where the matrix  $L^{(k,q,l)} = \underline{A}_{(k,k)}^{(k,q)} B_{(k)}^{(l)} \in \mathbb{R}^{M+1 \times N+1}$ ,  $\underline{A}_{(k,k)}^{(k,q)} \in \mathbb{R}^{M+1 \times N+1}$  and  $B_{(k)}^{(l)} \in$   
 460  $\mathbb{R}^{N+1 \times N+1}$ . Note that  $L^{(k,q,l)}$  has bandwidth  $1 + 2(l+q)$ , with the lower bandwidth  $q+l-k$   
 461 and upper bandwidth  $q+l+k$ . The bandwidth  $1 + 2(q+l)$  was given also in Theorem 2.1  
 462 of [7], and it follows since both  $\underline{A}$  and  $B$  are tri-diagonal matrices and there is a total of  
 463  $q+l$  matrix powers. The shift of the bandwidth from the centre is special for the current  
 464 method and due to the row-shifted  $B_{(k)}^{(l)}$ . For the Galerkin method there is also an additional  
 465 problem dependent bandwidth in (4.11) due to the stencil matrix  $K$ .

466 *Remark 4.3.* For any special orthogonal basis described as (2.28), the matrix  $L^{(k,q,l)}$  can  
 467 be computed explicitly simply from the Jacobi matrix and vector components  $a_{mn}^{(\alpha,\beta)}$ ,  $b_{mn}^{(\alpha,\beta)}$ ,  $h_m^{(k,\alpha,\beta)}$   
 468 and  $\psi_m^{(k,\alpha,\beta)}$  given in Sec. 2.1, and the scaling functions  $g_m^{(\alpha,\beta)}$ . ■

469 *Remark 4.4.* Any equation that can be written as Eq. (4.1) leads to an algebraic prob-  
 470 lem where the coefficient matrix is a sum of the strictly banded matrices  $L^{(k,q,l)}$ . This  
 471 includes also constant coefficient matrices, since  $\underline{A}_{(k,k)}^{(k,0)} = I$ . On this form Eq. (4.7) be-  
 472 comes

$$473 \quad (4.12) \quad \sum_{l=0}^k p_l L^{(k,0,l)} K^T \hat{\mathbf{u}} = \tilde{\mathbf{f}},$$

474 where  $L^{(k,0,0)} = I_{(k)}$  and  $p_0 = 1$ .

475 **4.1.3. The linear form and numerical implementations.** For a pure spectral  
 476 Petrov-Galerkin method the inner product integrals in (4.3) will be computed exactly, lead-  
 477 ing to analytical coefficient matrices that are sums of  $L^{(k,q,l)}$  matrices. A discrete inner  
 478 product in a space with  $N+1$  quadrature points is represented as  $(\cdot, \cdot)_{N,\omega}$  and (4.3) thus  
 479 becomes

$$480 \quad (4.13) \quad \sum_{l=0}^k (p_l \partial^{k-l}u, v)_{N+k,\omega} = (f, v)_{N+k,\omega},$$

481 using the  $N+k+1$  quadrature points of the test space  $V_{N+k}^{(k)}$ . Since Gaussian quadrature  
 482 of order  $N+k$  is exact for all polynomial integrands  $\in P_{2(N+k)+1}$ , the constant coefficient

483  $L^{(k,0,l)}$  will be exact also for a numerical approach. However, since the integrand of the  
 484 variable coefficient  $L^{(k,q,l)}$  are polynomials of order less than or equal to  $2N + k + q$ , a  
 485 numerical approach using  $N + k + 1$  quadrature points will only be exact for  $q \leq 2k + 1 - l$ .  
 486 Naturally, if  $q$  exceeds this limit we can simply increase the number of quadrature points  
 487 correspondingly.

488 A numerical approximation of the right hand side of (4.8) will use quadrature for the  
 489 integral and interpolation of  $f(x)$

$$490 \quad (4.14) \quad \tilde{\mathbf{f}} = B_{(k)}^{(k)} \bar{\mathbf{f}},$$

491 where the interpolation coefficients  $\bar{\mathbf{f}} = \{\bar{f}_{m,N+k}\}_{m=0}^{N+k} \in \mathbb{R}^{N+k+1}$  are defined as  $\bar{f}_{m,N+k} =$   
 492  $(I_{N+k}f, \bar{Q}_m)_{N+k,\omega}$ , and the interpolation operator is defined such that  $I_{N+k}f(x_j) = f(x_j)$   
 493 for all quadrature points  $\{x_j\}_{j=0}^{N+k}$ .

494 **4.1.4. Alternative new sparse method.** With a minor modification we can reformulate  
 495 the method presented in Eq. (4.3), such that the  $m$ 'th test and trial functions both  
 496 have the same polynomial order  $m + k$ , and test and trial spaces both are in  $P_N$ . In order  
 497 to achieve this we can simply pull  $k$  polynomial orders from the test function and put them  
 498 into the weight. For even order equations a Petrov-Galerkin formulation may then be to  
 499 find  $u \in S_N^{(k)}$  such that

$$500 \quad (4.15) \quad \sum_{l=0}^k (p_l \partial^{k-l} u, v)_{\omega^{(\alpha+k/2, \beta+k/2)}} = (f, v)_{\omega^{(\alpha+k/2, \beta+k/2)}}, \quad \forall v \in V_N^{(k/2)}.$$

501 In order to remain completely identical to (4.3) the additional weight will now have to be  
 502 removed from the test function, and we should use

$$503 \quad (4.16) \quad \bar{\phi}_m^{(k, \alpha, \beta)} = \frac{\phi_m^{(k, \alpha, \beta)}}{(1-x^2)^{k/2}} = \frac{(1-x^2)^{k/2} \partial^k Q_{m+k}^{(\alpha, \beta)}}{h_{m+k}^{(k, \alpha, \beta)}},$$

504 and  $V_N^{(k/2)} = \text{span}\{\bar{\phi}_m^{(k, \alpha, \beta)}\}_{m=0}^M$ . Note that we have simply shuffled the  $(1-x^2)^{k/2}$  term  
 505 around and the variational form (4.15) is still identical to (4.3) and we get exactly the  
 506 same matrices  $L^{(k,q,l)}$  as in Secs. 4.1.1 and 4.1.2. The only difference will be manifested  
 507 in numerical implementations of  $(f, v)_{N, \omega^{(\alpha+k/2, \beta+k/2)}}$ , that will naturally make use of  $N + 1$   
 508 quadrature points instead of  $N + k + 1$ . Furthermore, since  $\{Q_m^{(\alpha+k/2, \beta+k/2)}\}$  are orthogonal  
 509 with weight  $\omega^{(\alpha+k/2, \beta+k/2)}$ , it is more natural to rewrite the test functions  $\bar{\phi}_m^{(k, \alpha, \beta)}$  using (2.7)  
 510 as

$$511 \quad (4.17) \quad \bar{\phi}_m^{(k, \alpha, \beta)} = \gamma_m^{(k, \alpha, \beta)} \phi_m^{(k/2, \alpha+k/2, \beta+k/2)},$$

512 where the scaling function

$$513 \quad (4.18) \quad \gamma_m^{(k, \alpha, \beta)} = \frac{\psi_{m+k}^{(k/2, \alpha, \beta)} g_{m+k}^{(\alpha, \beta)} h_{m+k/2}^{(k/2, \alpha+k/2, \beta+k/2)}}{g_{m+k/2}^{(\alpha+k/2, \beta+k/2)} h_{m+k}^{(k, \alpha, \beta)}}.$$

514 Naturally, a numerical implementation of  $(f, v)_{N, \omega^{(\alpha+k/2, \beta+k/2)}}$  should use the quadrature  
 515 points of Jacobi polynomials with parameters  $(\alpha + k/2, \beta + k/2)$  instead of  $(\alpha, \beta)$ , which is  
 516 another discrepancy from the original method.



517 *Remark 4.5.* Equation (4.15) should only be considered for even order equations. For  
 518 odd equations we can still modify the test function and weight, but would have to treat  $\alpha$   
 519 and  $\beta$  separately, and depart from ultraspherical polynomials.

520 *Remark 4.6.* For  $k = 2$  and  $\alpha = \beta = -1/2$  this method corresponds to using Chebyshev  
 521 polynomials of the first kind for the trial functions and Chebyshev polynomials of the second  
 522 kind for the test functions, with inner products in  $L_{\omega^{1/2}}^2[-1, 1]$  and  $\gamma_m^{(2, -1/2, -1/2)} = \frac{1}{m+2}$ . A  
 523 similar approach is used, e.g., by Olver and Townsend [27] and Burns et al. [4].

524 **4.1.5. A comment on stability.** The stability of the new method depends mainly  
 525 on the condition numbers of the matrices  $\underline{L}^{(k,q,l)}K^T$ . Since the matrices  $\underline{L}^{(k,q,l)}$  are very  
 526 similar (index shifted) to those obtained by an integration preconditioner approach, and  
 527 since these have already been extensively analysed [8, 7, 21], we give here only a brief  
 528 comment, highlighting what is unique for the Petrov-Galerkin method.

529 The coefficient matrix for any problem described in this paper can be written as

$$530 \quad (4.19) \quad \underline{L}^{(k)}K^T \in \mathbb{R}^{M+1 \times M+1},$$

531 where  $\underline{L}^{(k)}$  is a weighted sum of matrices  $\underline{L}^{(k,q,l)}$ , with the exact form depending on the  
 532 polynomial coefficients  $p_l(x)$ . The 2-norm condition number of the matrix  $\underline{L}^{(k)}K^T$  is denoted  
 533 as  $\sigma(\underline{L}^{(k)}K^T)$ , and its upper bound can be estimated as

$$534 \quad (4.20) \quad \sigma(\underline{L}^{(k)}K^T) \leq \sigma(\underline{L}^{(k)})\sigma(K^T).$$

535 Coutsias et al. [8] prove that the condition numbers of integration operators (i.e., matrices  
 536 corresponding to  $\underline{L}^{(k)}$ ) will be bounded by a constant  $C$  as long as the leading coefficient  
 537 of the problem (i.e.,  $p_0(x)$ ) does not vanish within the problems interval. This condition is  
 538 also required to avoid singularities, and for problems with smooth solutions we immediately  
 539 get that  $\sigma(\underline{L}^{(k)}K^T) \leq C\sigma(K^T)$ . The Galerkin stencil matrix  $K$  is thus seen to play a very  
 540 important role for the stability of the new method. The stencil matrix is determined by the  
 541 choice of trial basis, which in turn depends on the boundary conditions of the given problem.  
 542 We may now follow Shen [35, Chapter 4] and choose the most compact basis function for any  
 543 set of boundary conditions, weighted such that all terms on the main diagonal of  $K$  are one.  
 544 For  $k = 2$  and Dirichlet boundary conditions we then get  $K = (\delta_{mn} - \delta_{m+2,n})_{m=0,n=0}^{N-2,N} \in$   
 545  $\mathbb{R}^{N-1 \times N+1}$ , and direct computation reveals that  $\sigma(K^T)$  scales as  $\mathcal{O}(N)$ . As such,  $\sigma(\underline{L}^{(k)}K^T)$   
 546 will also scale as  $\mathcal{O}(N)$  for large  $N$ . For the homogeneous biharmonic problem with  $k = 4$   
 547 we have the ultraspherical stencil matrix  $K = (\delta_{mn} - (1 + c_n)\delta_{m+2,n} + c_n\delta_{m+4,n})_{m=0,n=0}^{N-4,N} \in$   
 548  $\mathbb{R}^{N-3 \times N+1}$ , where  $c_n = \frac{2n+2\alpha+3}{2n+2\alpha+7}$ , see Eq. (3.29). Direct computation shows that the  
 549 condition number of this stencil matrix scales as  $\mathcal{O}(N^2)$ , which is thus also the upper bound  
 550 for  $\sigma(\underline{L}^{(k)}K^T)$ . A similar analysis may easily be performed for any stencil matrix.

551 **4.2. Multiple dimensions.** The methods described in Secs. 4.1 are all strictly banded  
 552 and easily extended to multiple dimensions through the use of tensor product methods. Let  
 553 us for illustration consider the two-dimensional Poisson's equation in Cartesian coordinates

$$554 \quad (4.21) \quad \nabla^2 u(x, y) = f(x, y),$$

555 for any type of boundary conditions on the domain  $\Omega = [-1, 1]^2$ . For the trial function  
 556 we choose the tensor product space  $\mathcal{S} = S_N^{(2)}(x) \otimes S_N^{(2)}(y)$ , with basis  $\{\psi_m(x)\psi_n(y) \mid m, n =$   
 557  $0, 1, \dots, M\}$ , where  $\psi_m(x) = (K_x \mathbf{Q}_N)_m$  and  $\psi_n(y) = (K_y \mathbf{Q}_N)_n$ . Here  $K_x \in \mathbb{R}^{M+1 \times N+1}$

558 and  $K_y \in \mathbb{R}^{M+1 \times N+1}$  are stencil matrices determined by the problems boundary conditions  
 559 in the  $x$  and  $y$ -directions, respectively. The test space is chosen as  $\mathcal{V} = V_{N+2}^{(2)} \otimes V_{N+2}^{(2)} =$   
 560  $\text{span}\{\phi_m^{(2)}(x)\phi_n^{(2)}(y) \mid m, n = 0, 1, \dots, M\}$  and we attempt to find  $u \in \mathcal{S}$  such that

$$561 \quad (4.22) \quad (\nabla^2 u, v)_\omega = (f, v)_\omega \quad \forall v \in \mathcal{V},$$

562 where the weight  $\omega = \omega(x)\omega(y)$  is the product of the weights in the  $x$  and  $y$  directions. The  
 563 expansion for the solution is now

$$564 \quad (4.23) \quad u(x, y) = \sum_{i=0}^M \sum_{j=0}^M \hat{u}_{ij} \psi_i(x) \psi_j(y) \in \mathcal{S},$$

565 with expansion coefficients  $\hat{U} = (\hat{u}_{ij}) \in \mathbb{R}^{M+1 \times M+1}$ . Inserting for test and trial functions it  
 566 is easy to show that Poisson's equation (4.22) in algebraic form becomes

$$567 \quad (4.24) \quad L_x^{(0,0)} \hat{U} L_y^{(0,2)T} + L_x^{(0,2)} \hat{U} L_y^{(0,0)T} = \tilde{F},$$

568 where  $(\tilde{F})_{ij} = (f, \phi_i^{(2)} \phi_j^{(2)})_\omega$  and  $L_s^{(q,l)} = L^{(2,q,l)} K_s^T$  for  $s \in (x, y)$ . We now use the row-  
 569 major vectorization, or  $\text{vec}^2$ , operation on (4.24) to arrive at

$$570 \quad (4.25) \quad \left( L_x^{(0,0)} \otimes L_y^{(0,2)} + L_x^{(0,2)} \otimes L_y^{(0,0)} \right) \text{vec}(\hat{U}) = \left( L_x^{(0,2)} \otimes L_y^{(0,2)} \right) \text{vec}(\tilde{F}),$$

571 where  $\otimes$  here represent a tensor product, or Kronecker product, of matrices,  $\text{vec}(\hat{U}) \in$   
 572  $\mathbb{R}^{(M+1)^2}$  is the column vector obtained by flattening the row-major two-dimensional  $\hat{U}$ , i.e.,  
 573  $\text{vec}(\hat{U}) = (\hat{u}_{00}, \dots, \hat{u}_{0M}, \hat{u}_{10}, \dots, \hat{u}_{1M}, \dots, \dots, \hat{u}_{M0}, \dots, \hat{u}_{MM})^T$  and the Kronecker product  
 574 matrices are all of shape  $\mathbb{R}^{(M+1)^2 \times (M+1)^2}$ .

575 The Kronecker product method is easily automated, also for higher dimensions, and  
 576 sparse and strictly banded matrices  $L_s^{(q,l)}$  lead to sparse and strictly banded Kronecker  
 577 product matrices. For a Dirichlet problem using ultraspherical polynomials and  $K_s =$   
 578  $(\delta_{mn} - \delta_{m+2,n})_{m=0,n=0}^{M,N} \in \mathbb{R}^{M+1 \times N+1}$  for both  $s \in (x, y)$ , the coefficient matrix on the left  
 579 of (4.25) will have 12 nonzero diagonals.

### 580 4.3. Numerical examples.

581 **4.3.1. First order problem.** We consider the first order problem

$$582 \quad (4.26) \quad u'(x) + \frac{1}{x^2 + 1} u(x) = s(x), \quad u(-1) = 0, \quad x \in [-1, 1],$$

583 using ultraspherical polynomials. For this first order problem we use the trial space  $S_N^{(1)} =$   
 584  $\{v \in P_N \mid v(-1) = 0\}$  with basis function  $\psi_n = Q_n^{(\alpha)} + Q_{n+1}^{(\alpha)}$ , corresponding to a stencil  
 585 matrix  $K = (\delta_{mn} + \delta_{m+1,n})_{m=0,n=0}^{N-1,N} \in \mathbb{R}^{N \times N+1}$ .

586 Next, we multiply through with  $x^2 + 1$  to get only polynomial coefficients, and attempt  
 587 to find  $u \in S_N^{(1)}$  such that

$$588 \quad (4.27) \quad ((x^2 + 1)u', v)_\omega + (u, v)_\omega = (f, v)_\omega, \quad \forall v \in V_{N+1}^{(1)} = \text{span}\{\phi_n^{(1)}\}_{n=0}^{N-1},$$

<sup>2</sup>i.e.,  $\text{vec}(AUB^T) = (A \otimes B)\text{vec}(U)$  for matrices  $A, U, B$  of appropriate shape.

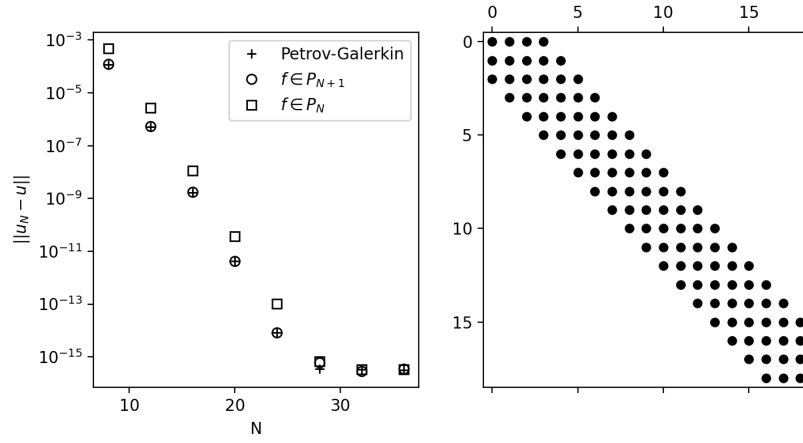


FIG. 1. Left: The  $L^2[-1, 1]$  error norm for the solution of Eq. (4.27) using  $u(x) = \exp(-0.25x^4)(x+1)$  and three different computations of  $\tilde{f}$ . Right: Sparsity pattern of the coefficient matrix.

589 where  $f(x) = (x^2 + 1)s(x)$ . Inserting for test and trial functions we get

$$590 \quad (4.28) \quad (L^{(1,2,0)} + L^{(1,0,0)} + L^{(1,0,1)})K^T \hat{u} = \tilde{f},$$

591 where the coefficient matrix on the left has 6 nonzero diagonals, with lower bandwidth 2  
592 and upper 3, see Fig. 1. We compute the right hand side both exactly and numerically  
593 with either  $f(x) \in P_{N+1}$  or  $f(x) \in P_N$ . The latter is computed merely as a curiosity,  
594 because it corresponds closely to using the IP method with a Galerkin trial function (see  
595 [23]). Note that if  $u \in P_N$ , then, due to the polynomial coefficient, the right hand side  
596  $f(x)$  will be a polynomial  $\in P_{N+1}$ . The larger test space of the current method thus has  
597 an advantage here. This is evident in the left hand panel of Figure 1, which shows the  
598  $L^2[-1, 1]$  error norm  $\|u_N - u\| = (\int_{-1}^1 (u_N - u)^2 dx)^{1/2}$  using the manufactured solution  
599  $u(x) = \exp(-0.25x^4)(x+1)$  and Chebyshev polynomials of the first kind. We see that for  
600 this problem one additional coefficient for  $f(x)$  leads to approximately one number extra in  
601 accuracy until machine precision is reached.

602 The current example is used in slightly different form by Olver and Townsend [27]

$$603 \quad (4.29) \quad u'(x) + \frac{1}{ax^2 + 1}u(x) = 0, \quad u(-1) = 1, \quad x \in [-1, 1],$$

604 with the analytical solution  $u(x) = \exp(-\frac{1}{\sqrt{a}}(\tan^{-1}(\sqrt{ax}) - \tan^{-1}(\sqrt{a})))$  and  $a = 5 \times 10^4$ .  
605 We can solve this problem as described above, but need to add one (constant) basis function  
606  $\psi_N = Q_0^{(a)} = 1$  to the trial basis and look for the solution

$$607 \quad (4.30) \quad u(x) = \sum_{n=0}^N \hat{u}_n \psi_n(x).$$

608 We immediately get that  $\hat{u}_N = u(-1) = 1$ , and solve for the remaining coefficients using the  
609 same matrices as before (4.28), only scaled appropriately by  $a$ . The right hand side vector  
610  $\tilde{f}_n = 0$  for  $n = 1, 2, \dots, N - 1$ . However, due to the boundary basis and  $(u, v)_\omega$  we get the

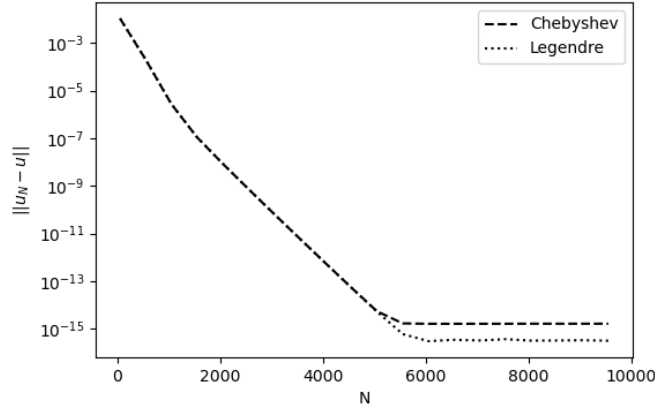


FIG. 2. The  $L^2[-1, 1]$  error norm for the solution of Eq. (4.27) using manufactured solution  $u(x) = \exp(-\frac{1}{\sqrt{a}}(\tan^{-1}(\sqrt{ax}) - \tan^{-1}(\sqrt{a})))$  and Legendre (dotted) and Chebyshev (dashed) basis functions.

611 following nonzero term on the right:  $\tilde{f}_0 = -(\psi_N, \phi_0^{(1)})_\omega \hat{u}_N = -1$ . We solve the problem  
 612 using both Chebyshev and Legendre polynomials, and the  $L^2$  error norm is shown in Figure  
 613 2. Not surprisingly, the problem is resolved to machine precision using approximately 5000  
 614 degrees of freedom, which was obtained also by Olver and Townsend.

615 *Remark 4.7.* The condition number of the coefficient matrix  $L^{(1,2,0)} + L^{(1,0,0)} + L^{(1,0,1)}$   
 616 is bounded by a constant, see Sec. 4.1.5 and Sec. 4 of [8]. Since the condition numbers of  
 617 the stencil matrix scale as  $\mathcal{O}(N)$ , the coefficient matrix of this problem also scales as  $\mathcal{O}(N)$   
 618 for large  $N$ , which is easily shown with direct computations.

619 **4.3.2. Second order problem.** We consider the Helmholtz problem

$$620 \quad (4.31) \quad u''(x) - \mu u(x) = f(x), \quad u(\pm 1) = 0, x \in [-1, 1],$$

621 where the constant coefficient  $\mu \geq 0$ . For this problem we can use the Dirichlet trial space  
 622  $S_N^{(2)} = V_N^{(1)}$ , with basis  $\{\psi_n\}_{n=0}^{N-2}$ , and  $\psi_n = Q_n^{(\alpha)} - Q_{n+2}^{(\alpha)}$ , corresponding to a stencil matrix  
 623  $K = (\delta_{mn} - \delta_{m+2,n})_{m=0,n=0}^{N-2,N} \in \mathbb{R}^{N-1 \times N+1}$ . The Petrov-Galerkin problem is formulated as:  
 624 find  $u \in V_N^{(1)}$  such that

$$625 \quad (4.32) \quad (u'', v)_\omega - \mu(u, v)_\omega = (f, v)_\omega, \quad \forall v \in V_{N+2}^{(2)} = \text{span}\{\phi_m^{(2)}\}_{m=0}^{N-2}.$$

626 Using Eq. (4.7) with  $k = 2$ ,  $p_1 = 0$  and  $p_2 = -\mu$ , we obtain

$$627 \quad (4.33) \quad (I_{(2)} - \mu B_{(2)}^{(2)})K^T \hat{\mathbf{u}} = \tilde{\mathbf{f}},$$

628 where the coefficient matrix consists of 4 nonzero diagonals. This sparsity matches the best  
 629 that has been reported for the Helmholtz problem with Chebyshev polynomials, see [23, 12].

630 *Remark 4.8.* Restricted to Chebyshev polynomials, and up to different scaling of the  
 631 basis functions, this method corresponds to the Petrov-Galerkin method described by El-  
 632 barbary [12].

633 An alternative formulation for this problem according to Sec. 4.1.4 is to find  $u \in V_N^{(1)}$   
 634 such that

$$635 \quad (4.34) \quad (u'', v)_{\omega^{(\alpha+1)}} - \mu(u, v)_{\omega^{(\alpha+1)}} = (f, v)_{\omega^{(\alpha+1)}}, \quad \forall v \in V_N^{(1)} = \text{span}\{\bar{\phi}_m^{(2, \alpha)}\}_{m=0}^{N-2}.$$

636 This is actually a regular Galerkin method (not Petrov-Galerkin), since the trial and test  
 637 spaces are the same, and it leads to exactly the same left hand side of the algebraic problem  
 638 (4.33) as before. The right hand side will differ only for a numerical implementation. For  
 639  $\alpha = -1/2$  this corresponds to using the trial function  $\psi_n = T_n - T_{n+2}$  and test function  
 640  $\bar{\phi}_m^{(2, -1/2)} = \frac{1}{m+2} \phi_m^{(1, 1/2)} = \frac{1}{\pi(m+2)} \left( \frac{U_m}{m+1} - \frac{U_{m+2}}{m+3} \right)$ .

641 Another second order problem is the Airy differential equation

$$642 \quad (4.35) \quad \epsilon u'' - xu = 0, \quad u(-1) = \text{Ai}\left(-\sqrt[3]{\frac{1}{\epsilon}}\right), \quad u(1) = \text{Ai}\left(\sqrt[3]{\frac{1}{\epsilon}}\right),$$

643 which has the Airy function  $u(x) = \text{Ai}\left(\sqrt[3]{\frac{1}{\epsilon}}x\right)$  as solution. Again we follow Olver and  
 644 Townsend [27] and choose  $\epsilon = 10^{-9}$  such that the solution becomes highly oscillatory. Be-  
 645 cause of the boundary conditions we also need to add two basis functions to the homogeneous  
 646 trial basis, and use  $\psi_{N-1} = \frac{1}{2}(Q_0^{(\alpha)} + Q_1^{(\alpha)})$  and  $\psi_N = \frac{1}{2}(Q_0^{(\alpha)} - Q_1^{(\alpha)})$ . The linear algebra  
 647 problem to solve becomes

$$648 \quad (4.36) \quad (\epsilon I_{(2)} - L^{(2, 1, 2)})K^T \hat{\mathbf{u}} = \tilde{\mathbf{f}},$$

649 where  $\tilde{f}_j = 0$  for  $j = 2, \dots, N-2$  and, due to the boundary functions,  $\hat{u}_{N-1} = u(-1)$ ,  
 650  $\hat{u}_N = u(1)$ ,  $\tilde{f}_0 = \sum_{j=N-1}^N (\psi_j, x\phi_0^{(2)})_{\omega} \hat{u}_j$  and  $\tilde{f}_1 = \sum_{j=N-1}^N (\psi_j, x\phi_1^{(2)})_{\omega} \hat{u}_j$ . Figure 3 shows  
 651 the Airy function and the  $L^2[-1, 1]$  error using Chebyshev polynomials for basis. The  
 652 results are similar to Olver and Townsend, and robust for large  $N$  due to good conditioning  
 653 of the matrix.<sup>3</sup> A notable difference from the almost banded matrix obtained by Olver and  
 654 Townsend is that the coefficient matrix here is strictly banded with 7 nonzero diagonals.

655 *Remark 4.9.* In agreement with the comment in Sec. 4.1.5 it can be shown with direct  
 656 computation that the coefficient matrices in this section have condition numbers that are  
 657 scaling as  $\mathcal{O}(N)$  (for large  $N$ ) for any ultraspherical basis with scaling as (2.32).

658 **4.3.3. A comment on sparsity.** The test function  $\phi_m^{(k)}$  guarantees a sparse and  
 659 strictly banded differentiation matrix of any order lower than or equal to  $k$ . This is a  
 660 generic sparse approach that applies to all orthogonal polynomials in the Jacobi family,  
 661 but there is no guarantee that this is the best, or most sparse, solution. Consider, for  
 662 example, the second order problem in Sec. 4.3.2 with  $\mu = 0$ . If we reformulate this as  
 663 a Galerkin problem, using the same space for both test and trial functions, we can find  
 664  $u \in V_N^{(1)} = \text{span}\{Q_m - Q_{m+2}\}_{m=0}^{N-2}$  such that

$$665 \quad (4.37) \quad (u'', v)_{\omega} = (f, v)_{\omega}, \quad \forall v \in V_N^{(1)} = \text{span}\{\phi_m^{(1)}\}_{m=0}^{N-2}.$$

666 Note that we here use  $\phi_m^{(1)}$  for the test space instead of  $\phi_m^{(2)}$ . For a Legendre basis we now  
 667 obtain a diagonal stiffness matrix (see [31])

$$668 \quad (4.38) \quad (\psi_n'', \phi_m^{(1)}) = (m+1)(m+2)\delta_{mn}.$$

<sup>3</sup>In fact, we obtain an  $L^2[-1, 1]$  error of  $1.7 \times 10^{-14}$  for the overresolved  $N = 10^6$ .

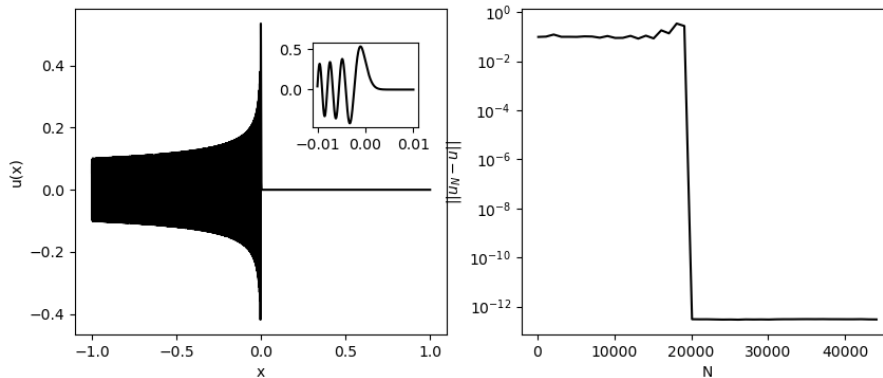


FIG. 3. The Airy function  $u(x) = \text{Ai}\left(\sqrt[3]{\frac{1}{\epsilon}}x\right)$  with  $\epsilon = 10^{-9}$  on the left, with an inset figure zoomed in on the region  $x \in [-0.01, 0.01]$ . The figure on the right shows the  $L^2[-1, 1]$  error norm using Chebyshev polynomials.

669 Since a diagonal stiffness matrix is better than the bi-diagonal  $I_{(2)}K^T$  that we found in Sec.  
 670 4.3.2, this is clearly a better approach for Legendre polynomials. However, for a Chebyshev  
 671 basis of the first kind, or any other ultraspherical basis using (2.32), the corresponding  
 672 stiffness matrix will be upper triangular and full (see, e.g., [32]). We note that the Legendre  
 673 basis is probably the only ultraspherical basis that can achieve a diagonal stiffness matrix for  
 674 (4.37), because a trial basis  $\{\phi_n\}$  (e.g., with  $\phi_n = Q_n - Q_{n+2}$ ) requires  $\{\phi_n''\}$  to be orthogonal  
 675 to a Dirichlet basis. For Legendre  $L_n'' - L_{n+2}'' = (2n+3)L_{n+1}'$ , which is orthogonal to the  
 676 Dirichlet basis  $\{(1-x^2)L_{n+1}'\}$ . This good fortune stems from the fact that  $b_{n+1,n} = -b_{n-1,n}$   
 677 (such that  $Q_n = b_{n-1,n}(Q_{n-1}' - Q_{n+1}')$ ), which can only be obtained for  $\alpha = 1/2$  with the  
 678 scaling used in (2.32).<sup>4</sup>

679 **5. Conclusions.** We have described a generic global spectral Petrov-Galerkin method  
 680 for linear ordinary differential equations with polynomial coefficients. The method leads  
 681 to highly sparse and strictly banded matrices, and is as such easy to implement using off-  
 682 the-shelf linear algebra softwares for banded matrices. Like most efficient methods that  
 683 have been described for orthogonal polynomials, the method relies on recursion relations of  
 684 Jacobi polynomials. The method is very easy to describe, because all it takes for a  $k$ 'th  
 685 order linear differential equation is the use of a specific test function

$$686 \quad (5.1) \quad \phi_n^{(k)} \sim (1-x^2)^k \partial^k Q_{n+k},$$

687 where  $\partial^k = \frac{d^k}{dx^k}$ , along with trial functions composed as compact combinations of the special-  
 688 ized Jacobi polynomials  $Q_n$ , satisfying a given problems boundary conditions. For efficient  
 689 implementations we have also described a new recursion relation for Jacobi polynomials

$$690 \quad (5.2) \quad (1-x^2)^k \partial^k Q = (C^{(k)})^T Q, \quad k > 0,$$

<sup>4</sup>The Chebyshev polynomials of second kind have  $b_{n+1,n} = -b_{n-1,n}$ , but use different scaling such that  $\{U_n - U_{n+2}\}$  is not a Dirichlet basis.

691 where  $\mathbf{Q}^{(\alpha,\beta)} = (Q_0^{(\alpha,\beta)}, Q_1^{(\alpha,\beta)}, \dots)^T$ , and the matrix  $C^{(k)}$ , which has bandwidth  $1 + 2k$ , is  
 692 easily computed from well-known, explicit Jacobi recursion operators.

693 The Petrov-Galerkin method leads naturally to coefficient matrices that consist of  
 694 banded stencil matrices and index shifted versions of the matrices obtained by the inte-  
 695 gration preconditioner (IP) method. However, there is no explicit need for preconditioners  
 696 (or "quasi-inverse" matrices) in the description of the method, only test and trial functions  
 697 and naturally assembled coefficient matrices. We have described the generic coefficient ma-  
 698 trix for an equation with polynomial coefficients, i.e.,  $(\partial^{k-l} Q_n, x^q \phi_m^{(k)})_\omega$  for integer  $k, l$  and  
 699  $q$  and indices  $m$  and  $n$ , through an explicit expression, which is easily computed simply from  
 700 already well-known recursion matrix operators for Jacobi polynomials.

701 Since all coefficient matrices are strictly banded, the extension of the method to multiple  
 702 dimensions is trivial through the use of Kronecker product methods. This is an advantage  
 703 over tau-based methods, where the coefficient matrices are almost-banded, using full rows to  
 704 implement boundary conditions. For the current method homogeneous boundary conditions  
 705 are built into the trial functions, and inhomogeneous conditions can be added through lifting  
 706 functions that do not interfere at all with the derived, strictly banded, coefficient matrices.

707 The Petrov-Galerkin method described in this paper has already been implemented in  
 708 the open source global spectral Galerkin software framework Shenfun [26] for any ultras-  
 709 pherical or Jacobi basis. It can be used for any linear differential equations with polynomial  
 710 coefficients, with any composition of Dirichlet and Neumann boundary conditions. For  
 711 higher dimensions it is using tensor product methods.

712 **Code availability.** For reproducibility, the examples in this paper have all been com-  
 713 puted with Shenfun (<https://github.com/spectralDNS/shenfun>), version 4.0.2. The public  
 714 repository <https://github.com/spectralDNS/PG-paper-2022> contains code used to create all  
 715 figures in the paper.

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