From Electrostatics To Almost Optimal Nodal Sets For Polynomial Interpolation In A Simplex

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FROM ELECTROSTATICS TO ALMOST OPTIMAL NODAL SETS
FOR POLYNOMIAL INTERPOLATION IN A SIMPLEX [*]

J. S. HESTHAVEN [†]

Abstract. The electrostatic interpretation of the Jacobi-Gauss quadrature points is exploited to obtain interpolation points suitable for approximation of smooth functions defined on a simplex. Moreover, several new estimates, based on extensive numerical studies, for approximation along the line using Jacobi-Gauss-Lobatto quadrature points as the nodal sets are presented.

The electrostatic analogy is extended to the two-dimensional case, with the emphasis being on nodal sets inside a triangle for which two very good matrices of nodal sets are presented. The matrices are evaluated by computing the Lebesgue constants and they share the property that the nodes along the edges of the simplex are the Gauss-Lobatto quadrature points of the Chebyshev and Legendre polynomials, respectively. This makes the resulting nodal sets particularly well suited for integration with conventional spectral methods and supplies a new nodal basis for $h - p$ finite element methods.

Key words. Polynomial Interpolation, Lebesgue Constants, Jacobi Polynomials, Triangular Elements, Spectral Methods.

AMS subject classifications. 41A10, 65D05, 41A63, 78A30

1. Introduction. In 1885, Stieltjes[1, 2] revealed a remarkable connection between Jacobi polynomials and electrostatics by asking the following question -

Problem: Let two unit mass charges, $p > 0$ and $q > 0$, be held fixed at the positions $x = \pm 1$. Assume also that N unit mass charges, positioned at $x_1, \ldots, x_N$, are allowed to move freely along the line connecting the two endpoint charges. What is the position of the charges that minimizes the electrostatic energy

$$W(x_1, \ldots, x_N) = -\sum_{i=1}^{N} \left(p \log |x_i + 1| + q \log |x_i - 1| + \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{N} \log |x_i - x_j| \right) .$$

He continued by showing that the energy is minimized when $x_1, \ldots, x_N$ are given as the zeros of the Jacobi-polynomial, $P_N^{\alpha,\beta}(x)$, with $\alpha = 2p - 1$ and $\beta = 2q - 1$. In 1939, Szegö[3] showed that this minimum indeed is the unique global minimum. Additionally, he showed that also the Hermite and Laguerre polynomials may be obtained through an electrostatic approach. Consequently, it was established that the Gauss quadrature points of the classical orthogonal polynomials can be determined as the steady state, minimum energy solution to a problem of electrostatics.

The symmetric Jacobi polynomials, $P_N^{\alpha,\alpha}(x) = P_N^{\alpha}(x)$, play a particularly important role in many areas of numerical analysis such as linear algebra and approximation theory. In particular, the special case of $P_N^{-1/2}(x) = T_N(x)$, known as the Chebyshev polynomials of the first kind, is used extensively for approximation of smooth functions. Indeed, the successful application of spectral methods to the solution of partial differential equations is mainly based on the superior approximation properties of the Chebyshev polynomials (see e.g. [4]).

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The apparent connection between steady state, minimum energy solutions to problems of electrostatics and polynomials, well suited for approximation of smooth functions, is the main inspiration of the present work.

The question we attempt to address is whether it is possible to formulate an electrostatic problem in a simplex, the minimum energy, steady state solution of which leads to the specification of polynomials suitable for approximating smooth functions defined on the simplex.

In particular, we shall focus the attention towards nodal sets and polynomial interpolation in an equilateral triangle. Such nodal sets are at the heart of the specification of high order element methods, e.g. the $h - p$ finite element method [5] or spectral element methods[6]. Also for the construction of diffeomorphic mapping functions, using transfinite blending functions, does the specification of high order shape functions play an important role.

In the present work we will restrict the attention to nodal sets which share certain properties. In order for the nodal sets to be useful in connection with high order element methods, it is important that the nodal sets include nodes along the boundaries of the simplex. In particular, along the line this implies that the endpoints should be included in the nodal set. This allows for imposing boundary conditions and enforcing continuity between elements. In the two-dimensional case the picture is a little more complicated. Our aim is to obtain nodal sets that can be integrated with more conventional spectral methods or provide a fundamental building block for a high order element method. In the latter case, the actual specification of the points along the edges of the simplex is less important as all elements are similar such that enforcing continuity becomes a straightforward procedure. However, in relation to spectral methods the picture is a little more complicated. Traditional spectral methods in more than one dimensional are based on tensor-products of one-dimensional approximations, with the most commonly used nodal sets being based on Gauss-Lobatto quadrature points of Chebyshev or Legendre polynomials. This has the additional advantage that Gauss quadrature rules exist for integration along the edges. Based on these observations we have chosen to restrict the attention to nodal sets in the simplex which share the property that the nodes along the edges are specified as Gauss-Lobatto quadrature points of symmetric Jacobi polynomials. Moreover, we require that the one-dimensional edge polynomial is of same order as the global multi-dimensional polynomial.

The remaining part of the paper is organized as follows. In Sec. 2 we recall a few results from approximation theory important to the present work and we introduce the Lebesgue constant as a measure of the quality of the interpolating polynomial. Section 3 is devoted to interpolation of functions defined along the line. The known estimates of the Lebesgue constant for approximation using symmetric Jacobi polynomials are briefly reviewed and several new estimates, based on extensive numerical studies, using the symmetric Jacobi-Gauss-Lobatto quadrature points as nodal sets are conjectured. In Sec. 4 we turn towards the problem of constructing high order interpolating polynomials in the triangle through the solution of a problem of electrostatics. Section 5 contains a short discussion and concluding remarks. In the appendices we give the barycentric coordinates of two nodal matrices well suited for interpolation in a triangle.

2. General Concepts and Notation. Throughout this paper we shall be concerned with the distribution of nodes in an m-dimensional simplex, $\mathsf{S}^m \subset \mathsf{R}^m$, leading to an almost optimal polynomial interpolation as measured through the Lebesgue

constant. For the sake of simplicity, we restrict the analysis to the one-dimensional, $m = 1$, and the two-dimensional case, $m = 2$, with the emphasis on S^2 being an equilateral triangle.

We define the space of n-degree polynomials in m variables, P_n^m, such that the dimension of the approximation space is

$$\dim \mathsf{P}_n^m \equiv N_n^m = \left(\begin{array}{c} m + n \\ m \end{array} \right) \ ,$$

being the minimum space in which P_n^m may be complete [7]. Let us also introduce the nodal set, $\Pi_n^m = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)$, where the nodal points, or collocation points, are termed $\boldsymbol{x}_i \in \mathsf{S}^m$. Here, and in the following, we will used $N = N_n^m$ to simplify the notation unless clarification is deemed necessary.

Interpolation of smooth functions, $f[\mathsf{S}^m] : \mathsf{R}^m \to \mathsf{R}$, where $f[\mathsf{S}^m] \in C[\mathsf{S}^m]$ and $f \in \mathsf{H}$ is square integrable and belongs to the Hilbert space, H, can now be viewed as for a given Π_n^m find the polynomial, $\mathcal{I}_n^m f \in \mathsf{P}_n^m$ such that $\forall \boldsymbol{x}_i \in \mathsf{S}^m, \mathcal{I}_n^m f(\boldsymbol{x}_i) = f(\boldsymbol{x}_i)$, where we have introduced the projector, $\mathcal{I}_n^m[\mathsf{S}^m] : \mathsf{H} \to \mathsf{P}_n^m$. The solution to this problem is obtained by introducing the complete polynomial basis, $p_i(\boldsymbol{x}) \in \mathsf{P}_n^m$ and $\mathsf{P}_n^m = \text{span}\{p_i(\boldsymbol{x})\}_{i=1}^N$, such that $\forall i \in [1, \dots, N] : f(\boldsymbol{x}_i) = \sum_{j=1}^N a_j p_j(\boldsymbol{x}_i)$. Finding the expansion coefficients, a_j, is then accomplished by solving the linear problem

$$\left[\begin{array}{ccc} p_1(\boldsymbol{x}_1) & \dots & p_N(\boldsymbol{x}_1) \\ \vdots & & \vdots \\ p_1(\boldsymbol{x}_N) & \dots & p_N(\boldsymbol{x}_N) \end{array} \right] \left[\begin{array}{c} a_1 \\ \vdots \\ a_N \end{array} \right] = \left[\begin{array}{c} f(\boldsymbol{x}_1) \\ \vdots \\ f(\boldsymbol{x}_N) \end{array} \right] \ ,$$

or $\text{VDM}\boldsymbol{a} = \boldsymbol{f}$, where the matrix is denoted $\text{VDM} = \text{VDM}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)$ in recognition of the fact that in the one-dimensional case it equals the Vandermonde matrix if $p_j(x_i) = (x_i)^{j-1}$. Existence and uniqueness of the interpolating polynomial is guaranteed if and only if the Vandermonde determinant, $|\text{VDM}|$, is different from zero.

In the one-dimensional case this is ensured if the nodal points are distinct. However, for $m \geq 2$ no such simple results exist. A geometric characterization of distributions of points in S^m ensuring a non-zero determinant is given in [8]. However, these considerations lead to sufficient conditions only and are certainly not necessary.

If we simply assume that $|\text{VDM}| \neq 0$, we may express the polynomial approximation, $\mathcal{I}_n^m f(\boldsymbol{x}) \in \mathsf{P}_n^m$, using interpolating Lagrange polynomials, $L_i(\Pi_n^m, \boldsymbol{x}) \in \mathsf{P}_n^m$, with the property $L_i(\Pi_n^m, \boldsymbol{x}_j) = \delta_{ij}$. Thus, the polynomial interpolation is given as

$$\mathcal{I}_n^m f(\boldsymbol{x}) = \sum_{i=1}^N f(\boldsymbol{x}_i) L_i(\Pi_n^m, \boldsymbol{x}) \ .$$

This relation is naturally true for any smooth $f(\boldsymbol{x}) \in \mathsf{H}$, and in particular for the basis, $p_i(\boldsymbol{x})$, itself. Consequently, the interpolating Lagrange polynomials may in general be found as the solution to the dual interpolation problem

$$(1) \quad \left[\begin{array}{ccc} p_1(\boldsymbol{x}_1) & \dots & p_1(\boldsymbol{x}_N) \\ \vdots & & \vdots \\ p_N(\boldsymbol{x}_1) & \dots & p_N(\boldsymbol{x}_N) \end{array} \right] \left[\begin{array}{c} L_1(\Pi_n^m, \boldsymbol{x}) \\ \vdots \\ L_N(\Pi_n^m, \boldsymbol{x}) \end{array} \right] = \left[\begin{array}{c} p_1(\boldsymbol{x}) \\ \vdots \\ p_N(\boldsymbol{x}) \end{array} \right] \ ,$$

through which, using Cramers rule, we obtain the direct solution

$$(2) \qquad L_i(\Pi_n^m, \boldsymbol{x}) = \frac{|\mathrm{VDM}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{i-1}, \boldsymbol{x}, \boldsymbol{x}_{i+1}, \ldots, \boldsymbol{x}_N)|}{|\mathrm{VDM}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)|} .$$

The solution of Vandermonde systems, Eq.(1), is notoriously difficult due to exponential-like growth of the condition-number. Therefore, direct solution of the linear system, Eq.(1), should only be done for cases where no explicit formula for the Lagrange polynomials is known, however complicated it may be. If, indeed, it is necessary to solve the Vandermonde problem great care must be exercised for large values of N. We refer to [9] for a discussion of this topic and for references to work dealing with the accurate solution of Vandermonde systems.

We equip the polynomial space, P_n^m, with the supremum-norm, $\|\cdot\|$, and introduce the measures

$$\|\mathcal{I}_n^m\| = \sup_{f \neq 0} \frac{\|\mathcal{I}_n^m f\|}{\|f\|_\infty} \;\;, \;\; \|f\|_\infty = \max_{\mathbf{x} \in \mathsf{S}^m} |f(\boldsymbol{x})| .$$

The interpolation error is uniformly bounded from below by the best approximation as

$$\|f(\boldsymbol{x}) - p^*(\boldsymbol{x})\|_\infty \leq \|f(\boldsymbol{x}) - \mathcal{I}_n^m f(\boldsymbol{x})\|_\infty ,$$

where $p^*(\boldsymbol{x})$ signifies the best approximating polynomial ensured to exist since f is assumed smooth [10]. For $m = 1$, the rate of convergence of $p^*(x)$ is guaranteed to be at least geometric in N through Jacksons theorem. For $m \geq 2$, no such results exist for the simplex.

Unfortunately, determination of $p^*(\boldsymbol{x})$ is even for $m = 1$ an unsolved problem in the general case and for $m \geq 2$ virtually nothing is known. A powerful way of estimating the quality of alternative approximations as compared to $p^*(\boldsymbol{x})$ appears as a result of the following theorem.

THEOREM 2.1 (LEBESGUE). *Assume that $f[\mathsf{S}^m] \in C[\mathsf{S}^m]$ and that we consider the nodal set, Π_n^m, then*

$$\|f(\boldsymbol{x}) - \mathcal{I}_n^m f(\boldsymbol{x})\|_\infty \leq [1 + \Lambda(\Pi_n^m)] \|f(\boldsymbol{x}) - p^*(\boldsymbol{x})\|_\infty ,$$

where

$$\Lambda(\Pi_n^m) = \|\mathcal{I}_n^m\| = \max_{\mathbf{x} \in \mathsf{S}^m} \sum_{i=1}^{N} |L_i(\Pi_n^m, \boldsymbol{x})| ,$$

is termed the Lebesgue constant.

Consequently, by computing the Lebesgue constant we obtain a measure of how close the approximation is to the best polynomial approximation. It is noteworthy that the value of the Lebesgue constant depends solely on the interpolating Lagrange polynomials and, therefore, is determined completely by the nodal set, Π_n^m.

For interpolation of smooth functions on S^1, we learn from Theorem 2.1 that convergence can be expected only when the function is sufficiently smooth such that the approximation error decays faster than the growth of the Lebesgue constant. Another motivation for searching for nodal sets resulting in small Lebesgue constants

is that due to finite precision of digital computers, given through the machine accuracy, ε_M, one can only expect valid results when $[\Lambda(\Pi_n^m)]^{-1} \gg \varepsilon_M$, independent of the smoothness of the function being approximated. It is therefore of significant importance to specify methods for obtaining nodal sets resulting in small and slowly growing Lebesgue constants. The study of this is the subject of the remaining part of the paper.

3. Interpolation Points in S^1 Using Electrostatics. The interpolation problem in S^1 has received extensive attention in the past and we shall not attempt to fully account for the large amount of results, but rather selectively present the relevant theory. For a general introduction we refer to [10, 11, 12].

For $m = 1$, we introduce the polynomial space, $\mathsf{P}_n^1 = \mathrm{span}\{p_i(x)|p_i(x) = x^{i-1}\}_{i=1}^{n+1}$, since $N_n^1 = N = n + 1$, and the corresponding nodal set, $\tilde{\Pi}_n^1 = \{x_i\}_{i=1}^{n+1}$, where it is assumed that the nodes are ordered as $a = x_1 < \ldots < x_{n+1} = b$.

For $\mathsf{S}^1 = [a, b]$, VDM becomes the regular Vandermonde matrix with the determinant given as

$$|\mathrm{VDM}(x_1, \ldots x_{n+1})| = \prod_{i=1}^{n+1} \prod_{j=i+1}^{n+1} (x_i - x_j) \ ,$$

and, consequently, the interpolating Lagrange polynomials exist and are unique provided only that the nodes are distinct. Moreover, the interpolating Lagrange polynomial in S^1 is given on explicit form as

$$L_i(\tilde{\Pi}_n^1, x) = \prod_{\substack{j=1 \\ j \neq i}}^{n+1} \frac{x - x_j}{x_i - x_j} \ .$$

If no further constraints are imposed on the position of the nodes, the nodal configuration leading to an optimal Lebesgue constant is non-unique [13].

If we, however, restrict the permissible nodal sets by requiring the endpoints to be fixed at $x_1 = -1$ and $x_{n+1} = 1$, the setting becomes considerably more firm. Sets endowed with this constrain are known as canonical sets. Any degree N_n^1 nodal set, $\tilde{\Pi}_n^1 = [a = x_1 < \ldots < x_{n+1} = b]$ may be mapped to the canonical nodal set, Π_n^1, through a linear mapping. Moreover, since the Lagrange polynomials are invariant under the linear mapping, i.e. $\Lambda(\Pi_n^1) \leq \Lambda(\tilde{\Pi}_n^1)$, it is sufficient to consider the properties of the canonical nodal sets to which we shall mainly direct the attention in what remains.

The equioscillatory property of the Lebesgue functions, defined as

$$\lambda(\Pi_n^m, \boldsymbol{x}) = \sum_{i=1}^{N} |L_i(\Pi_n^m, \boldsymbol{x})| \ ,$$

characterizing the optimal canonical nodal set was first conjectured in the famous Bernstein-Erdös conjecture and later proved in [14, 15]. This result establishes existence and uniqueness of the optimal set and, among other properties, shows that the optimal nodal set, Π_n^1, is symmetric around $x = 0$. A numerical procedure for computing the optimal nodal set in S^1 is given in [16].

Bounds for the Lebesgue constant of the optimal canonical nodal set was first obtained in [17].

THEOREM 3.1. *For all permissible nodal sets, Π_n^1, and all n there exists a positive constant, c, such that*

$$\Lambda(\Pi_n^1) > \frac{2}{\pi} \log(n+1) - c \ .$$

This has later been refined considerably [12] as

THEOREM 3.2. *The Lebesgue constant, $\Lambda(\Pi_n^1)$, for the optimal canonic nodal set, Π_n^1, in S^1 is bounded as*

$$c \left(\frac{\log\log(n+1)}{\log(n+1)} \right)^2 > \Lambda(\Pi_n^1) - \frac{2}{\pi} \log(n+1) - \chi > \begin{cases} \frac{\pi}{18(n+1)^2} + \mathcal{O}\left(\frac{1}{(n+1)^4} \right) & \text{for } n \text{ odd} \\ -\frac{2}{\pi(n+1)} + \mathcal{O}\left(\frac{1}{(n+1)^2} \right) & \text{for } n \text{ even} \end{cases}$$

where

$$\chi = \frac{2}{\pi} \left(\gamma + \log\frac{4}{\pi} \right) = 0.52125162\dots \ ,$$

and $\gamma = 0.57721566\dots$ represents Euler's constant.

The value of the Lebesgue constant for various choices of nodal sets has been given much attention in the past. However, as we have discussed previously, we are primarily interested in nodal sets obtained as Gauss-Lobatto quadrature points for the symmetric Jacobi polynomials due to their extensive use in connection with spectral methods. We have therefore chosen to restrict the discussion in the following to results obtained for the Jacobi polynomials only.

Equally Distributed Nodal Sets. For reasons of comparison, let us, however, first focus the attention towards the interpolation problem at an equidistant grid and introduce the equally distributed nodal set, $\Pi_n^{\mathrm{Eq}} = \{x_i | x_i = -1 + 2(i-1)/n\}_{i=1}^{n+1}$, with the associated Lebesgue constant, $\Lambda_n^{\mathrm{Eq}} = \Lambda(\Pi_n^{\mathrm{Eq}})$. The well known Runge-phenomenon associated with interpolation at an equidistant grid manifests itself through a very rapid growth of the Lebesgue constant [18, 19, 20]

THEOREM 3.3. *The Lebesgue constant, Λ_n^{Eq}, for interpolation in S^1 with an equally distributed nodal set, Π_n^{Eq}, is bounded for $n \geq 1$ as*

$$\frac{2^{n-2}}{n^2} < \Lambda_n^{\mathrm{Eq}} < \frac{2^{n+3}}{n} \ ,$$

with the asymptotic estimate

$$\Lambda_n^{\mathrm{Eq}} \simeq \frac{2^{n+1}}{en(\log n + \gamma)} \quad \text{for } n \to \infty \ ,$$

where γ represents Euler's constant.

Clearly, the very fast growth of Λ_n^{Eq} with n confirms that interpolation in S^1 using Π_n^{Eq} results in a very poor approximation for increasing n. Indeed, for $n \geq 65$, we find that $\mathcal{O}((\Lambda_n^{\mathrm{Eq}})^{-1}) \sim 10^{-16}$, rendering the approximation useless on most contemporary computers. For reasons of comparison, we list Λ_n^{Eq} for $n \in [1, 24]$ in Table 1.

Lebesgue constants for various choices of nodal sets. Listed is the minimum Lebesgue constant, $\Lambda_n^{\mathrm{JGL},\alpha}$, for the optimal value of α using the Jacobi-Gauss-Lobatto nodal set, $\Pi_n^{\mathrm{JGL},\alpha}$. Also given is Λ_n^{LGL} and Λ_n^{CGL} representing the Lebesgue constants for the Legendre-Gauss-Lobatto, Π_n^{LGL}, and the Chebyshev-Gauss-Lobatto, Π_n^{CGL}, nodal sets. For comparison we also list the the Lebesgue constants,Λ_n^{Opt}, for the optimal nodal set [27] and the Lebesgue constant, Λ_n^{Eq}, corresponding to an equally distributed nodal set, Π_n^{Eq}.

n	α	$\Lambda_n^{\mathrm{JGL},\alpha}$	Λ_n^{LGL}	Λ_n^{CGL}	Λ_n^{Opt}	Λ_n^{Eq}
1	*All*	1.0000	1.0000	1.0000	1.0000	1.0000
2	*All*	1.2500	1.2500	1.2500	1.2500	1.2500
3	0.364636	1.4229	1.5000	1.6667	1.4229	1.6311
4	0.390667	1.5595	1.6359	1.7988	1.5595	2.2078
5	0.410978	1.6746	1.7786	1.9889	1.6722	3.1063
6	0.420531	1.7709	1.8737	2.0826	1.7681	4.5493
7	0.428904	1.8560	1.9724	2.2022	1.8516	6.9297
8	0.433838	1.9301	2.0456	2.2747	1.9255	10.945
9	0.438665	1.9973	2.1210	2.3619	1.9917	17.848
10	0.441695	2.0575	2.1805	2.4210	2.0517	29.899
11	0.444993	2.1129	2.2415	2.4894	2.1066	51.214
12	0.446733	2.1636	2.2917	2.5393	2.1571	89.324
13	0.448718	2.2109	2.3428	2.5957	2.2040	158.09
14	0.450689	2.2545	2.3862	2.6388	2.2476	283.19
15	0.451792	2.2958	2.4303	2.6867	2.2884	512.35
16	0.453426	2.3341	2.4684	2.7247	2.3268	934.50
17	0.453893	2.3707	2.5072	2.7664	2.3630	1716.4
18	0.454938	2.4049	2.5412	2.8003	2.3973	3171.1
19	0.456111	2.4375	2.5758	2.8371	2.4298	5889.4
20	0.456752	2.4685	2.6065	2.8677	2.4608	10986.
21	0.457683	2.4980	2.6377	2.9008	-	20574.
22	0.459342	2.5260	2.6658	2.9288	-	38667.
23	0.459593	2.5532	2.6942	2.9587	-	72908.
24	0.459831	2.5792	2.7200	2.9844	-	137852.

Chebyshev Distributed Nodal Sets. Let us now turn towards nodal sets associated with zeros of Jacobi polynomials and begin by considering the Cauchy remainder for polynomial interpolation

$$f(x) - \mathcal{I}_n^1 f(x) = \prod_{i=1}^{n+1} (x - x_i) \frac{1}{(n+1)!} \frac{d^{n+1} f(x)}{dx^{n+1}} \ ,$$

indicating that a good choice for interpolation may be the nodal set minimizing $\| \prod_{i=1}^{n+1} (x - x_i) \|_\infty$. This uniquely determined nodal set, Π_n^{CG}, is recognized as the Chebyshev-Gauss quadrature points, i.e., the zeros of the Chebyshev polynomial, $P_{n+1}^{-1/2}(x) = T_{n+1}(\cos\theta) = \cos((n+1)\theta)$.

As realized by Stieltjes [1, 2], these points may found as a solution to the electrostatic problem with $p = q = 1/4$. Note, however, that this nodal set is not canonical since $\Pi_n^{\mathrm{CG}} = \{x_i | x_i = -\cos((2i-1)\pi/2(n+1))\}_{i=1}^{n+1}$. The Lebesgue constant, $\Lambda_n^{\mathrm{CG}} = \Lambda(\Pi_n^{\mathrm{CG}})$, for the Chebyshev-Gauss nodal set is given as [21, 22]

THEOREM 3.4. *The Lebesgue constant, Λ_n^{CG}, for interpolation using the Chebyshev-Gauss nodal set, Π_n^{CG}, is bounded for $n \geq 1$ as*

$$\Lambda_n^{\mathrm{CG}} = \frac{2}{\pi} \log(n+1) + A + \alpha_n \ ,$$

where

$$A = \frac{2}{\pi} \left(\gamma + \log \frac{8}{\pi} \right) \quad and \quad 0 < \alpha_n < \frac{\pi}{72(n+1)^2} \quad .$$

The asymptotic behavior of Λ_n^{CG} *is given by*

$$\Lambda_n^{\mathrm{CG}} \simeq \frac{2}{\pi} \log(n+1) + A + \frac{8}{\pi} \sum_{s=1}^{\infty} \frac{(-1)^{s+1} A_s}{[2(n+1)]^{2s}} \quad ,$$

where

$$A_s = \left(2^{2s-1} - 1 \right)^2 \frac{\pi^{2s}}{2s} \frac{B_{2s}^2}{(2s)!} \quad ,$$

and B_p *signifies the Bernoulli numbers.*

Comparing with the optimal values of the Lebesgue constant given in Theorem 3.2, is it clear that interpolation using Π_n^{CG} results in an approximation error being close to that of the optimal canonical nodal set.

However, if we consider the canonical Chebyshev-Gauss or extended Chebyshev-Gauss nodal set, Π_n^{ECG}, obtained through the linear mapping

$$\Pi_n^{\mathrm{ECG}} = \left\{ x_i \left| x_i = -\frac{\cos\left(\frac{2i-1}{2(n+1)}\pi\right)}{\cos\left(\frac{\pi}{2(n+1)}\right)} \right. \right\}_{i=1}^{n+1} \quad ,$$

the Lebesgue constant, $\Lambda_n^{\mathrm{ECG}} = \Lambda(\Pi_n^{\mathrm{ECG}})$, is bounded by [21]

THEOREM 3.5. *The Lebesgue constant,* Λ_n^{ECG}, *for interpolation using the extended Chebyshev-Gauss nodal set,* Π_n^{ECG}, *is bounded for* $n \geq 4$ *as*

$$\Lambda_n^{\mathrm{ECG}} = \frac{2}{\pi} \log(n+1) + A - \frac{4}{3\pi} + \beta_n \quad ,$$

where

$$0 < \beta_n < 0.01 \left[\log\left(\frac{n+1}{4} \right) \right]^{-1} \quad .$$

By expressing the two constants in the Theorems 3.4 and 3.5 as

$$A - \chi = \frac{2}{\pi} \log 2 \quad and \quad A - \frac{4}{3\pi} - \chi = \frac{2}{\pi} \left(\log 2 - \frac{2}{3} \right) = 0.01685801 \ldots \quad ,$$

it becomes clear that both nodal sets are close to the optimal set for large values of n. However, in particular the extended Chebyshev-Gauss nodal set, Π_n^{ECG}, results in an approximation that is very close to that obtained using the optimal nodal set. Indeed, to the best of our knowledge, the extended Chebyshev-Gauss nodal set is the best known nodal set with the position of the nodes given on closed form.

However, Π_n^{ECG}, does not represent a nodal set associated with the zeros of a Jacobi polynomial. As discussed previously, this issue is important in connection

with the solution of partial differential equations using spectral methods where high-order integration is required. Consequently, in such cases it is desirable that the nodal set is related to a Gauss quadrature formula, explaining why the extended Chebyshev-Gauss nodal set plays a less important role in this context.

Also, the Chebyshev-Gauss nodal set is less attractive for use in connection with spectral methods as the endpoints of the interval are not included, thereby making it hard to enforce boundary conditions. For these reasons, the most used nodal set for constructing approximate solutions to partial differential equations using spectral methods is the canonical Chebyshev-Gauss-Lobatto set being obtained as the zeros of the polynomial , $(1-x^2)T_n'(x)$, and is given on closed form as $\Pi_n^{CGL} = (-1, \{x_i\}_{i=2}^n, 1)$ where $x_i = -\cos((i-1)\pi/n)$.

To return to the electrostatic analogy, we recall that the Jacobi-Gauss quadrature points appear from the original work. However, since the Jacobi-Gauss-Lobatto quadrature points are obtained as the interior zeros of the polynomial $(P_n^\alpha(x))'$ and using the identity for Jacobi-polynomials [23],

$$2\frac{d}{dx}P_n^\alpha(x) = (n+1+2\alpha)P_{n-1}^{\alpha+1}(x) \ ,$$

we realize that also the Jacobi-Gauss-Lobatto quadrature points appear as solutions to the original electrostatic problem by using the relation, $\alpha = 2(p-1)$ and including the endpoints in the nodal set, e.g. using $p = q = 3/4$ results in the Chebyshev-Gauss-Lobatto nodal set ($\alpha = -\frac{1}{2}$).

Estimation of the Lebesgue constant, $\Lambda_n^{\text{CGL}} = \Lambda(\Pi_n^{\text{CGL}})$, for the Chebyshev-Gauss-Lobatto nodal set is done in [24], yielding the following result

THEOREM 3.6. *The Lebesgue constant, Λ_n^{CGL}, using the Chebyshev-Gauss-Lobatto nodal set, Π_n^{CGL}, is bounded as*

$$\Lambda_n^{\text{CGL}} < \Lambda_{n-1}^{\text{CG}} \quad n \ even$$
$$\Lambda_n^{\text{CGL}} = \Lambda_{n-1}^{\text{CG}} \quad n \ odd$$

where Λ_n^{CG} represents the Lebesgue constant obtained for the Chebyshev-Gauss nodal set, Π_n^{CG}, as given in Theorem 3.4.

We immediately observe that in addition to the desirable property that the Gauss-Lobatto nodal sets includes the endpoints of S^1, the Lebesgue constants are also uniformly bounded by those obtained using the Gauss nodal set.

The tight bound on Λ_n^{CGL} for n being odd is possible due to the observation [24] that $\Lambda_n^{\text{CGL}} = \lambda(\Pi_n^{\text{CGL}}, 0)$, where $\lambda(\Pi_n^{\text{CGL}}, x)$ represents the Lebesgue function. Based on extensive numerical evidence, we conjecture that

CONJECTURE 3.1. *The Lebesgue constant, Λ_n^{CGL}, using the Chebyshev-Gauss-Lobatto nodal set, Π_n^{CGL}, is given as*

$$n \ even \ : \Lambda_n^{\text{CGL}} = \lambda\left(\Pi_n^{\text{CGL}}, \frac{\pi}{2n}\right) \ , \ n \to \infty \ .$$

For n being even, $x = 0$ is always part of the nodal set as $x_{n/2}$. Consequently, it is conjectured that the Lebesgue function attains it maximum value exactly between the center node, $x_{n/2}$, and $x_{(n+2)/2}$, since

$$\frac{x_{(n+2)/2}}{2} = -\frac{1}{2}\cos\left(\frac{\pi}{2}\frac{n+2}{n}\right) = \frac{1}{2}\sin\left(\frac{\pi}{n}\right) \sim \frac{\pi}{2n} ,$$

for large values of n. This result conforms well with the result that for n being odd the maximum of the Lebesgue function is also found exactly between the two center nodes, i.e. at $x = 0$.

Values of the Lebesgue constant, Λ_n^{CGL}, is given in Table 1 for $n \in [1, 24]$, and in Fig. 1 we have plot Λ_n^{CGL} for large n confirming the logarithmic dependence on n.

Legendre Distributed Nodal Sets. Based on the general expression for the interpolating Lagrange polynomials, Eq.(2), it appears that the nodal set maximizing the Vandermonde determinant, $|\mathrm{VDM}|$, could be expected to yield an interpolating polynomial with a small value of the Lebesgue constant. As shown in [25] this nodal set is given as $\Pi_n^{\mathrm{LGL}} = (-1, \{x_i\}_{i=2}^n, 1)$ where $\{x_i\}_{i=2}^n = \{x_i | (P_n^0(x_i))' = 0\}_{i=2}^n$, i.e. the extrema of $P_n^0(x)$ also known as the Legendre polynomial. This nodal set, Π_n^{LGL}, is known as the Legendre-Gauss-Lobatto or the Fekete/Fejér nodal set.

Estimates for the Lebesgue constant, $\Lambda_n^{\mathrm{LGL}} = \Lambda(\Pi_n^{\mathrm{LGL}})$ are sparse, the problem being that no explicit formula for the nodal set is known. The first estimate is possibly given in [25] as $\Lambda_n^{\mathrm{LGL}} \leq \sqrt{n+1}$, which is also obtained simply by applying the Cauchy-Schwartz inequality and the fact $\sum_{i=1}^{n+1} |L_i(\Pi_n^{\mathrm{LGL}}, x)|^2 \leq 1$. This, however, is very pessimistic, as evidenced by the conjecture in [13] that $\Lambda_n^{\mathrm{LGL}} < \Lambda_n^{\mathrm{CG}}$, and an estimate as $\Lambda_n^{\mathrm{LGL}} \leq c\log(n+1)$ was put forward in [26] although the constant, c, remains undetermined. Based on numerical experiments, we conjecture the following

CONJECTURE 3.2. *The Lebesgue constant, Λ_n^{LGL}, using the Legendre-Gauss-Lobatto nodal set, Π_n^{LGL}, is bounded as*

$$\Lambda_n^{\mathrm{LGL}} \leq \frac{2}{\pi}\log(n+1) + 0.685 ,$$

and

$$\Lambda_n^{\mathrm{LGL}} = \lambda(\Pi_n^{\mathrm{LGL}}, 0) \qquad n \ odd$$

$$\Lambda_n^{\mathrm{LGL}} \simeq \lambda\left(\Pi_n^{\mathrm{LGL}}, \frac{\pi}{2n}\right) \quad n \ even$$

This conjecture is consistent with those put forward in [13] and does indeed confirm that $\Lambda_n^{\mathrm{LGL}} < \Lambda_n^{\mathrm{CG}}$ uniformly in n. Additionally, we also find $\Lambda_n^{\mathrm{LGL}} < \Lambda_n^{\mathrm{CGL}}$ uniformly in n as is illustrated in Fig. 1. Numerical values of Λ_n^{LGL} are given in Table 1 for $n \in [1, 24]$ supporting the conjecture.

Jacobi Distributed Nodal Sets. Let us finally focus the attention at the general case, for which very little is known. If we first consider the Jacobi-Gauss nodal set, $\Pi_n^{\mathrm{JG},\alpha}$, being given as $\Pi_n^{\mathrm{JG},\alpha} = \{x_i | P_{n+1}^\alpha(x_i) = 0\}_{i=1}^{n+1}$ the most general result is [3]

THEOREM 3.7. *The Lebesgue constant, $\Lambda_n^{\mathrm{JG},\alpha}$, using the Jacobi-Gauss nodal set, Π_n^{LGL}, scales as*

$$\begin{array}{ll} \Lambda_n^{\mathrm{JG},\alpha} \sim \mathcal{O}(\log(n+1)) & \alpha \leq -\frac{1}{2} \\ \Lambda_n^{\mathrm{JG},\alpha} \sim \mathcal{O}(\sqrt{n+1}) & \alpha > -\frac{1}{2} \end{array} ,$$
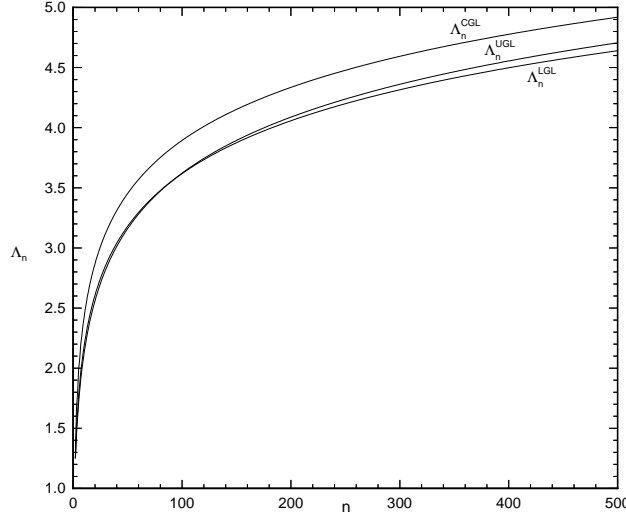
FIG. 1. *The Lebesgue constants as a function of n for various choices of Jacobi-Gauss-Lobatto nodal sets. Shown are the Lebesgue constants for the Legendre polynomials, Λ_n^{LGL}, and for Chebyshev polynomials of the first, Λ_n^{CGL}, and second kind, Λ_n^{UGL}, respectively.*

Unfortunately, no such general results exist when considering the nodal sets, $\Pi_n^{\mathrm{JGL},\alpha}$, based on the Jacobi-Gauss-Lobatto quadrature points, given as $\Pi_n^{\mathrm{JGL},\alpha} = (-1, \{x_i\}_{i=2}^n, 1)$ where we have $\{x_i\}_{i=2}^n = \{x_i | (P_n^\alpha(x_i))' = 0\}_{i=2}^n$. We have previously discussed the two special cases of the Chebyshev-Gauss-Lobatto nodal set, $\alpha = -1/2$, and the Legendre-Gauss-Lobatto nodal set, $\alpha = 0$. An interesting question arises: Among all $\Pi_n^{\mathrm{JGL},\alpha}$, which value of α minimizes the Lebesgue constant, $\Lambda_n^{\mathrm{JGL},\alpha}$ for a given n?

In attempting to address this question, we give in Table 1 the value of α leading to the minimum Lebesgue constant, $\Lambda_n^{\mathrm{JGL},\alpha}$, among all the nodal sets based on the Jacobi-Gauss-Lobatto quadrature points, $\Pi_n^{\mathrm{JGL},\alpha}$ for various values of n. By comparing with the Lebesgue constants, Λ_n^{Opt}, for the optimal nodal set [27], is it clear that the computed Jacobi-Gauss-Lobatto nodal sets are very close to the optimal nodal set. We observe that the value of α leading to the optimal nodal set varies with n, although, it seems that it asymptotes towards a fixed value around $\alpha \simeq 0.5$. This tendency is found to be maintained for $n \leq 60$. However, we have been unable to continue the computation beyond this point as the computation of the optimal value of α becomes prohibitively expensive due to the many required computations of the corresponding Lebesgue constant.

The value of $\alpha = 1/2$ corresponds to a nodal set, Π_n^{UGL}, based on the Gauss-Lobatto quadrature points for the Chebyshev polynomial of the second kind being given as $U_n(\cos(\theta)) = \sin((n+1)\theta)/\sin\theta$. Unfortunately, as we will see shortly, the hypothesis that Π_n^{UGL} is close to the optimal nodal set is only valid for small n. We recall that the nodal set is given on explicit form as $\Pi_n^{\mathrm{UGL}} = \{-1, \{x_i\}_{i=2}^n, 1\}$ where $x_i = -\cos((2i-1)\pi/2(n+1))$.

We are not aware of any results estimating the Lebesgue constant, $\Lambda_N^{\mathrm{UGL}} = \Lambda(\Pi_n^{\mathrm{UGL}})$, using the Gauss-Lobatto nodal set of the Chebyshev polynomials of the second kind. Based on extensive numerical studies we conjecture the following

CONJECTURE 3.3. *The Lebesgue constant, Λ_n^{UGL}, using the Chebyshev-Gauss-Lobatto nodal set, Π_n^{UGL}, is bounded as*

$$\Lambda_n^{\mathrm{UGL}} \leq \frac{2}{\pi} \log(n+1) + \beta_n \ ,$$

with

$$0 < \beta_n < 0.525 f(n+1) \ ,$$

where f is a weak function of n behaving asymptotically as

$$n \to \infty \ : \ \frac{f(n)}{\log n} \to \infty \ , \ \frac{f(n)}{\sqrt{n}} \to 0 \ .$$

We have been unable to estimate the unknown function, $f(n)$, more accurately. However, numerical studies indicate that asymptotically, $f(n) \simeq n^\alpha$, where $\alpha \sim \mathcal{O}(0.1)$.

We observe that for small values of n, the nodal sets associated with Chebyshev polynomials of the second kind results in a Lebesgue constant that is very close to the optimal one as given in Theorem 3.2. However, the slow growth of Λ_n^{UGL} with n renders this property invalid for increasing n. In Fig. 1 we compare Λ_n^{UGL} with Λ_n^{LGL} and Λ_n^{CGL} to find that the former is superior to the more commonly used Chebyshev-Gauss-Lobatto points for any practical value of n, while it is superior to the Legendre-Gauss-Lobatto points only for small n. An attractive property of Π_n^{UGL} is , however, that it is given on explicit form contrary to Π_n^{LGL}.

In the present section we have summarized and extended the results for interpolation on nodal sets with particular emphasis on nodal sets appearing as solutions to an electrostatic problem and related to the symmetric Jacobi-polynomials. The results may most easily be summarized as

$$\Lambda_n^{\mathrm{Eq}} > \Lambda_n^{\mathrm{CG}} > \Lambda_n^{\mathrm{CGL}} > \Lambda_n^{\mathrm{LGL}} \sim \Lambda_n^{\mathrm{UGL}} > \Lambda_n^{\mathrm{ECG}} \ ,$$

which we believe is valid for all practical values of n in the context of spectral methods and is consistent with results put forward in [13, 28].

Although there remains many open questions to be answered when considering interpolation in S^1 using Jacobi-Gauss-Lobatto nodal sets, it seems clear, however, that some of the nodal sets obtainable through the solution of an electrostatic problem are very close to what is theoretically possible.

4. Interpolation Points in S^2 Using Electrostatics. The problem of polynomial interpolation in S^2 is considerable more complex than in S^1 and very little is known. Hence, in the present work we shall focus the attention on polynomial interpolation of functions defined on an equilateral triangle, S^2, as pictured in Fig. 2.

In the present context, it is convenient to use barycentric coordinates. Let us denote $\boldsymbol{v}_i$, $i \in [1,3]$, as the three vertices, i.e., in this case $\boldsymbol{v}_1 = (-1,0)$, $\boldsymbol{v}_2 = (0,\sqrt{3})$ and $\boldsymbol{v}_3 = (1,0)$, such that any $\boldsymbol{x} \in \mathsf{S}^2$ can be expressed using a convex combination of the barycentric coordinates, (b_1, b_2, b_3), as

$$\boldsymbol{x} = \sum_{i=1}^{3} \boldsymbol{v}_i b_i \quad \text{and} \quad \sum_{i=1}^{3} b_i = 1 \ ,$$

and $0 \leq b_i \leq 1$.
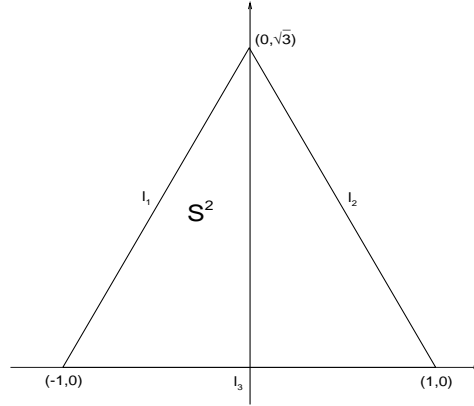
FIG. 2. *The standard equilateral triangle,* S^2.

We introduce the polynomial space, $\mathsf{P}_n^2 = \mathrm{span}\{p_{ij}(\boldsymbol{x}) = x^i y^j; i, j \geq 0; i + j \leq n\}$. The basis functions spanning the polynomial space may conveniently be thought of as

$$
\begin{array}{ccccccc}
& & & 1 & & & \\
& & x & & y & & \\
& x^2 & & xy & & y^2 & \\
x^3 & & x^2 y & & y^2 x & & y^3 \\
& & & \vdots & & &
\end{array}
$$

Estimation of the Lebesgue constant for interpolation in S^2 is extremely difficult and only for the equidistant grid in barycentric coordinates, given as

$$
\Pi_n^{\mathrm{Eq}} = \left\{ \boldsymbol{x}_i \, \middle| \, (b_1, b_2, b_3) = \left(1 - \frac{k+l}{n}, \frac{k}{n}, \frac{l}{n} \right) ; k \geq 0, l \geq 0, k + l \leq n \right\}_{i=1}^{N} \;,
$$

do results exist. We recall that n represents the order of the polynomial approximation and also signifies the order of the polynomial employed along the edges. The explicit expression for the interpolating Lagrange polynomial, $L_i(\Pi_n^{\mathrm{Eq}}, \boldsymbol{x})$, is given in [29], where also the bound for the Lebesgue constant, Λ_n^{Eq}, is derived

THEOREM 4.1. *The Lebesgue constant,* Λ_n^{Eq}, *using the nodal set,* Π_n^{Eq}, *for polynomial interpolation in* S^2 *is bounded as*

$$
\Lambda_n^{\mathrm{Eq}} \leq \binom{2n-1}{n} \;.
$$

As for interpolation along the line, we observe an extremely rapid growth of Λ_n^{Eq} essentially rendering this nodal set useless for high order polynomial interpolation. For reasons of comparison, we list the Lebesgue constants for $n \in [1, 16]$ in Table 2. The question naturally raises as to whether it is possible to obtain nodal sets better suited than Π_n^{Eq} for interpolation in S^2.

This question was first addressed in [29] by realizing from Eq.(2) that a good nodal set could be obtained by maximizing the Vandermonde determinant, |VDM|, much like the procedure that leads to the Legendre-Gauss-Lobatto points discussed previously. However, the study was quite restricted and nodal sets was computed only for $n \leq 7$.

Recently, a more thorough study was published in [27], where nodal sets, resulting in a significantly slower growth of the Lebesgue constant than obtained for Π_n^{Eq}, were obtained by minimizing over the L_2-norm of the Lebesgue-function for $n \in [2, 13]$. As is evident from the computed Lebesgue constants, Λ_n^{Opt}, as reproduced in Table 2, the suggested procedure yields very good nodal sets, although there is no way one can know whether these are the optimal sets. Indeed, as we will show shortly, at least for $n \leq 5$ is it possible to find sets with a smaller Lebesgue constant. However, the main reason for our interest in obtaining alternative nodal sets is the fact that the sets given in [27] does not have nodal distributions along the edges that can be identified as Jacobi-Gauss-Lobatto quadrature points. As we have argued previously, this latter property is advantageous if one wishes to apply the polynomials on the simplex in connection with spectral methods which are almost exclusively based on Jacobi polynomials.

Inspired by the success of polynomial interpolation in S^1 when using nodal sets appearing as solutions to an electrostatic problem, we now propose to consider the following scenario.

Assume that the edges of the simplex, S^2, labeled l_l as illustrated in Fig. 2, are fragments of a continuous line-charge with the charge density, $\rho_l^L > 0$. Consider now an arbitrary edge, l_l, connecting the two vertices, $\boldsymbol{v}_a = (x_a, y_a)$ and $\boldsymbol{v}_b = (x_b, y_b)$. The electrostatic force, $\boldsymbol{F}_l(\boldsymbol{x})$, from the line acting on a particle with the charge, ρ_p, held at the position $\boldsymbol{x}$, is then given as $\boldsymbol{F}_l^L(\boldsymbol{x}) = \rho_p \boldsymbol{E}_l^L(\boldsymbol{x}) = -\rho_p \nabla \phi_l^L$, where ϕ_l^L is the electrostatic potential from the edge, l_l. Contrary to the approach used in S^1, where the potential is logarithmic, we assume the potential to be algebraic, such that the potential from the line-fragment at $\boldsymbol{x}$ is given as

$$\phi_l^L(\boldsymbol{x}) = \rho_l^L \int_0^1 \frac{1}{|\boldsymbol{x} - \boldsymbol{x}_L|} \, dt \ ,$$

where $\boldsymbol{x}_L = \boldsymbol{v}_a + t(\boldsymbol{v}_b - \boldsymbol{v}_a)$, $t \in [0, 1]$ represents the edge. It is straightforward to perform this integration analytically.

We also assume that a number, N_p, of unit mass charges, ρ_p, are allowed to move freely inside the simplex, mutually interacting according to the potential

$$\phi(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{\rho_p^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|} \ .$$

Let us now propose to consider the following problem -

Problem: Let the line charge density be given as $\rho_l^L > 0$. Assume also that N_p unit mass charges with unit charge, $\rho_p = 1$, are allowed to move freely inside the simplex. What is the steady state position of the charges that minimize the electrostatic energy

$$W(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{N_p}) = \sum_{i=1}^{N_p} \left(\sum_{l=1}^{3} \phi_l^L(\boldsymbol{x}_i) + \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{N_p} \phi(\boldsymbol{x}_i, \boldsymbol{x}_j) \right) \quad .$$

The problem is clearly very similar to the one originally put forward by Stieltjes[1, 2], however with significantly more complexity.

Contrary to the $m = 1$ case, we have no prior knowledge of a proper choice of the line charge density of the line, ρ_l^L, in order to obtain nodal sets well suited for polynomial interpolation. Indeed, we will later use this free parameter for optimizing the nodal sets. However, based on the knowledge gained from S^1 we believe that the most appropriate choice is $\rho_1^L = \rho_2^L = \rho_3^L = \rho^L$, i.e., the external potential field imposed by the line-charges is symmetric.

As the aim is to construct nodal sets well suited for approximating partial differential equations in a multi-domain setting, we require that the edges contain interpolation points. However, the specification of these points is at this point undetermined.

We also remind that the aim is to construct interpolating polynomials with the edge polynomials having the same order as that of the global interpolating polynomials, i.e. the total number of nodal points should be related to the number of freely moving charges as $N_p = N_n^2 - 3n$, where $3n$ is the number of nodal points reserved for the edges. This value of N_p allows for the construction of a complete basis as discussed in Section 2.

We have chosen to approach the problem by solving it numerically as an N-body problem by integrating Newtons 2nd law as

$$\ddot{\boldsymbol{x}}_i = -\left(\sum_{l=1}^{3} \nabla \phi_l^L(\boldsymbol{x}_i) + \sum_{\substack{j=1 \\ j \neq i}}^{N_p} \nabla \phi(\boldsymbol{x}_i, \boldsymbol{x}_j) \right) - \varepsilon \dot{\boldsymbol{x}}_i \quad ,$$

where the last term, $\dot{\boldsymbol{x}}_i$, corresponds to a small friction in order to make the problem slightly dissipative. This equation is advanced in time using a 7(6) embedded Nyström-Runge-Kutta scheme with error control [30]. The resulting solution is passed on as an initial guess to a nonlinear solver to find the true steady state solution. We have used a algorithm based on a modification of Powell's hybrid algorithm [31].

The single most important remaining point is how to chose the initial conditions. Finding the global minimum of the energy function is in general extremely complicated in particular for increasing N_p. However, since we are interested in solutions suitable for polynomial interpolation, we restrict the attention to steady-state solutions that process a high degree of symmetry. Inside the simplex, we consider solutions that are constructed of three symmetry patterns. A charge can be situated at the center of the triangle, termed a 1-symmetry; it can be positioned along one of the three meridians, termed a 3-symmetry; or it can be inside one of the six sub-triangles bounded by the symmetry-axes, referred to as a 6-symmetry. If we denote the number of charges with a 1-symmetry, n_1, the number of charges with a 3-symmetry, n_3, and

TABLE 2

Lebesgue constants for various choices of nodal sets in the simplex. Listed is the computed Lebesgue constants for the nodal set, $\Lambda_n^{\mathrm{JGL},\alpha}$ with the optimal Jacobi-Gauss-Lobatto quadrature points along the edges. Λ_n^{LGL} and Λ_n^{CGL} represents the Lebesgue constants for the nodal sets with the Legendre-Gauss-Lobatto and Chebyshev-Gauss-Lobatto nodes along the edges, respectively. For comparison, we also give the Lebesgue constants, Λ_n^{Opt}, for the nodal sets presented in [27], and the Lebesgue constants, Λ_n^{Eq}, for the equidistant nodal set, Π_n^{Eq}.

n	N_n^2	$\Lambda_n^{\mathrm{JGL},\alpha}$	Λ_n^{LGL}	Λ_n^{CGL}	Λ_n^{Opt}	Λ_n^{Eq}
1	3	1.0000	1.0000	1.0000	1.0000	1.0000
2	6	1.6667	1.6667	1.6667	1.6667	1.6667
3	10	2.1299	2.1125	2.1150	2.1115	2.2698
4	15	2.6033	2.5878	2.6050	2.6920	3.4748
5	21	3.2171	3.1958	3.2096	3.3010	5.4522
6	28	4.1291	4.0752	4.0736	3.7910	8.7477
7	36	4.8848	4.7753	4.7846	4.3908	14.345
8	45	6.0127	5.8518	5.8786	5.0893	24.007
9	55	7.1075	6.8717	6.9174	5.9181	40.923
10	66	8.371	8.4412	8.3963	7.0851	70.891
11	78	10.603	10.075	10.091	8.3383	124.53
12	91	13.550	12.628	12.517	10.082	221.41
13	105	-	-	15.336	12.046	397.70
14	120	-	-	22.184	-	720.70
15	136	-	-	29.691	-	1315.9
16	153	-	-	41.726	-	2418.5

those with a 6-symmetry as n_6, the total number of charges is then obtained as $N_p = (n-1)(n-2)/2 = n_1 + 3n_3 + 6n_6$.

The integer solution to this equation is non-unique for $n > 4$. Different solutions correspond to different symmetry patterns inherent in the distribution of the charges. We have used these initial symmetry patterns to construct the initial conditions and then searched for the specific symmetry pattern that results in a steady state solution with the minimum energy among all the possible symmetry patterns for a given n.

Having established the computational framework, let us now return to the two outstanding problems - specification of the line-charge, ρ^L, and the distribution of the nodes along the edges. As mentioned previously, we are primarily interested in having a distribution of nodal points along the edges that is related to Jacobi-Gauss-Lobatto quadrature points, i.e. they are uniquely determined by the parameter, α, of the Jacobi polynomial. At this point we realize that the problem of finding the best nodal distribution inside the simplex is reduced to a two-parameter minimization problem in ρ^L and α. This is much like the original problem, however, with the unfortunate difference that in S^2 we do not know how they are related or even if they are.

In the following we have used the approach outlined above to find symmetric, steady state solutions to the electrostatic problem. However, doing a full two-dimensional optimization is out of reach and we have restricted the attention to a few special cases of α that is of most interest within the present context.

For a fixed value of α, the problem is reduced to a one-dimensional minimization problem in ρ^L, which is feasible. In all problems we find that $\rho^L \sim \mathcal{O}(1)$, but varies slightly with n as well as with α.

As the most natural choice of α in relation to spectral methods, we have computed the nodal sets for $\alpha = -1/2$, corresponding to the Chebyshev-Gauss-Lobatto nodal set along the edge. In Table 2, we give the corresponding Lebesgue constant, Λ_n^{CGL},
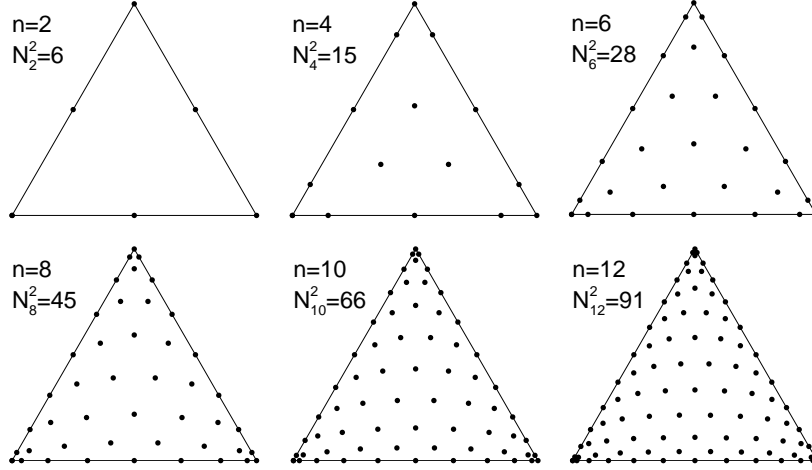
FIG. 3. *Nodal sets in the equilateral triangle with Chebyshev-Gauss-Lobatto nodal sets along the edges.*

for increasing n, confirming the soundness of the electrostatic approach. Indeed, we observe that the computed nodal sets are very good as compared to the corresponding equidistant nodal set and compare well also with the nodal sets presented in [27], indeed being superior for small values of n. In Appendix A we give the barycentric coordinates for the computed nodal sets for $n \in [2, 16]$.

Another widely used nodal set for spectral methods is based on the Legendre-Gauss-Lobatto nodal set, i.e. corresponding to $\alpha = 0$. We have obtained nodal sets with the Legendre-Gauss-Lobatto nodal set along the edges and the corresponding Lebesgue constants, Λ_n^{LGL}, is also given in Table 2. Not surprisingly, we observe that these nodal sets seems to be slightly better than those related to the Chebyshev nodal sets, being consistent with the findings in S^1. The barycentric coordinates of the computed nodal sets are given in Appendix B, although we give them only for $n \in [2, 12]$. For larger values of n the optimal interior nodal sets are virtually identical to those obtained when using the Chebyshev-Gauss-Lobatto quadrature points along the edges since the contribution of the edges to the value of the Lebesgue constant becomes less and less significant for increasing n. Consequently, the nodal sets obtained when optimizing in ρ^L for different values of α are very similar for large n. We therefore advocate using the nodal sets given in Appendix A also for $\alpha = 0$ and $n > 12$.

For comparison, we also give the Lebesgue constant, $\Lambda_n^{JGL,\alpha}$, for nodal sets optimized for use with the optimal one-dimensional Jacobi-Gauss-Lobatto nodal set along the edges and in Table 2, showing that both of the former nodal sets are superior to this latter set, which we therefore discard.

Regarding the value of the optimal line-charge, we find that for small values n, ρ^L is highly dependent on the choice of α. However, for increasing n, i.e. $n > 10$, the optimal value of ρ^L is virtually independent on α and attains a value of $\rho^L \simeq 0.75$.

In Fig. 3 we illustrate the resulting nodal sets for $\alpha = -0.5$ and various values of n, clearly showing the high degree of symmetry characterizing the nodal sets.

5. Concluding Remarks. In this paper we have exploited the remarkable connection between solutions to problems of electrostatics and nodal sets well suited for polynomial interpolation along the line. The emphasis has been on nodal sets con-

structed from the Jacobi-Gauss-Lobatto quadrature points and we have shown how they relate to the solution of a problem of electrostatics. Based on extensive numerical evidence we have also conjectured several estimates of the variation of the Lebesgue constant with n for the Jacobi-Gauss-Lobatto quadrature points for which only few analytical results exist. In particular, our results indicate that the nodal sets based on the Gauss-Lobatto quadrature points of the Chebyshev polynomial of the second kind is the best choice among the Jacobi polynomials for which there exists a closed form expression of the nodal set. This suggests that the Chebyshev polynomial of the second kind, rather that the extensively used Chebyshev polynomials of the first kind, could be used with advantage as the basis functions for solving partial differential equations using spectral methods, at least for small values of N where fast transforms are of less importance.

The possibility of formulating an electrostatic problem leading to very good nodal sets for polynomial interpolation along the line inspired us to attempt a similar approach in a 2-simplex with the emphasis being on an equilateral triangle. We have formulated a natural extension of the original approach and found that the solution of that electrostatic problem leads to nodal sets which are very close to the best known sets, thus confirming that the electrostatic analogy seems to carry over to the multi-dimensional case, provided the problem is properly posed. Indeed, there are many ways this can be done, in particular with respect to the treatment of the bounding edges, where we chose the simplest possible approach in order to minimize the computational workload required to find the sought after steady state solutions. However, our results clearly show that there is a connection between the solution to problems of electrostatics and nodal sets well suited for polynomial interpolation in the multi-dimensional simplex. It is our belief that a very similar approach can be applied for finding suitable nodal sets in a higher dimensional simplex as well.

When computing the nodal sets for polynomial interpolation in the equilateral triangle, we chose to restrict the attention to solutions where the nodes along the edges were distributed as Gauss-Lobatto quadrature points of Chebyshev or Legendre polynomials. The reason for this being that Chebyshev and Legendre polynomials are the most commonly used polynomial basis used for obtaining solutions to partial differential equations through spectral methods. Consequently, the computed nodal sets can easily be combined with more conventional multi-domain spectral methods or even provide the basic building block for a triangular spectral element method with unstructured grids interior to the triangle [32]

Appendix A: Nodal Matrix for the Triangle with Chebyshev-Gauss-Lobatto Nodal Sets Along the Edges. In the following we give the barycentric coordinates for the nodal sets optimized for use with Chebyshev-Gauss-Lobatto nodal sets of order n along the edges, i.e., they are distributed as the zeros of the polynomial, $(1-x^2)T'_n(x)$. Only the nodes interior to the simplex are given and nodes processing symmetries are only given once. The remaining nodes can be found by permutations of the barycentric coordinates.

n	n_1	n_2	n_3	b_1	b_2	b_3
3	1			0.3333333333	0.3333333333	0.3333333333
4		1		0.2410021998	0.2410021998	0.5179956004
5		2		0.1591570023	0.1591570023	0.6816859954
				0.4099016620	0.4099016620	0.1801966760
6	1			0.3333333333	0.3333333333	0.3333333333
		1		0.1048904342	0.1048904342	0.7902191316
			1	0.3095036860	0.5582114022	0.1322849118
7		3		0.0666479037	0.0666479037	0.8667041924
				0.4474963910	0.4474963910	0.1050072180
				0.2606379453	0.2606379453	0.4787241094
			1	0.2328951264	0.6750593997	0.0920454739
8		3		0.0467325482	0.0467325482	0.9065349036
				0.2031909379	0.2031909379	0.5936181242
				0.3906323571	0.3906323571	0.2187352858
			2	0.3618069634	0.5544121321	0.0837809045
				0.1799524415	0.7523326932	0.0677148653
9	1			0.3333333333	0.3333333333	0.3333333333
		3		0.0354284515	0.0354284515	0.9291430970
				0.4641239296	0.4641239296	0.0717521408
				0.1632684184	0.1632684184	0.6734631632
			3	0.2965866112	0.6351919517	0.0682214371
				0.1437685751	0.8034472485	0.0527841764
				0.3225938344	0.4969468296	0.1804593360
10		4		0.0267617465	0.0267617465	0.9464765070
				0.1333154550	0.1333154550	0.7333690900
				0.4230209738	0.4230209738	0.1539580524
				0.2834641787	0.2834641787	0.4330716426
			4	0.3934497870	0.5469389728	0.0596112402
				0.2464304982	0.6986850110	0.0548844908
				0.1165696792	0.8422416956	0.0411886252
				0.2707661899	0.5807728926	0.1484609175
11		5		0.0205770993	0.0205770993	0.9588458014
				0.4745463805	0.4745463805	0.0509072390
				0.1106491928	0.1106491928	0.7787016144
				0.2422912395	0.2422912395	0.5154175210
				0.3764104927	0.3764104927	0.2471790146
			5	0.3362467835	0.6143637919	0.0493894246
				0.2075057639	0.7480004251	0.0444938110
				0.0961598440	0.8711975595	0.0326425965
				0.3648517435	0.5058451075	0.1293031490
				0.2299937315	0.6463450688	0.1236611997
12	1			0.3333333333	0.3333333333	0.3333333333
		4		0.0157664060	0.0157664060	0.9684671880
				0.0927641836	0.0927641836	0.8144716328
				0.4451055330	0.4451055330	0.1097889340
				0.2092594550	0.2092594550	0.5814810900
			7	0.4144591572	0.5428398510	0.0427009918
				0.2891782274	0.6704310002	0.0403907724
				0.1766396330	0.7874226099	0.0359377571
				0.0801575546	0.8939792746	0.0258631708
				0.3176588844	0.5750391576	0.1073019580
				0.1970549373	0.6986253330	0.1043197297
				0.3292289528	0.4566354051	0.2141356421

n	n_1	n_2	n_3	b_1	b_2	b_3
13		6		0.0125158559	0.0125158559	0.9749682882
				0.4814041934	0.4814041934	0.0371916132
				0.0791069148	0.0791069148	0.8417861704
				0.1831015613	0.1831015613	0.6337968774
				0.4068245409	0.4068245409	0.1863509182
				0.2954002632	0.2954002632	0.4091994736
			8	0.3615540438	0.6022119116	0.0362340446
				0.2513189999	0.7149811088	0.0336998913
				0.1523482839	0.8179762698	0.0296754463
				0.0680753374	0.9108476566	0.0210770060
				0.3944786597	0.5151527485	0.0903685918
				0.2767319260	0.6304802457	0.0927878283
				0.1706952037	0.7399484931	0.0893563032
				0.2915934740	0.5215057084	0.1869008176
14		6		0.4587977340	0.4587977340	0.0824045320
				0.3671908093	0.3671908093	0.2656183814
				0.2595748224	0.2595748224	0.4808503552
				0.1603773315	0.1603773315	0.6792453370
				0.0685768901	0.0685768901	0.8628462198
				0.0103478215	0.0103478215	0.9793043570
			10	0.9234057833	0.0588664441	0.0177277726
				0.8416660290	0.1330619104	0.0252720607
				0.7521462903	0.2191316332	0.0287220764
				0.6425344401	0.3256595455	0.0318060144
				0.5379997781	0.4292596705	0.0327405513
				0.4692799339	0.3610693351	0.1696507310
				0.7721478696	0.1494014554	0.0784506750
				0.5652822600	0.3505856755	0.0841320645
				0.6781794781	0.2494595411	0.0723609808
				0.5834887797	0.2550816171	0.1614296032
15	1			0.3333333333	0.3333333333	0.3333333333
		6		0.4852528832	0.4852528832	0.0294942336
				0.4255990820	0.4255990820	0.1488018360
				0.2320836842	0.2320836842	0.5358326316
				0.1405179457	0.1405179457	0.7189641086
				0.0599963506	0.0599963506	0.8800072988
				0.0085857218	0.0085857218	0.9828285564
			12	0.9337196169	0.0512926813	0.0149877018
				0.8617284617	0.1169291070	0.0213424313
				0.7794706504	0.1957424109	0.0247869387
				0.6834546988	0.2890601702	0.0274851310
				0.5886608293	0.3824865582	0.0288526124
				0.8006726315	0.1325472687	0.0667800998
				0.7134213061	0.2207559648	0.0658227291
				0.6135939037	0.3123505510	0.0740555453
				0.5171616793	0.4145995177	0.0682388030
				0.6286428956	0.2270147509	0.1443423535
				0.5244220875	0.3265860871	0.1489918254
				0.4324830342	0.3299898010	0.2375271649

n	n_1	n_2	n_3	b_1	b_2	b_3
16		7		0.4692881367	0.4692881367	0.0614237267
				0.3932305456	0.3932305456	0.2135389089
				0.3025577746	0.3025577746	0.3948844509
				0.2078492229	0.2078492229	0.5843015542
				0.1284932701	0.1284932701	0.7430134598
				0.0529388222	0.0529388222	0.8941223556
				0.0072437614	0.0072437614	0.9855124772
			14	0.9419105656	0.0452492885	0.0128401458
				0.8772044870	0.1042200005	0.0185755125
				0.8060459745	0.1727546471	0.0211993784
				0.7198500717	0.2560058606	0.0241440677
				0.6256312013	0.3487602527	0.0256085459
				0.5343544917	0.4393591499	0.0262863584
				0.8214366546	0.1173927115	0.0611706338
				0.7464832409	0.1959218281	0.0575949309
				0.6578452111	0.2860606787	0.0560941102
				0.5620632423	0.3743524772	0.0635842805
				0.6657283975	0.1263493158	0.2079222867
				0.5755509622	0.2921362629	0.1323127749
				0.4806452274	0.3853613574	0.1339934152
				0.4883520007	0.2978352313	0.2138127680

Appendix B: Nodal Matrix for the Triangle with Legendre-Gauss-Lobatto Nodal Sets Along the Edges. In the following we give the barycentric coordinates for the nodal sets optimized for use with Legendre-Gauss-Lobatto nodal sets of order n along the edges, i.e., they are distributed as the zeros of the polynomial, $(1 - x^2)P_n'(x)$. Only the nodes interior to the simplex are given and nodes processing symmetries are only given once. The remaining nodes can be found by permutations of the barycentric coordinates.

n	n_1	n_2	n_3	b_1	b_2	b_3
3	1			0.3333333333	0.3333333333	0.3333333333
4		1		0.2371200168	0.2371200168	0.5257599664
5		2		0.1575181512	0.1575181512	0.6849636976
				0.4105151510	0.4105151510	0.1789696980
6	1			0.3333333333	0.3333333333	0.3333333333
		1		0.1061169285	0.1061169285	0.7877661430
			1	0.3097982151	0.5569099204	0.1332918645
7		3		0.0660520784	0.0660520784	0.8678958432
				0.4477725053	0.4477725053	0.1044549894
				0.2604038024	0.2604038024	0.4791923952
			1	0.2325524777	0.6759625951	0.0914849272
8		3		0.0469685351	0.0469685351	0.9060629298
				0.2033467796	0.2033467796	0.5933064408
				0.3905496216	0.3905496216	0.2189007568
			2	0.3617970895	0.5541643672	0.0840385433
				0.1801396087	0.7519065566	0.0679538347
9	1			0.3333333333	0.3333333333	0.3333333333
		3		0.0355775717	0.0355775717	0.9288448566
				0.4640303025	0.4640303025	0.0719393950
				0.1633923069	0.1633923069	0.6732153862
			3	0.2966333890	0.6349633653	0.0684032457
				0.1439089974	0.8031490682	0.0529419344
				0.3225890045	0.4968009397	0.1806100558

n	n_1	n_2	n_3	b_1	b_2	b_3
10		4		0.0265250690	0.0265250690	0.9469498620
				0.1330857076	0.1330857076	0.7338285848
				0.4232062312	0.4232062312	0.1535875376
				0.2833924371	0.2833924371	0.4332151258
			4	0.3934913008	0.5472380443	0.0592706549
				0.2462883939	0.6991456238	0.0545659823
				0.1163195333	0.8427538829	0.0409265838
				0.2707097521	0.5811217960	0.1481684519
11		5		0.0204278105	0.0204278105	0.9591443790
				0.4746683133	0.4746683133	0.0506633734
				0.1104863580	0.1104863580	0.7790272840
				0.2422268680	0.2422268680	0.5155462640
				0.3764778430	0.3764778430	0.2470443140
			5	0.3361965758	0.6146545276	0.0491488966
				0.2073828199	0.7483396985	0.0442774816
				0.0959885136	0.8715407373	0.0324707491
				0.3649298091	0.5060795425	0.1289906484
				0.2299163838	0.6466193522	0.1234642640
12	1			0.3333333333	0.3333333333	0.3333333333
		4		0.0156346170	0.0156346170	0.9687307660
				0.0926054449	0.0926054449	0.8147891102
				0.4452623516	0.4452623516	0.1094752968
				0.2091994115	0.2091994115	0.5816011770
			7	0.4145270405	0.5430117044	0.0424612551
				0.2890538328	0.6707932601	0.0401529071
				0.1765067641	0.7877603302	0.0357329057
				0.0799959921	0.8942989924	0.0257050155
				0.3177076680	0.5753716491	0.1069206829
				0.1969473706	0.6989024696	0.1041501598
				0.3292603428	0.4567841256	0.2139555316

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