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2006 J. Phys. A: Math. Gen. 39 5563

(http://iopscience.iop.org/0305-4470/39/19/S14)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 5563–5584 doi:10.1088/0305-4470/39/19/S14

On group Fourier analysis and symmetry preserving discretizations of PDEs

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Received 12 October 2005, in final form 3 February 2006
Published 24 April 2006
Online at stacks.iop.org/JPhysA/39/5563

Abstract
In this paper we review some group theoretic techniques applied to discretizations of PDEs. Inspired by the recent years active research in Lie group- and exponential-time integrators for differential equations, we will in the first part of the paper present algorithms for computing matrix exponentials based on Fourier transforms on finite groups. As an example, we consider spherically symmetric PDEs, where the discretization preserves the 120 symmetries of the icosahedral group. This motivates the study of spectral element discretizations based on triangular subdivisions. In the second part of the paper, we introduce novel applications of multivariate non-separable Chebyshev polynomials in the construction of spectral element bases on triangular and simplicial sub-domains. These generalized Chebyshev polynomials are intimately connected to the theory of root systems and Weyl groups (used in the classification of semi-simple Lie algebras), and these polynomials share most of the remarkable properties of the classical Chebyshev polynomials, such as near-optimal Lebesgue constants for the interpolation error, the existence of FFT-based algorithms for computing interpolants and pseudo-spectral differentiation and existence of Gaussian integration rules. The two parts of the paper can be read independently.

PACS numbers: 02.20.Qs, 02.30.Jr, 02.60.Jh

1. Introduction

As an introductory motivation, we briefly review some recent developments of numerical time integration based on computing exponentials. A detailed understanding of this introduction is not necessary for reading the rest of the paper. Classical numerical integrators (e.g., Runge–Kutta and multistep) assumes an ODE $y'(t) = F(y(t))$, where $y(t) \in \mathbb{R}^n$ and the basic time-step updates the solution are obtained by translations on $\mathbb{R}^n$. Indeed all classical one-step methods are of the form $y_{n+1} = y_n + \Psi_{h,F}(y_n)$, where h denotes the timestep and $\Psi_{h,F}$ is given by the method.

In the last decade, there has been a significant development of numerical *Lie group integrators* (LGI) (Iserles *et al* 2000). These are based on the more general assumption that the domain of $y(t)$ is a manifold $\mathcal{M}$ acted upon transitively by a Lie group G. Let $\mathfrak{g}$ be the corresponding Lie algebra and $\exp: \mathfrak{g} \to G$ the exponential map. A vectorfield F on $\mathcal{M}$ can be expressed in terms of a map $A: \mathcal{M} \to \mathfrak{g}$ as $F(y) = A(y) \cdot y$ (Munthe-Kaas 1989). It is assumed that the group action $p \mapsto \exp(A) \cdot p$ can be computed accurately and efficiently for all $p \in \mathcal{M}$ and $A \in \mathfrak{g}$. The basic time-step update in many LGI methods is obtained from the group action as $y_{n+1} = \exp(\Psi_{h,A}(y_n)) \cdot y_n$, where $\Psi_{h,A}(y_n) \in \mathfrak{g}$ depends on the particular LGI. For matrix Lie groups, exp denotes the matrix exponential. As a simple example, consider $y'(t) = A(y) \cdot y$, where $A \in \mathbb{R}^{n\times n}$, $y \in \mathbb{R}^n$ and the action is the matrix-vector product. The *exponentiated Euler method* is the simplest possible LGI given as $y_{n+1} = \exp(hA(y_n)) \cdot y_n$. If A is a skew-symmetric matrix, this yields a first-order integrator for equations evolving on a sphere, where the update is done by the action of the orthogonal rotation matrix $\exp(hA)$. The order theory of high-order LGI is now well understood (Owren 2006). The basic difference between the classical-order theory and the order theory of LGI arises from the fact that translations on $\mathbb{R}^n$ form a commutative group, whereas more general group actions are non-commutative. Corrections for non-commutativity is necessary in any LGI of order higher than 2.

LGI methods enjoy a number of nice geometrical properties, of which we will focus here on their *symmetry* and *equivariance* properties. Fundamental in the theory of differential equations is the equivariance of the solution curves with respect to any diffeomorphism $\phi: \mathcal{M} \to \mathcal{M}$ acting on the domain. Let $\phi_* F$ denote the *push forward* of the vectorfield F, i.e. $(\phi_* F)(z) = T\phi \cdot F(\phi^{-1}(z))$ for all $z \in \mathcal{M}$, where $T\phi$ denotes the tangent map (in coordinates the Jacobian matrix). Then the two differential equations $y'(t) = F(y(t))$, $y(0) = y_0$ and $z'(t) = (\phi_* F)(z(t))$, $z(0) = \phi(y_0)$ have analytical solution curves related by $z(t) = \phi(y(t))$. In particular, if $\phi_* F = F$, we say that ϕ is a symmetry of the vectorfield, and in that case ϕ maps solution curves to other solution curves of the same equation.

For numerical integrators, it is in general impossible to satisfy equivariance with respect to arbitrary diffeomorphisms, since this would imply an analytically correct solution. (There always exists a local diffeomorphism which straighten the flow to a constant flow in x_1 direction, and this is integrated exactly by any numerical method).

The *equivariance group* of a numerical scheme is the largest group of diffeomorphisms under which the numerical solutions transform equivariantly. It is known that the equivariance group of classical Runge–Kutta methods is the group of all affine linear transformations of $\mathbb{R}^n$. LGI methods based on exact computation of exponentials have equivariance groups which include the Lie group G on which the method is based, hence if some elements $g \in G$ are symmetries of the differential equation, then G-equivariant LGIs will exactly preserve these symmetries. However, if the exact exponential is replaced with approximations, care must be taken in order not to destroy G-equivariance and symmetry preservation of the numerical scheme. In the case of PDEs, symmetry preservation is also depending on symmetry preserving spatial discretizations.

In the recent years, there has been a significant interest in the application of LGI and other exponential-based integrators for solving PDEs (Hochbruck and Lubich 1998, Krogstad 2005). A starting point for many of these methods are differential equations of the form $u'(t) = \mathcal{L}(u) + \mathcal{N}(u)$, where $\mathcal{L}$ is a stiff linear differential operator, and $\mathcal{N}$ is a non-stiff and non-linear part of the PDE. In important cases, methods based on computing $\exp(\mathcal{L})$ can replace implicit treatment of such stiff PDEs. Of particular interest to us in this paper are cases where $\mathcal{L}$ commutes with a group of symmetries, so that $\mathcal{L}(u \circ g) = \mathcal{L}(u) \circ g$ for all $g \in G$. This is a typical situation for many differential operators arising from physical systems (e.g., the Laplace operator commutes with the group of Euclidean transformations of the domain).

The paper is organized as follows. In section 2 we will discuss the use of Fourier transforms on finite groups in the computation of the exponential of discretized linear operators commuting with a finite group of domain symmetries. In particular, we will discuss the icosahedral symmetry group, which is the largest finite subgroup of the full group of all rotations of a sphere. In section 3 we will discuss issues related to spectral element discretizations with icosahedral symmetries, in particular we will present a novel approach to constructing high-order bi-variate polynomial bases on triangles. This approach is based on the beautiful properties of non-separable multivariate Chebyshev polynomials. These polynomials are constructed by symmetric 'caleidoscopic' foldings of Fourier basis functions, and both the theory and also practical computations (discretizations and FFTs) are depending on group theoretical ideas.

2. Symmetries and the matrix exponential

The topic of this section is applications of Fourier analysis on groups in the computation of matrix exponentials. Assuming that the domain is discretized with a symmetry respecting discretization, we will show that by a change of basis derived from the irreducible representations of the group, the operator is block diagonalized. This simplifies the computation of matrix exponentials. The basic mathematics behind this chapter is *representation theory of finite groups* (James and Liebeck 2001, Lomont 1959, Serre 1977). Applications of this theory in scientific computing is discussed by a number of authors, see e.g. Allgower *et al* (1992), Allgower *et al* (1998), Bossavit (1986), Douglas and Mandel (1992), Georg and Miranda (1992). Our exposition, based on the *group algebra*, is explained in detail in Åhlander and Munthe-Kaas (2005), which is intended to be a self-contained introduction to the subject.

2.1. $\mathcal{G}$-equivariant matrices

A *group* is a set $\mathcal{G}$ with a binary operation $g, h \mapsto gh$, inverse $g \mapsto g^{-1}$ and identity element e, such that $g(ht) = (gh)t$, $eg = ge = g$ and $gg^{-1} = g^{-1}g = e$ for all $g, h, t \in \mathcal{G}$. We let $|\mathcal{G}|$ denote the number of elements in the group. Let $\mathcal{I}$ denote the set of indices used to enumerate the nodes in the discretization of a computational domain. We say that a group $\mathcal{G}$ *acts on* a set $\mathcal{I}$ (from the right) if there exists a product $(i, g) \mapsto ig : \mathcal{I} \times \mathcal{G} \to \mathcal{I}$, such that

$$ie = i \qquad \text{for all} \quad i \in \mathcal{I}, \tag{1}$$

$$i(gh) = (ig)h \qquad \text{for all} \quad g, h \in \mathcal{G} \quad \text{and} \quad i \in \mathcal{I}. \tag{2}$$

The map $i \mapsto ig$ is a permutation of the set $\mathcal{I}$, with the inverse permutation being $i \mapsto ig^{-1}$. An action partitions $\mathcal{I}$ into disjoint *orbits*

$$\mathcal{O}_i = \{j \in \mathcal{I} \mid j = ig \quad \text{for some} \quad g \in \mathcal{G}\}, i \in \mathcal{I}.$$

We let $\mathcal{S} \subset \mathcal{I}$ denote a selection of *orbit representatives*, i.e. one element from each orbit. The action is called *transitive* if $\mathcal{I}$ consists of just a single orbit, $|\mathcal{S}| = 1$. For any $i \in \mathcal{I}$, we let the *isotropy subgroup at i*, $\mathcal{G}_i$ be defined as

$$\mathcal{G}_i = \{g \in \mathcal{G} \mid ig = i\}.$$

The action is *free* if $\mathcal{G}_i = \{e\}$ for every $i \in \mathcal{I}$, i.e. there are no fixed points under the action of $\mathcal{G}$.

Definition 1. *A matrix $\boldsymbol{A} \in \mathbb{C}^{\mathcal{I}\times\mathcal{I}}$ is $\mathcal{G}$-equivariant if*

$$\boldsymbol{A}_{i,j} = \boldsymbol{A}_{ig,jg} \qquad \textit{for all} \quad i, j \in \mathcal{I} \quad \textit{and all} \quad g \in \mathcal{G}. \tag{3}$$

The definition is motivated by the result that if $\mathcal{L}$ is a linear differential operator commuting with a group of domain symmetries $\mathcal{G}$, and if we can find a set of discretization nodes $\mathcal{I}$ such that every $g \in \mathcal{G}$ acts on $\mathcal{I}$ as a permutation $i \mapsto ig$, then $\mathcal{L}$ can be discretized as a $\mathcal{G}$-equivariant matrix A, see Allgower *et al* (1998), Bossavit (1986).

2.2. *The group algebra*

We will establish that $\mathcal{G}$ equivariant matrices are associated with (scalar or block) convolutional operators in the *group algebra*.

Definition 2. *The group algebra $\mathbb{C}\mathcal{G}$ is the complex vectorspace $\mathbb{C}^{\mathcal{G}}$ where each $g \in \mathcal{G}$ corresponds to a basis vector $\boldsymbol{g} \in \mathbb{C}\mathcal{G}$. A vector $a \in \mathbb{C}\mathcal{G}$ can be written as*

$$a = \sum_{g\in\mathcal{G}} a(g)\boldsymbol{g} \qquad \textit{where} \quad a(g) \in \mathbb{C}.$$

The convolution product $* : \mathbb{C}\mathcal{G} \times \mathbb{C}\mathcal{G} \to \mathbb{C}\mathcal{G}$ is induced from the product in $\mathcal{G}$ as follows. For basis vectors $\boldsymbol{g}, \boldsymbol{h}$, we set $\boldsymbol{g} * \boldsymbol{h} \equiv \boldsymbol{gh}$, and in general if $a = \sum_{g\in\mathcal{G}} a(g)\boldsymbol{g}$ and $b = \sum_{h\in\mathcal{G}} b(h)\boldsymbol{h}$, then

$$a * b = \left(\sum_{g\in\mathcal{G}} a(g)\boldsymbol{g}\right) * \left(\sum_{h\in\mathcal{G}} b(h)\boldsymbol{h}\right) = \sum_{g,h\in\mathcal{G}} a(g)b(h)(\boldsymbol{gh}) = \sum_{g\in\mathcal{G}} (a * b)(g)\boldsymbol{g},$$

where

$$(a * b)(g) = \sum_{h\in\mathcal{G}} a(gh^{-1})b(h) = \sum_{h\in\mathcal{G}} a(h)b(h^{-1}g). \tag{4}$$

Consider a $\mathcal{G}$-equivariant $\boldsymbol{A} \in \mathbb{C}^{n\times n}$ in the case where $\mathcal{G}$ acts freely and transitively on $\mathcal{I}$. In this case there is only one orbit of size $|\mathcal{G}|$ and hence $\mathcal{I}$ may be identified with $\mathcal{G}$. Corresponding to $\boldsymbol{A}$ there is a unique $A \in \mathbb{C}\mathcal{G}$, given as $A = \sum_{g\in\mathcal{G}} A(g)g$, where A is the first column of $\boldsymbol{A}$, i.e.

$$A(gh^{-1}) = \boldsymbol{A}_{gh^{-1},e} = \boldsymbol{A}_{g,h}. \tag{5}$$

Similarly, any vector $\boldsymbol{x} \in \mathbb{C}^n$ corresponds uniquely to $x = \sum_{g\in\mathcal{G}} x(g)g \in \mathbb{C}\mathcal{G}$, where $x(g) = \boldsymbol{x}_g$ for all $g \in \mathcal{G}$. Consider the matrix vector product

$$(\boldsymbol{Ax})_g = \sum_{h\in\mathcal{G}} \boldsymbol{A}_{g,h}\boldsymbol{x}_h = \sum_{h\in\mathcal{G}} A(gh^{-1})x(h) = (A * x)(g).$$

If $\boldsymbol{A}$ and $\boldsymbol{B}$ are two equivariant matrices, then $\boldsymbol{AB}$ is the equivariant matrix where the first column is given as

$$(\boldsymbol{AB})_{g,e} = \sum_{h\in\mathcal{G}} \boldsymbol{A}_{g,h}\boldsymbol{B}_{h,e} = \sum_{h\in\mathcal{G}} A(gh^{-1})B(h) = (A * B)(g).$$

We have shown that *if $\mathcal{G}$ acts freely and transitively, then the algebra of $\mathcal{G}$-equivariant matrices acting on $\mathbb{C}^n$ is isomorphic to the group algebra $\mathbb{C}\mathcal{G}$ acting on itself by convolutions from the left.*

In the case where $\boldsymbol{A}$ is $\mathcal{G}$-equivariant w.r.t. a free, but not transitive, action of $\mathcal{G}$ on $\mathcal{I}$, we need a block version of the above theory. Let $\mathbb{C}^{m\times\ell}\mathcal{G} \equiv \mathbb{C}^{m\times\ell} \otimes \mathbb{C}\mathcal{G}$ denote the space of vectors consisting of $|\mathcal{G}|$ matrix blocks, each block of size $m \times \ell$, thus $A \in \mathbb{C}^{m\times\ell}\mathcal{G}$ can be written as

$$A = \sum_{g\in\mathcal{G}} A(g) \otimes g \qquad \text{where} \qquad A(g) \in \mathbb{C}^{m\times\ell}. \tag{6}$$

The convolution product (4) generalizes to a block convolution $* : \mathbb{C}^{m\times\ell}\mathcal{G} \times \mathbb{C}^{\ell\times k}\mathcal{G} \to \mathbb{C}^{m\times k}\mathcal{G}$ given as

$$A * B = \left(\sum_{g\in\mathcal{G}} A(g) \otimes g\right) * \left(\sum_{h\in\mathcal{G}} B(h) \otimes h\right) = \sum_{g\in\mathcal{G}} (A * B)(g) \otimes g,$$

where

$$(A * B)(g) = \sum_{h\in\mathcal{G}} A(gh^{-1})B(h) = \sum_{h\in\mathcal{G}} A(h)B(h^{-1}g), \tag{7}$$

and $A(h)B(h^{-1}g)$ denotes a matrix product.

If the action of $\mathcal{G}$ on $\mathcal{I}$ is free, but not transitive, then $\mathcal{I}$ split in m orbits, each of size $|\mathcal{G}|$. We let $\mathcal{S}$ denote a selection of one representative from each orbit. We will establish an isomorphism between the algebra of $\mathcal{G}$-equivariant matrices acting on $\mathbb{C}^n$ and the block-convolution algebra $\mathbb{C}^{m\times m}\mathcal{G}$ acting on $\mathbb{C}^m\mathcal{G}$. We define the mappings $\mu : \mathbb{C}^n \to \mathbb{C}^m\mathcal{G}$, $\nu : \mathbb{C}^{n\times n} \to \mathbb{C}^{m\times m}\mathcal{G}$ as

$$\mu(\boldsymbol{y})_i(g) = y_i(g) = \boldsymbol{y}_{ig}\ \forall i \in \mathcal{S}, \qquad g \in \mathcal{G}, \tag{8}$$

$$\nu(\boldsymbol{A})_{i,j}(g) = A_{i,j}(g) = \boldsymbol{A}_{ig,j}\ \forall i, \qquad j \in \mathcal{S} g \in \mathcal{G}. \tag{9}$$

In Åhlander and Munthe-Kaas (2005) we show:

Proposition 1. *Let $\mathcal{G}$ act freely on $\mathcal{I}$. Then μ is invertible and ν is invertible on the subspace of $\mathcal{G}$-equivariant matrices. Furthermore, if $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{C}^{n\times n}$ are $\mathcal{G}$-equivariant and $\boldsymbol{y} \in \mathbb{C}^n$, then*

$$\mu(\boldsymbol{A}\boldsymbol{y}) = \nu(\boldsymbol{A}) * \mu(\boldsymbol{y}), \tag{10}$$

$$\nu(\boldsymbol{A}\boldsymbol{B}) = \nu(\boldsymbol{A}) * \nu(\boldsymbol{B}). \tag{11}$$

To complete the connection between $\mathcal{G}$-equivariance and block convolutions, we need to address the general case where the action is not free, hence some of the orbits in $\mathcal{I}$ have reduced size. One way to treat this case is to duplicate the nodes with non-trivial isotropy subgroups, thus a point $j \in \mathcal{I}$ is considered to be $|\mathcal{G}_j|$ identical points, and the action is extended to a free action on this extended space. Equivariant matrices on the original space is extended by duplicating the matrix entries, and scaled according to the size of the isotropy. We define

$$\mu(\boldsymbol{x})_i(g) = x_i(g) = \boldsymbol{x}_{ig}\ \forall i \in \mathcal{S}, \qquad g \in \mathcal{G}, \tag{12}$$

$$\nu(\boldsymbol{A})_{i,j}(g) = A_{i,j}(g) = \frac{1}{|\mathcal{G}_j|}\boldsymbol{A}_{ig,j}\ \forall i, \qquad j \in \mathcal{S} g \in \mathcal{G}. \tag{13}$$

With these definitions it can be shown that (10) and (11) still hold. It should be noted that μ and ν are no longer invertible, and the extended block convolutional operator $\nu(\boldsymbol{A})$ becomes singular. This poses no problems for the computation of exponentials since this is a forward computation. Thus we just exponentiate the block convolutional operator and restrict the result back to the original space. However, for inverse computations such as solving linear systems, the characterization of the image of μ and ν as subspaces of $\mathbb{C}^m\mathcal{G}$ and $\mathbb{C}^{m\times m}\mathcal{G}$ is an important issue for finding the correct solution (Åhlander and Munthe-Kaas 2005, Allgower *et al* 1993).

2.3. The generalized Fourier transform (GFT)

So far we have argued that a symmetric differential operator becomes a $\mathcal{G}$-equivariant matrix under discretization, which again can be represented as a block convolutional operator. In this section we will show how convolutional operators are block diagonalized by a Fourier transform on $\mathcal{G}$. This is the central part of Frobenius' theory of group representations from 1897–1899. We recommend the monographs (Fässler and Stiefel 1992, James and Liebeck 2001, Lomont 1959, Serre 1977) as introductions to representation theory with applications.

Definition 3. *A d-dimensional group representation is a map* $R : \mathcal{G} \to \mathbb{C}^{d\times d}$ *such that*

$$R(gh) = R(g)R(h) \qquad \text{for all} \quad g, h \in \mathcal{G}. \tag{14}$$

Generalizing the definition of *Fourier coefficients*, we define for any $A \in \mathbb{C}^{m\times k}\mathcal{G}$ and any d-dimensional representation R a matrix $\hat{A}(R) \in \mathbb{C}^{m\times k} \otimes \mathbb{C}^{d\times d}$ as

$$\hat{A}(R) = \sum_{g\in\mathcal{G}} A(g) \otimes R(g). \tag{15}$$

Proposition 2 (The convolution theorem). *For any* $A \in \mathbb{C}^{m\times k}\mathcal{G}$, $B \in \mathbb{C}^{k\times \ell}\mathcal{G}$ *and any representation* R*, we have*

$$(\widehat{A * B})(R) = \hat{A}(R)\hat{B}(R). \tag{16}$$

Proof. The statement follows from

$$\begin{aligned}\hat{A}(R)\hat{B}(R) &= \left(\sum_{g\in\mathcal{G}} A(g)\otimes R(g)\right)\left(\sum_{h\in\mathcal{G}} B(h)\otimes R(h)\right)\\ &= \sum_{g,h\in\mathcal{G}} A(g)B(h)\otimes R(g)R(h) = \sum_{g,h\in\mathcal{G}} A(g)B(h)\otimes R(gh)\\ &= \sum_{g,h\in\mathcal{G}} A(gh^{-1})B(h)\otimes R(g) = (\widehat{A * B})(R).\end{aligned}$$

□

Let d_R denote the dimension of the representation. For use in practical computations, it is important that $A * B$ can be recovered by knowing $(\widehat{A * B})(R)$ for a suitable selection of representations, and furthermore that their dimensions d_R are as small as possible. Note that if R is a representation and $X \in \mathbb{C}^{d_R\times d_R}$ is non-singular, then also $\tilde{R}(g) = XR(g)X^{-1}$ is a representation. We say that R and $\tilde{R}$ are equivalent representations. If there exists a similarity transform $\tilde{R}(g) = XR(g)X^{-1}$, such that $\tilde{R}(g)$ has a block diagonal structure, independent of $g \in \mathcal{G}$, then R is called *reducible*, otherwise it is *irreducible*.

Theorem 3 (Frobenius). *For any finite group* $\mathcal{G}$ *there exists a complete list* $\mathcal{R}$ *of non-equivalent irreducible representations, such that*

$$\sum_{R\in\mathcal{R}} d_R^2 = |\mathcal{G}|.$$

Defining the GFT for $a \in \mathbb{C}\mathcal{G}$ *as*

$$\hat{a}(R) = \sum_{g\in\mathcal{G}} a(g)R(g) \qquad \text{for every} \quad R \in \mathcal{R}, \tag{17}$$

Table 1. Gain in computational complexity for matrix exponential via GFT.

Domain	$\mathcal{G}$	$\lvert\mathcal{G}\rvert$	$\{d_R\}_{R\in\mathcal{R}}$	$W_{\text{direct}}/W_{\text{fspace}}$
Triangle	$\mathcal{D}_3$	6	$\{1, 1, 2\}$	21.6
Tetrahedron	$\mathcal{S}_4$	24	$\{1, 1, 2, 3, 3\}$	216
Cube	$\mathcal{S}_4 \times \mathcal{C}_2$	48	$\{1, 1, 1, 1, 2, 2, 3, 3, 3, 3\}$	864
Icosahedron	$\mathcal{A}_5 \times \mathcal{C}_2$	120	$\{1, 1, 3, 3, 3, 3, 4, 4, 5, 5\}$	3541

we may recover a by the inverse GFT (IGFT)

$$a(g) = \frac{1}{|\mathcal{G}|}\sum_{R\in\mathcal{R}} d_R \operatorname{trace}(R(g^{-1})\hat{a}(R)). \tag{18}$$

For the block transform of $A \in \mathbb{C}^{m\times k}\mathcal{G}$ given in (15), the GFT and the IGFT are given componentwise as

$$\hat{A}_{i,j}(R) = \sum_{g\in\mathcal{G}} A_{i,j}(g)R(g) \in \mathbb{C}^{d_R\times d_R}, \tag{19}$$

$$A_{i,j}(g) = \frac{1}{|\mathcal{G}|}\sum_{R\in\mathcal{R}} d_R \operatorname{trace}(R(g^{-1})\hat{A}_{i,j}(R)). \tag{20}$$

Complete lists of irreducible representations for a selection of common groups are found in Lomont (1959).

2.4. *Applications to the matrix exponential*

We have seen that via the GFT, any $\mathcal{G}$-equivariant matrix is block diagonalized. Corresponding to an irreducible representation R, we obtain a matrix block $\hat{A}(R)$ of size $md_R \times md_R$, where m is the number of orbits in $\mathcal{I}$ and d_R the size of the representation. Let W_{direct} denote the computational work, in terms of floating point operations, for computing the matrix exponential on the original data A, and let W_{fspace} be the cost of doing the same algorithm on the corresponding block diagonal GFT-transformed data $\hat{A}$. Thus $W_{\text{direct}} = c(m|\mathcal{G}|)^3 = cm^3\left(\sum_{R\in\mathcal{R}} d_R^2\right)^3$, $W_{\text{fspace}} = cm^3\sum_{R\in\mathcal{R}} d_R^3$ and the ratio becomes

$$\mathcal{O}(n^3):\quad W_{\text{direct}}/W_{\text{fspace}} = \left(\sum_{R\in\mathcal{R}} d_R^2\right)^3 \Big/ \sum_{R\in\mathcal{R}} d_R^3.$$

Table 1 lists this factor for the symmetries of the triangle, the tetrahedron, the 3D cube and the maximally symmetric discretization of a 3D sphere (icosahedral symmetry with reflections).

The cost of computing the GFT is not taken into account in this estimate. There exists fast GFT algorithms of complexity $\mathcal{O}(|\mathcal{G}|\log^{\ell}(|\mathcal{G}|))$ for a number of groups, but even if we use a slow transform of complexity $\mathcal{O}(|\mathcal{G}^2|)$, the total cost of the GFT becomes just $\mathcal{O}(m^2|\mathcal{G}|^2)$, which is much less than W_{fspace}.

2.4.1. Example: Equilateral triangle. The smallest noncommutative group is $\mathcal{D}_3$, the symmetries of an equilateral triangle. There are six linear transformations that map the triangle onto itself, three pure rotations and three rotations combined with reflections. In figure 1(*a*), we indicate the two generators α (rotation 120° clockwise) and β (right–left reflection). These satisfy the algebraic relations $\alpha^3 = \beta^2 = e$, $\beta\alpha\beta = \alpha^{-1}$, where e denotes the identity transform. The whole group is $\mathcal{D}_3 = \{e, \alpha, \alpha^2, \beta, \alpha\beta, \alpha^2\beta\}$.

Given an elliptic operator $\mathcal{L}$ on the triangle such that $\mathcal{L}(u\circ\alpha) = \mathcal{L}(u)\circ\alpha$ and $\mathcal{L}(u\circ\beta) = \mathcal{L}(u)\circ\beta$ for any u satisfying the appropriate boundary conditions on the triangle, let the domain

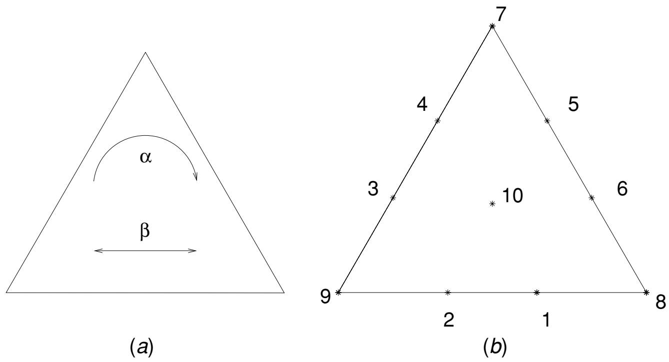


Figure 1. Equilateral triangle with a symmetry preserving set of ten nodes.

Table 2. A complete list of irreducible representations for $\mathcal{D}_3$.

	α	β
ρ_0	1	1
ρ_1	1	−1
ρ_2	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

be discretized with a *symmetry respecting discretization*, see figure 1(*b*). In this example we consider a finite difference discretization represented by the nodes $\mathcal{I} = \{1, 2, \ldots, 10\}$, such that both α and β map nodes to nodes. In finite element discretizations, one would use basis functions mapped to other basis functions by the symmetries. We define the action of $\mathcal{D}_3$ on $\mathcal{I}$ as

$$(1, 2, 3, 4, 5, 6, 7, 8, 9, 10)\alpha = (5, 6, 1, 2, 3, 4, 9, 7, 8, 10),$$
$$(1, 2, 3, 4, 5, 6, 7, 8, 9, 10)\beta = (2, 1, 6, 5, 4, 3, 7, 9, 8, 10),$$

and extend to all of $\mathcal{D}_3$ using (2). As orbit representatives, we may pick $\mathcal{S} = \{1, 7, 10\}$. The action of the symmetry group is free on the orbit $\mathcal{O}_1 = \{1, 2, 3, 4, 5, 6\}$, while the points in the orbit $\mathcal{O}_7 = \{7, 8, 9\}$ have isotropy subgroups of size 2, and finally $\mathcal{O}_{10} = \{10\}$ has isotropy of size 6.

The operator $\mathcal{L}$ is discretized as a matrix $\boldsymbol{A} \in \mathbb{C}^{10\times 10}$ satisfying the equivariances $\boldsymbol{A}_{ig,jg} = \boldsymbol{A}_{i,j}$ for $g \in \{\alpha, \beta\}$ and $i, j \in \mathcal{S}$. Thus we have e.g. $\boldsymbol{A}_{1,6} = \boldsymbol{A}_{3,2} = \boldsymbol{A}_{5,4} = \boldsymbol{A}_{4,5} = \boldsymbol{A}_{2,3} = \boldsymbol{A}_{6,1}$.

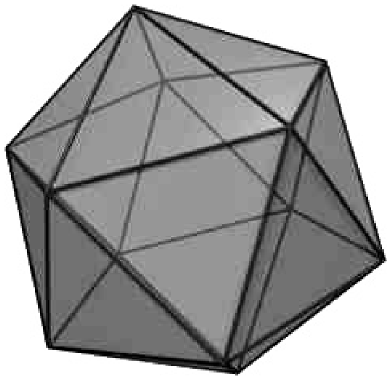
$\mathcal{D}_3$ has three irreducible representations given in table 2 (extended to the whole group using (14)). To compute $\exp(\boldsymbol{A})$, we find $A = \nu(\boldsymbol{A}) \in \mathbb{C}^{3\times 3}\mathcal{G}$ from (13) and find $\hat{A} = \mathrm{GFT}(A)$ from (19). The transformed matrix $\hat{A}$ has three blocks, $\hat{A}(\rho_0), \hat{A}(\rho_1) \in \mathbb{C}^{m\times m}$ and $\hat{A}(\rho_2) \in \mathbb{C}^{m\times m} \otimes \mathbb{C}^{2\times 2} \simeq \mathbb{C}^{2m\times 2m}$, where $m = 3$ is the number of orbits. We exponentiate each of these blocks, and find the components of $\exp(\boldsymbol{A})$ using the inverse GFT (20).

We should remark that in Lie group integrators, it is usually more important to compute $y = \exp(A) \cdot x$ for some vector x. In this case, we compute $\hat{y}(\rho_i) = \exp(\hat{A}(\rho_i)) \cdot \hat{x}(\rho_i)$, and recover y by the inverse GFT. Note that $\hat{x}(\rho_2), \hat{y}(\rho_2) \in \mathbb{C}^m \otimes \mathbb{C}^{2\times 2} \simeq \mathbb{C}^{2m\times 2}$.

2.4.2. Example: Icosahedral symmetry. As a second example illustrating the general theory, we solve the simple heat equation

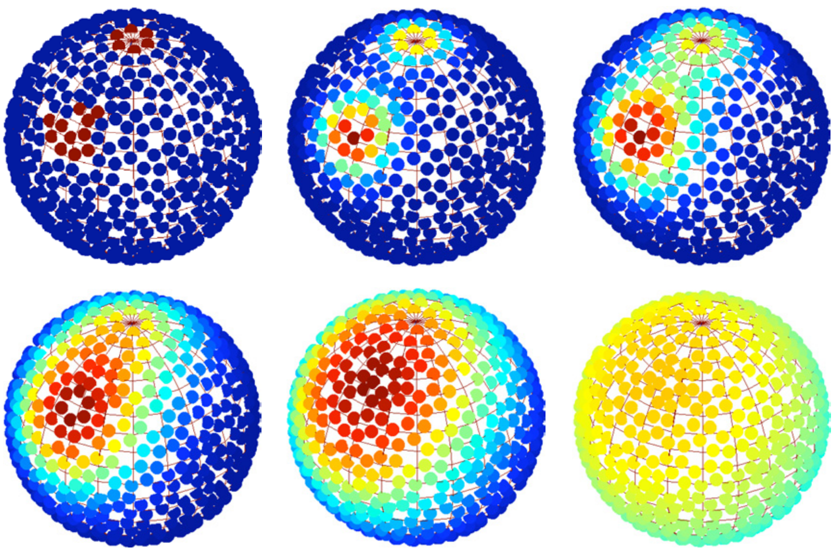
$$u_t = \nabla^2 u$$

on the surface of a unit sphere. The programming in this example is done by Trønnes (2005) in his master thesis.



The sphere is divided into 20 equilateral triangles, and each triangle subdivided in a finite difference mesh respecting all the 120 symmetries of the full icosahedral symmetry group (including reflections). To understand this group, it is useful to realize that five tetrahedra can be simultaneously embedded in the icosahedron, so that the 20 triangles correspond to the in total 20 corners of these five tetrahedra. From this one sees that the icosahedral rotation group is isomorphic to A_5, the group of all 60 even permutations of the five tetrahedra. The 3D reflection matrix $-I$ obviously commutes with any 3D rotation, and hence we realize that the full icosahedral group is isomorphic to the direct product $C_2 \times A_5$, where $C_2 = \{1, -1\}$. The irreducible representations of A_5, listed in Lomont have dimensions $\{1, 3, 3, 4, 5\}$, and the representations of the full icosahedral group are found by taking tensor products of these with the two one-dimensional representations of C_2. The fact that the full icosahedral group is a direct product is also utilized in faster computation of the GFT. This is, however, not of major importance, since the cost of the GFT in any case is much less than the cost of the matrix exponential.

The figures below show the solution of the heat equation at times 0, 2, 5, 10, 25 and 100. The initial condition consists of two located heat sources in the northern hemisphere.



This example serves as a simple toy example to check the practical issues of programming the group-based diagonalization techniques discussed above. In future work, we aim at solving more interesting equations such as shallow water equations and Euler flow equations on spherical geometries, using high-order Lie group integrators for the time integration and high-order spectral element discretizations in the space. For this purpose, we are interested in spectral element methods based on triangular subdivisions. In the remaining part of this paper, we will overview a novel approach to this topic, based on families of non-separable multivariate Chebyshev polynomials obtained from group theory.

3. Multivariate Chebyshev and triangular spectral elements

Bivariate Chebyshev polynomials were constructed independently by Koornwinder (1974) and Lidl (1975) by folding exponential functions. Multidimensional generalizations (the A_2 family) appeared first in Eier and Lidl (1982). In Hoffman and Withers (1988), a general folding construction was presented. Characterization of such polynomials as eigenfunctions of differential operators is found in Beerends (1991), Koornwinder (1974). Although the fundamental mathematical properties of multivariate Chebyshev polynomials are developed in the above papers, they are to our knowledge not appearing in any works on numerical analysis, approximation theory nor any other areas of computational science. It is our goal to show that these polynomials have significant roles to play in computations, similar to the famous univariate case. A more detailed exposition of the theory of this paper will appear in Munthe-Kaas (2006).

3.1. Multivariate Chebyshev polynomials: a general construction

To motivate a general construction of multivariate Chebyshev polynomials, we consider the classical univariate case obtained by 'folding' the exponential functions to cosine functions, and applying a change of variables to turn cosine functions into Chebyshev polynomials. Define the Fourier basis functions $(k, \theta) = \exp(2\pi i k\theta)$ for $\theta \in G = \mathbb{R}/\mathbb{Z} = [0, 1)$ and $k \in \widehat{G} = \mathbb{Z}$. Let $W = \{1, -1\}$ be a symmetry group acting on G, and consider the 'folded' exponentials

$$(k, \theta)_s = \frac{1}{|W|}\sum_{\gamma\in W}(k, \gamma\theta) = \frac{1}{|W|}\sum_{\gamma\in W}(\gamma k, \theta) = \frac{1}{2}\left((k, \theta) + (-k, \theta)\right) = \cos(2\pi k\theta).$$

Define the change of variables $x(\theta) = (1, \theta)_s = \cos(2\pi\theta)$. This defines Chebyshev polynomials $T_k(x) = (k, \theta)_s$ for $k = \{0, 1, \ldots\}$. Note that $T_0(x) = 1$ and $T_1(x) = x$. The fact that all $T_k(x)$ are polynomials follows from the recursion $2T_1(x) \cdot T_k(x) = T_{k+1}(x) + T_{k-1}(x)$, which is a special case of (29). It should be noted that the beautiful computational properties of Chebyshev polynomials, such as existence of FFT-based fast algorithms, recursion relations, orthogonality (continuous and discrete) and excellent interpolation properties can all be explained in terms of group theory and can be generalized to multivariate cases.

Let $G = \mathbb{R}^d/\mathbb{Z}^d$ denote a d-dimensional domain, one-periodic in each direction, thus $\langle G, +\rangle$ is an Abelian (commutative) group where + denotes componentwise addition modulo 1. Let $\widehat{G} = \mathbb{Z}^d$ denote the Abelian group of d-dimensional integer vectors, and define the *dual pairing* $(\cdot, \cdot)\colon \widehat{G}\times G \to \mathbb{C}$ as

$$(k, \theta) = \exp(2\pi \mathrm{i} k^T\theta) \tag{21}$$

satisfying

$$(k, \theta + \theta') = (k, \theta) \cdot (k, \theta'), \qquad (k + k', \theta) = (k, \theta) \cdot (k', \theta). \tag{22}$$

Note that $\{(k,\cdot)\colon k \in \widehat{G}\}$ is the Fourier basis on G (a complete list of irreducible representations), while $\{(\cdot,\theta)\colon \theta \in G\}$ is the Fourier basis on $\widehat{G}$, thus G and $\widehat{G}$ are *dual* Abelian groups (Rudin 1962).

Let $W \subset Z^{d\times d}$ be a finite group of integer matrices, defining a left action $\theta \mapsto \gamma\theta$ on G and a right action $k^T \mapsto k^T\gamma$ on $\widehat{G}$. Define the symmetrized Fourier basis

$$(k,\theta)_s = \frac{1}{|W|}\sum_{\gamma\in W}(k,\gamma\theta) = \frac{1}{|W|}\sum_{\gamma\in W}(\gamma^T k,\theta), \tag{23}$$

and introduce a change of variables

$$x_j(\theta) = (\boldsymbol{e}_j,\theta)_s, \tag{24}$$

where $\boldsymbol{e}_j = (0,\ldots,1,\ldots,0)^T$ and $j \in \{1,\ldots,d\}$. We define a family of functions

$$T_k(x) = (k,\theta)_s \qquad \text{for} \quad k \in \widehat{G}. \tag{25}$$

We will impose enough structure on W to ensure that $T_k(x)$ form a complete family of d-variate polynomials, which we will call the *multivariate Chebyshev polynomials* associated with W.

First some properties that hold regardless of W. From the definition it follows immediately that $T_k(x)$ satisfy

$$T_0(x) = 1 \tag{26}$$

$$T_{e_j}(x) = x_j \tag{27}$$

$$T_k(x) = T_{\gamma^T k}(x) \qquad \text{for all} \quad \gamma \in W. \tag{28}$$

The *mother of all* recurrence relations between $T_k(x)$ is the following:

$$T_k(x)T_\ell(x) = \sum_{m\in\widehat{G}}\alpha_{k,\ell}(m)T_m(x) = \sum_{m\in\mathcal{S}}|m^T W|\alpha_{k,\ell}(m)T_m(x), \tag{29}$$

where $\mathcal{S}$ denotes a selection of one element from each orbit of W in $\widehat{G}$ and $|m^T W|$ denotes the size of the orbit represented by $m \in \mathcal{S}$. The function α is given by a convolution

$$\alpha_{k,\ell}(m) = \frac{1}{|W|^2}\sum\sum_{\gamma,\eta\in W}\delta_{\gamma^T k+\eta^T\ell,m}, \tag{30}$$

where δ is the Kronecker-δ. To understand (29), recall the convolution formula for the (Abelian) Fourier transform $\widehat{(fg)}(k) = (\widehat{f}*\widehat{g})(k) = \sum_{m\in\widehat{G}}\widehat{f}(k-m)\widehat{g}(m)$, where $f,g \in \mathbb{C}G$ and $\widehat{f},\widehat{g} \in \mathbb{C}\widehat{G}$. The Fourier transform of $T_k(x(\theta))$ is

$$\widehat{T}_k(m) = \frac{1}{|W|}\sum_{\gamma\in W}\delta_{\gamma^T k,m},$$

and by defining

$$\alpha_{k,\ell}(m) = \widehat{T_k T_\ell}(m) = (\widehat{T_k}*\widehat{T_\ell})(m), \tag{31}$$

we obtain (30). Due to symmetry, it is sufficient to sum over just one element in each W-orbit and scale with the size of the orbit.

The reader is encouraged to verify that (29) implies the common recurrence among classical Chebychev polynomials in the case where $d = 1$ and $W = \{1,-1\}$.

A trivial example of these formulae is obtained when $d = 1$ and $W = \{1\}$. In this case we get $x = \exp(2\pi i\theta)$, $T_k(x) = x^k$ for $k \in \mathbb{Z}$, and (29) becomes $T_k(x)\cdot T_\ell(x) = T_{k+\ell}(x)$. Thus T_k are not polynomials when $k < 0$, because W is too small and lacks symmetries sending negative k to positive. On the other hand, if W is too large, then $\{T_k(x)\}$ may not generate the full space of all multivariate polynomials, but just certain linear combinations of these.

In the following section we will introduce the Weyl groups W associated with *root systems*. These groups are just the right size to guarantee that $\{T_k(x)\colon k \in \mathcal{S}\}$ form complete bases for the space of multivariate polynomials.

3.2. Root systems and Weyl groups

A *root system* is a subset Φ of a Euclidean space $E = \mathbb{R}^d$ such that

(i) Φ is finite, spans E and does not contain 0.
(ii) If $\alpha \in \Phi$ then the only multiples of α in Φ are $\pm\alpha$.
(iii) If $\alpha \in \Phi$ then the reflection $\sigma_\alpha = I - 2\frac{\alpha\alpha^T}{\alpha^T\alpha}$ leaves Φ invariant.
(iv) If $\alpha, \beta \in \Phi$ then $2\frac{\alpha^T\beta}{\alpha^T\alpha} \in \mathbb{Z}$.

The (finite) group generated by the reflections $W = \langle \sigma_\alpha \mid \alpha \in \Phi \rangle$ is called the *Weyl group*. The integer linear combination of all the roots $\alpha \in \Phi$ is called the *root lattice* Λ_r. The *affine Weyl group* is the group generated by W and all the translations in the root lattice.

A root system always has a *basis*, defined as d linearly independent vectors $\{\alpha_1, \dots, \alpha_d\} \subset \Phi$ so that any $\alpha \in \Phi$ can be written as $\alpha = \sum_{j=1}^d c_j \alpha_j$, where $c_j \in \mathbb{Z}$ are either all non-negative or all non-positive. α_j are called the *simple roots*. We let

$$A = (\alpha_1, \dots, \alpha_d)$$

denote the matrix with columns formed by the simple roots, hence $\Lambda_r = \{A \cdot \kappa : \kappa \in \mathbb{Z}^d\}$.

Given any lattice $\Lambda \subset \mathbb{R}^d$, we define the *dual lattice* $\Lambda^\perp \subset \mathbb{R}^d$ as the set of all vectors whose inner-product with vectors in Λ yield integer values, thus $\Lambda_r^\perp = \{A^{-T} \cdot \kappa : \kappa \in \mathbb{Z}^d\}$. A well-known result of Fourier analysis is that periodization of $\mathbb{R}^d$ with respect to a lattice Λ is equivalent to restricting the Fourier coefficients to the dual lattice $\Lambda^\perp$.

According to the general construction of section 3.1, we construct the Chebyshev polynomials $T_k(x)$ from Φ as follows:

- *Primal and dual spaces:* The root lattice Λ_r defines a periodic domain $\mathbb{R}^d/\Lambda_r$. Via the basis A for Λ_r, this domain is isomorphic to $G = \mathbb{R}^d/\mathbb{Z}^d$. Using the dual basis A^{-T}, the Fourier space becomes $\widehat{G} = \mathbb{Z}^d$.
- *Weyl group:* Using the A basis, the group W becomes a group of integer matrices acting on G. We find $\sigma_{\alpha_i} A = A\tilde{\sigma}_i$, where $\tilde{\sigma}_i$ is the integer matrix

  $$\tilde{\sigma}_i = I - \boldsymbol{e}_i \boldsymbol{e}_i^T C,$$

  and C is the *Cartan matrix* of the root system, defined as

  $$C_{j,\ell} = 2\frac{\alpha_j^T \alpha_\ell}{\alpha_j^T \alpha_j}.$$

  Thus, from the Cartan matrix of the root system, we immediately find the integer matrices $\{\tilde{\sigma}_i\}_{i=1}^d$ generating the Weyl group W. Given W, we construct the Chebyshev family $\{T_k(x) : k \in \mathcal{S}\}$.
- *Fundamental domain in $\widehat{G}$:* It can be shown that a selection of orbit representatives can always be taken as the first quadrant of $\widehat{G} = \mathbb{Z}^d$, i.e.

  $$\mathcal{S} = \{k \in \mathbb{Z}^d : k_i \geqslant 0 \text{ for all } i\}.$$

  Furthermore, there exists a partial ordering $\prec$ on $\mathcal{S}$ such that the monomials can be written as

  $$x^k = x_1^{k_1} \cdots x_d^{k_d} = c_k T_k(x) + \sum_{\substack{\ell \in \mathcal{S} \\ \ell \prec k}} c_\ell T_\ell(x) \qquad \text{for} \quad c_k, c_\ell \in \mathbb{C}, \quad c_k \neq 0\,.$$

  Hence $\{T_k(x) : k \in \mathcal{S}\}$ is a basis for the space of multivariate polynomials.

- *Fundamental domain in G:* Let Δ denote the fundamental domain of W acting on G. The domain Δ has a simple characterization in terms of A and C. If the root system is *irreducible*, then Δ is always a simplex, and for reducible root systems, Δ becomes a Cartesian product of the fundamental domains for each of the irreducible components of Φ, see Munthe-Kaas (2006) for details. It can be shown that the coordinate map $\theta \mapsto x$ is invertible between Δ and the codomain $\delta = x(\Delta)$. The Jacobian of $x(\theta)$ is nonsingular inside Δ and singular on the boundary. It is important to note that while Δ are simplexes, this is not the case for the transformed domain $\delta = x(\Delta)$. This poses challenges for the construction of spectral element bases that we will address in the case A_2 in section 3.4.
- *Continuous orthogonality:* The exponentials are orthogonal under the standard inner product on G, and therefore the symmetrized exponentials are orthogonal on Δ. Thus the Chebyshev polynomials satisfy a continuous orthogonality
$$\int_\delta T_k(x)\cdot\overline{T_\ell(x)}\omega(x)\,\mathrm{d}x = 0 \qquad \text{for} \quad k,\ell\in\mathcal{S}, \quad k\neq\ell,$$
where $\omega(x)$ is the Jacobian determinant of the coordinate map $x(\theta)$. For the 1D case, $\omega(x) = (2\pi\sqrt{1-x^2})^{-1}$ (the normal Chebyshev weight function scaled with 2π).
- *Discrete orthogonality:* For fast computations, it is important to find a good discretization of $\Delta\subset G$. Up to a band-limit, the exponentials (k,θ) are orthogonal with on a uniform lattice in G, and uniform lattices provide Gaussian integration rules for the exponentials (with equal Gaussian weights). For the symmetrized exponentials, we need a lattice which is invariant under W. One such lattice with maximal symmetries is obtained by downscaling the root lattice with an integer factor $m = k|C|$. We include the determinant of the Cartan matrix to ensure that the lattice contains both the root lattice, and also the *weights lattice*, which are all the points with maximal symmetry under the action of the affine Weyl group on $\mathbb{R}^d$ (Humphreys 1970). Let $\Delta_m\subset G$ denote the down-scaled root lattice, restricted to Δ. Since G is expressed in terms of the basis A, this becomes
$$\Delta_m = \left\{\theta\in\Delta{:}\,\theta = \frac{\kappa}{m}, \kappa\in\mathbb{Z}^d\right\}.$$
The symmetrized exponentials $(k,\theta)_s$ satisfy a discrete orthogonality on Δ_m, where the Gaussian weight in a point θ is proportional to the size of the orbit $|W\theta|$. Thus the Chebyshev polynomials satisfy orthogonality under the discrete inner product
$$\langle T_k(x), T_\ell(x)\rangle_m = \frac{1}{c}\sum_{\theta\in\Delta_m}|W\theta|\cdot T_k(x(\theta))\;\cdot\;\overline{T_\ell(x(\theta))},$$
where $c = |W|\sum_{\theta\in\Delta_m}|W\theta|$. The Gaussian quadrature formula
$$\int_{x\in\delta} f(x)\omega(x)\,\mathrm{d}x \approx c\sum_{\theta\in\Delta_m}|W\theta| f(x(\theta))$$
is exact whenever $f(x) = T_k(x)$, $k\neq m\kappa$ for some $0\neq\kappa\in\mathbb{Z}^d$. The formula fails if k is in the dual lattice $(\Lambda_r/m)^\perp$, except $k=0$, since these T_k alias to T_0 on Δ_m. It should be noted that our lattice Δ_m is a generalization of Chebyshev–Gauss–Lobatto points in 1D (i.e., Chebyshev extremal points, with half weights on the boundary points). We can also generalize Chebyshev–Gauss points (zeros of Chebyshev polynomials) by using lattices obtained by taking appropriate cosets of the downscaled root lattice.

To complete this section, we want to characterize all root systems, and present the irreducible cases in 2D. A root system is called *reducible*, if the roots can be separated into two sets, such that the roots in one subset is orthogonal to all the other roots. Any root

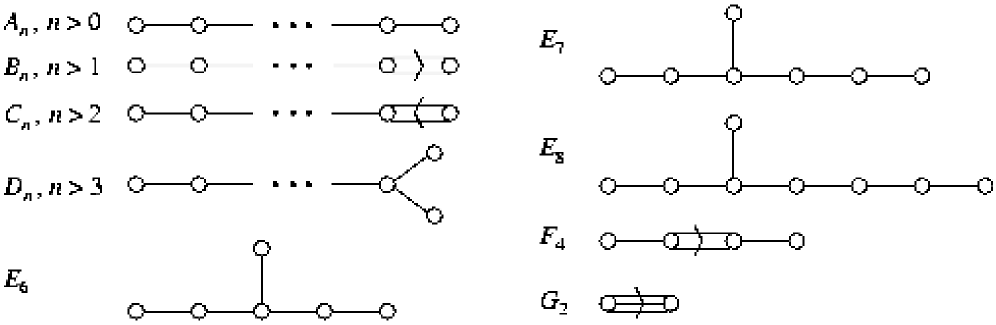


Figure 2. Dynkin diagrams.

system can be decomposed into irreducible components, and it is sufficient to study these. If a root system can be decomposed, then the corresponding fundamental domains become tensor products of the corresponding irreducible subdomains, and all the Chebyshev polynomials become tensor products of Chebyshev polynomials on the irreducible components. Thus the standard construction of the tensor product Chebyshev bases on box-shaped domains corresponds to a root system which can be completely decomposed into 1D roots.

Irreducible root systems are uniquely characterized in terms of their *Dynkin diagrams*, figure 2. These diagrams have one node for each simple root $\alpha_j \in \Delta$. The only possible angles between the simple roots are 90°, 60°, 45° or 30°. We draw no line between the nodes if the corresponding simple roots are orthogonal, one line if the angle is 60°, two lines for 45° and three lines for 30°. Roots may come in different lengths, but in an irreducible root system, there are at most two different lengths of the roots. To indicate short and long roots an arrow is inserted in the diagram, thus on the left of $<$ are the short roots, on the right the long ones. The 2D irreducible root systems are shown in figure 3.

The sequence of diagrams A_1, A_2, A_3, D_4, D_5, E_6, E_7 and E_8 are of particular interest in sampling theory. The root lattices corresponding to these are known to be the *densest lattice packings* in spaces of dimensions 1–8 (Conway and Sloane 1988). Suppose we seek a sampling lattice A on $\mathbb{R}^d$ so that the Euclidean distance in the Fourier space between 0 and the closest non-zero point in the dual lattice $A^{\perp}$ is some given constant c, i.e. we seek a sampling exact on $\|k\|_2 < c$ band limited functions. How can we choose such a lattice A with the lowest sampling density? The solution is: *choose a lattice from the sequence above!* To explain this, we note that all these lattices are self-dual (dual of same type). In the Fourier space, maximizing grid density $|A^{-T}|^{-1}$ (for a given lattice constant c) is equivalent to minimizing the density $|A|^{-1}$ in primal space. For dimensions 2, 3, 4 and 5, going from a rectangular to optimal grid saves 13%, 29%, 50% and 65% of the gridpoints.

3.3. Chebyshev expansions and symmetric FFTs

The (infinite) Chebychev expansion of a well-behaved function $f(x)$ defined for $x \in \delta$ is given as

$$f(x) = \sum_{k \in \mathcal{S}} |k^T W| \widehat{f}(k) T_k(x),$$

where $\widehat{f} \in \mathbb{C}\widehat{G}$ is the Fourier transform of $f(x(\theta))$ considered as a symmetric function in $\mathbb{C}G$. If we restrict x to the finite set $\{x(\theta) : \theta \in \Delta_m\}$, then we obtain a finite interpolating Chebyshev series of the form

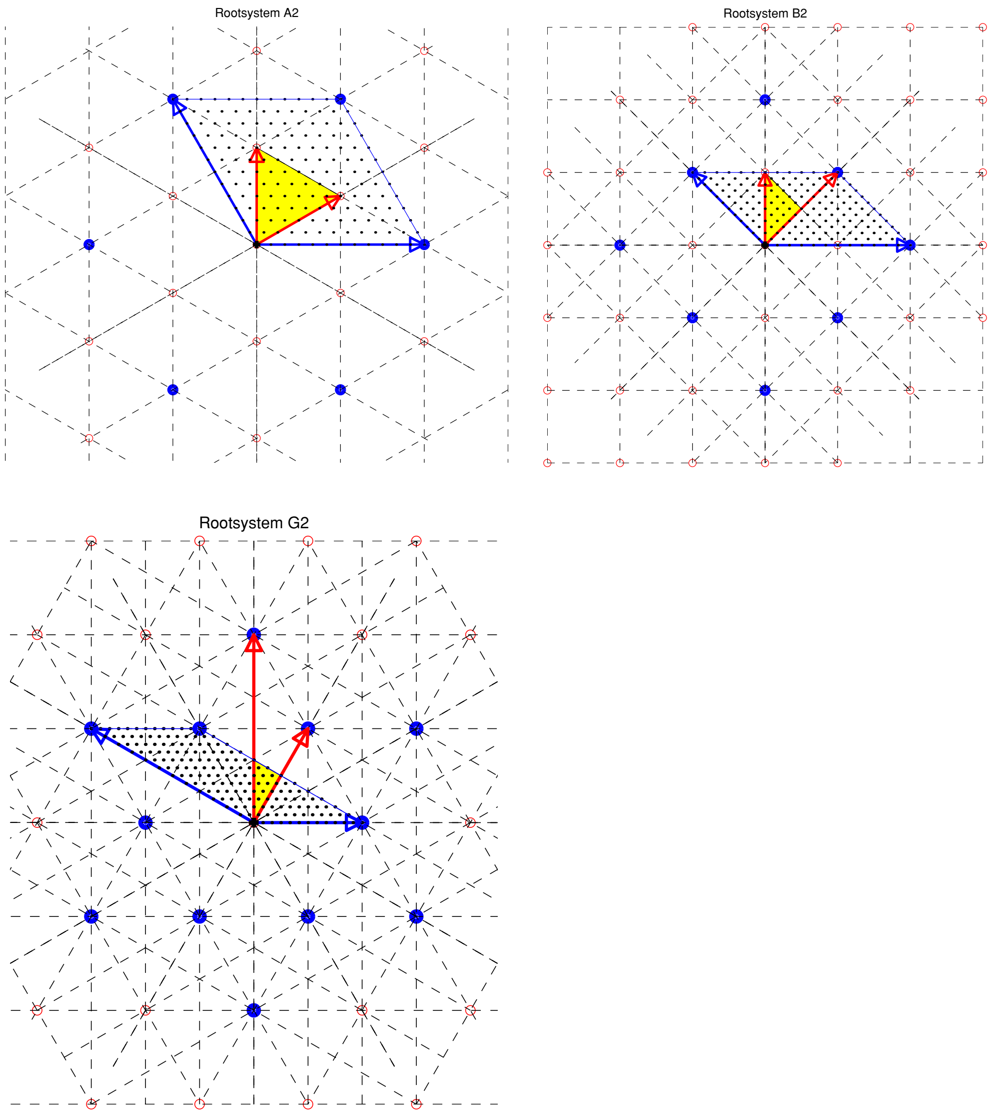


Figure 3. Irreducible root systems in 2D. The irreducible 2D root systems given by A_2, B_2 and G_2, corresponding to fundamental domains $\Delta \subset G$ given as equilateral triangle, $45^\circ - 45^\circ - 90^\circ$ triangle and $30^\circ - 60^\circ - 90^\circ$ triangle (yellow colour). Blue dots are the roots, blue arrows the simple roots, red dots the weights lattice and red arrows the fundamental dominant weights, the dotted lines are the mirrors in the affine Weyl group and the black dots indicate a downscaling of the root lattice by a factor $m = 12$. The parallelograms show the periodicity of the root lattice, and hence the fundamental domain of the (unsymmetrized) Fourier basis.

$$f(x(\theta)) = \sum_{k \in \mathcal{S}_m} |k^T W| \widehat{f}(k) T_k(x(\theta)).$$

Sampling at m-downscaled root lattice can be described as going from the continuous Abelian group G to the finite subgroup $G_m = \mathbb{Z}_m^d$. In the Fourier space, the sampling is described by going from the infinite group $\widehat{G}$ to the finite quotient $\widehat{G}_m = \widehat{G}/m\widehat{G} \simeq \mathbb{Z}_m^d$. The finite set

$\mathcal{S}_m \subset \mathcal{S}$ denotes the fundamental domain of the right action of W on $\widehat{G}_m$, see Munthe-Kaas (2006) for details.

Computationally the discrete Chebyshev interpolation problem is solved by computing a symmetric discrete Fourier transform $f \mapsto \widehat{f}$. A simple solution to this problem is just to form the full symmetrized $f \in \mathbb{C}G_m$, computing $\widehat{f}$ with a standard FFT, and restrict the result to $\mathcal{S}_m$. The cost is $5N\log_2(N)$ real flops, where $N = m^d$.

In Munthe-Kaas (1989), we provide group theoretic symmetric FFTs that can utilize all the symmetries in W and real symmetry in f. A related approach is found in Puschel and Rötteler (2004). A group theoretical explanation of the classical Cooley–Tukey algorithm is the result that if $H < G$ (subgroup of Abelian group) then $\widehat{H} = \widehat{G}/H^{\perp}$. So, the Cooley–Tukey algorithm can be generalized to any subgroup decomposition. The sequence

$$G_{|C|} < G_{2|C|} < \cdots < G_{2^k|C|}$$

preserves all the symmetries in W. Symmetries may be lost in the cosets, but in that case two different cosets will be identified by a symmetry. By carefully using all the symmetries both in primal space and in the Fourier space, we obtain an algorithm saving a factor $2|W|$ both in flops and in storage with respect to the full non-symmetric complex FFT. The cost of the symmetrized algorithm is $\frac{5}{2}M\log_2(M)$, where $M = |\Delta_m|$ is the number of lattice points in the fundamental domain.

3.4. The Chebyshev A_2 family

Of the three non-separable cases in 2D, the A_2 family is the most promising for building spectral elements. In the other two cases, the shape of the domains δ seem less suitable for patching.

3.4.1. Symmetry, recurrence and coordinate transformation. For A_2, we have simple roots and the Cartan matrix is given as

$$A = \begin{pmatrix} 2 & -1 \\ 0 & \sqrt{3} \end{pmatrix}, \qquad C = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}.$$

The action of W on $G = \mathbb{R}^2/\mathbb{Z}^2$ is generated by $\sigma_i = I - \boldsymbol{e}_i\boldsymbol{e}_i^T C$,

$$\sigma_1 = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix},$$

yielding a group with in total $|W| = 6$ elements. In general, the Chebyshev polynomials satisfy the symmetries $T_{-k} = \overline{T_k}$ and $T_{\gamma^T k} = T_k$ for all $\gamma \in W$, $k \in \widehat{G}$. Thus, when W does not contain the inversion $\theta \mapsto -\theta$, then $T_k(x)$ and the coordinates $x_i(\theta)$ are complex. In the A_2 case

$$x_1(\theta) = \tfrac{1}{3}(\mathrm{e}^{2\pi \mathrm{i}\theta_1} + \mathrm{e}^{-2\pi \mathrm{i}\theta_2} + \mathrm{e}^{2\pi \mathrm{i}(\theta_2-\theta_1)}), \qquad x_2(\theta) = \overline{x_1(\theta)}.$$

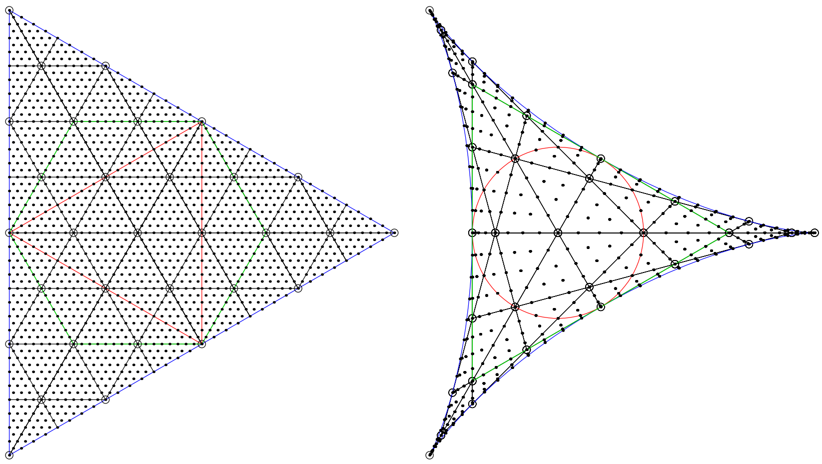
It is convenient to replace these with the real coordinates

$$x_{\mathrm{re}} = \tfrac{1}{2}(x_1 + x_2) = \tfrac{1}{3}(\cos(2\pi\theta_1) + \cos(2\pi\theta_2) + \cos 2\pi(\theta_1 - \theta_2)) \tag{32}$$

$$x_{\mathrm{im}} = \tfrac{1}{2}(x_1 - x_2) = \tfrac{1}{3}(\sin(2\pi \mathrm{i}\theta_1) - \sin(2\pi \mathrm{i}\theta_2) - \cos 2\pi \mathrm{i}(\theta_1 - \theta_2)). \tag{33}$$

Let $z = x_1$, $\overline{z} = x_2$, and write $T_{m,n}$ for T_k where $k = (m, n)^T$. We find the recurrences

$$T_{-1,0} = \overline{z}, \qquad T_{0,0} = 1, \qquad T_{1,0} = z \tag{34}$$



(*a*) (*b*)

Figure 4. The equilateral domain Δ maps to the Deltoid δ under coordinate change.

$$T_{n,0} = 3zT_{n-1,0} - 3\overline{z}T_{n-2,0} + T_{n-3,0} \tag{35}$$

$$T_{n,m} = (3T_{n,0}\overline{T_{m,0}} - T_{n-m,0})/2. \tag{36}$$

The fundamental domains of W are in the primal space $\Delta \subset G$ the triangle limited by $(0, 0)$, $\left(\frac{1}{3}, \frac{2}{3}\right)$, $\left(\frac{2}{3}, \frac{1}{3}\right)$ (the yellow triangle in figure 3(*a*)), and in the Fourier space $\mathcal{S} \subset \widehat{G}$ is the first quadrant of $\mathbb{Z}^2$. Under the discretization to Δ_m in the primal space, we find in the Fourier space $\mathcal{S}_m$ to be the quadrilateral with vertices in $(0, 0)$, $(m/2, 0)$, $(m/3, m/3)$, $(0, m/2)$. By also invoking the conjugation symmetry $T_{m,n} = \overline{T_{n,m}}$, we can reduce the fundamental domain in the Fourier space to the triangle $(0, 0)$, $(m/2, 0)$, $(m/3, m/3)$. The polynomials $T_{\ell,\ell}$ are all real, while the polynomials T_k for k on the line $(m/2, 0)$, $(m/3, m/3)$ are real on the lattice Δ_m. All the other T_k are complex.

In figure 4, we see the domain Δ_{12} and its image δ under change of variables (32) and (33). The domain δ is a shape known as the *deltoid*, or 3-cusp Steiner hypocycloid. It has many characterizations, and many interesting geometrical properties. The deltoid was introduced by L Euler in 1745 in a study of caustic patterns in optics, figure 5(*a*). The deltoid can also be drawn using a spirograph. Let a circle of diameter 2/3 roll inside a circle of diameter 1. Then the diameter of the inner circle fills the interior of the deltoid, figure 5(*b*). A line of constant length can be rotated inside the deltoid, so that it always touches all the three sides of the deltoid. Another property of the deltoid, which is interesting for approximation theory, is the fact that the straight lines of Δ pointing in the directions θ_1, θ_2 and $\theta_1 + \theta_2$ are mapped to straight lines in δ. In δ, these lines cross in points which are located as either 1D Gauss–Chebyshev points or Gauss–Chebyshev–Lobatto points. Other lines in Δ are not mapped to straight lines. We see for instance that the red triangle in Δ is mapped to the circle in δ, and importantly the green hexagon in Δ is mapped to a perfectly inscribed equilateral triangle in δ.

3.4.2. Approximation properties. For using Chebyshev A_2 in spectral elements, we must overcome the problem that T_k naturally lives on the deltoid and not triangles. We will discuss two approaches; either to straighten the deltoid to a triangle, or patching together deltoids with overlap.

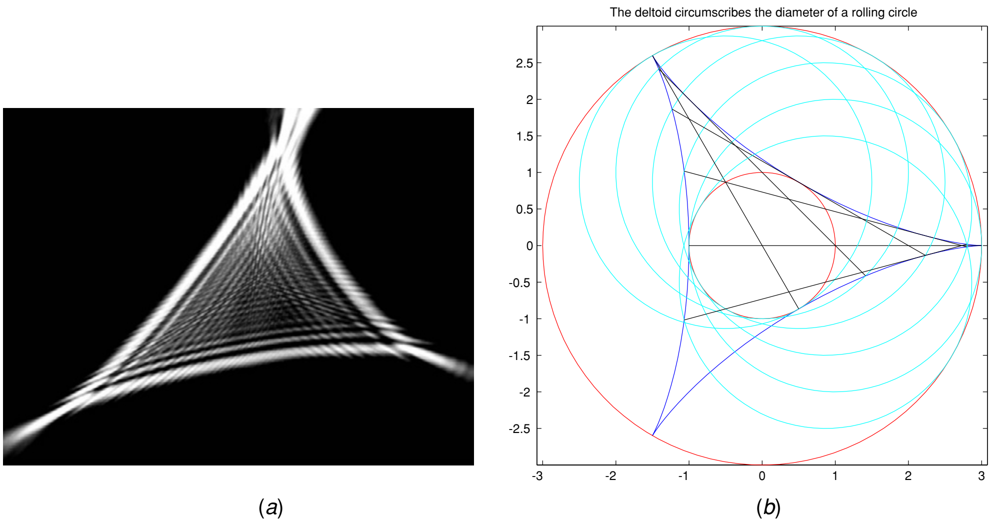


Figure 5. (*a*) A sunbeam refracted in a bathroom mirror. (*b*) Spirograph drawing.

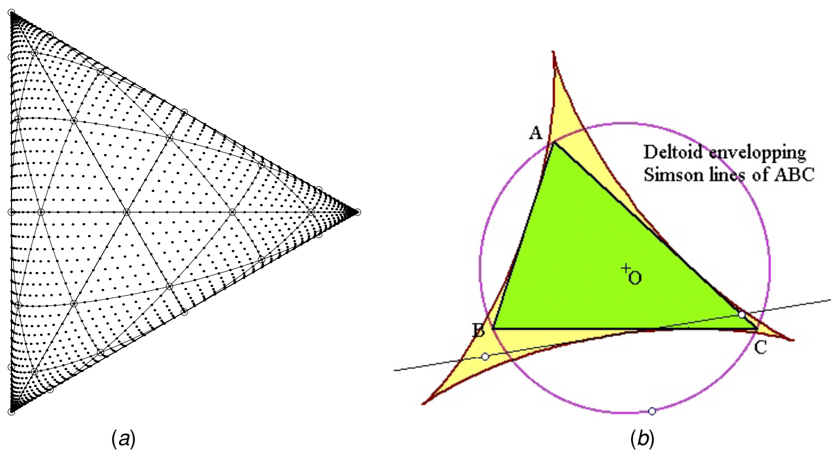


Figure 6. (*a*) Straightened deltoid. (*b*) Deltoid circumscribing arbitrary triangle.

Any straightening map from δ to a triangle must have singularities in the corners of δ, but can otherwise be well-behaved. We have constructed several different maps. A simple coordinate map taking $x(\theta) \in \delta$ to $[t_1, t_2]^T$ in an equilateral triangle, is given as

$$\boldsymbol{d} = [1 - \cos(\pi(2\theta_1 - \theta_2)), 1 - \cos(\pi(2\theta_2 - \theta_1)), 1 + \cos(\pi(\theta_1 + \theta_2))]^T \tag{37}$$

$$\begin{bmatrix} t_1 \\ t_2 \end{bmatrix} = \begin{bmatrix} -1/2 & -1/2 & 1 \\ -\sqrt{3}/2 & \sqrt{3}/2 & 0 \end{bmatrix} \cdot \boldsymbol{d}/\|\boldsymbol{d}\|_1, \tag{38}$$

The vector $\boldsymbol{d}$ represents the distances from x to the three sides of δ, measured along the three natural straight lines through x. In (38), these three numbers are taken as barycentric coordinates on an equilateral triangle with vertices given by the columns of the matrix. The resulting straight triangle is shown in figure 6(*a*).

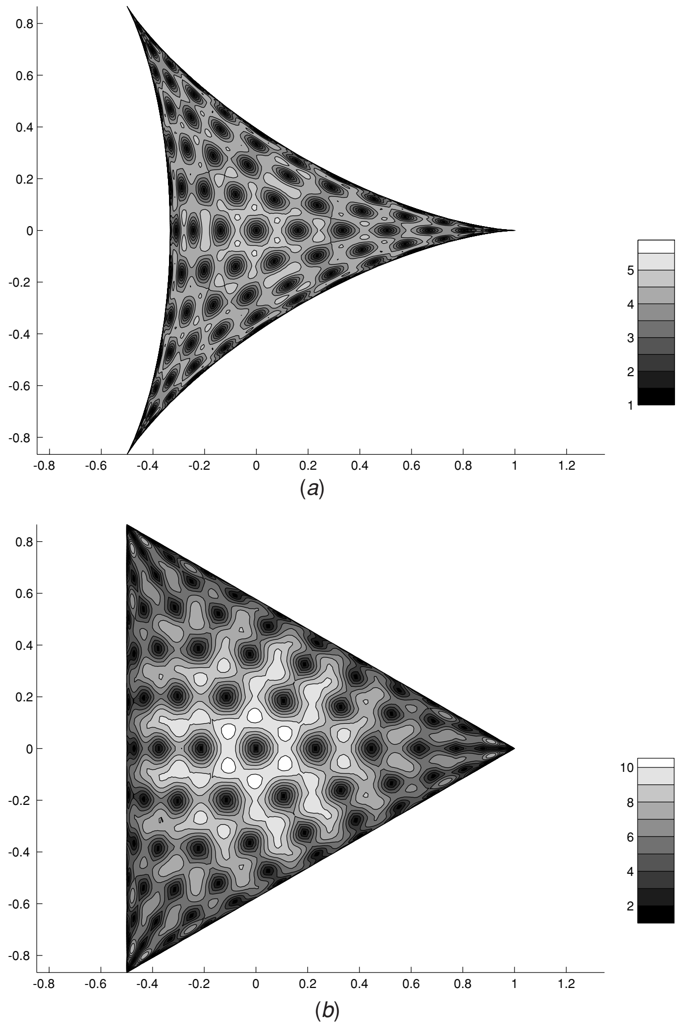


Figure 7. (*a*) Lebesgue function on deltoid. (*b*) Lebesgue function on straightened triangle.

Patching deltoids with overlap is an attractive alternative. The deltoid has the remarkable property of circumscribing *any* triangle such that each side of the triangle is tangent to a side of the deltoid, figure 6(*b*). It is not difficult to match nodes in two different patches along the naturally straight lines of the deltoid.

We want to numerically study the quality of interpolation on the deltoid and the straightened deltoid. Approximation theory on triangles is far less developed than on separable domains, and very little is known about choice of good interpolation points on triangles. Hesthaven (1998) has studied generalizations of Stieltjes electrostatic characterization of Jacobi–Gauss–Lobatto points from 1D to 2D, and produced interpolation points by numerical computations. In Taylor *et al* (2000), *Fekete interpolation points* are found by maximizing a Vandermonde determinant in a numerical optimization, see also Bos (1983), Chen and Babuska (1995), Fekete (1923). Fekete triangle points and icosahedral subdivisions of the

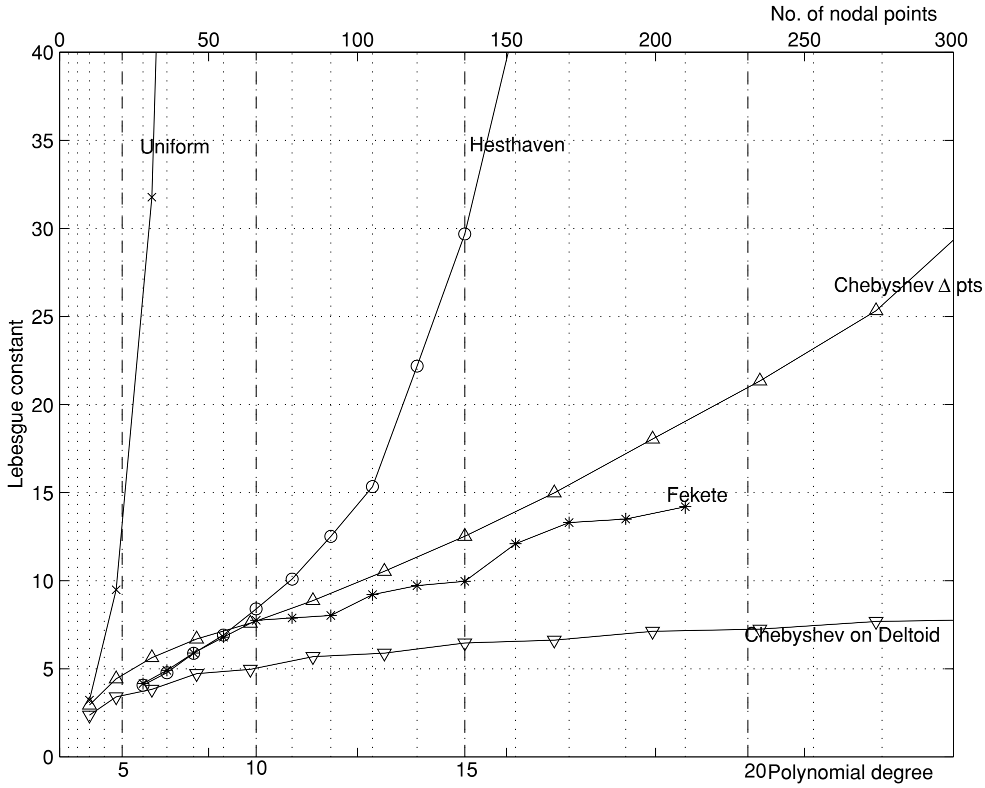


Figure 8. Lebesgue constants for various nodal points on the triangle and deltoid. Bottom curve: points $x(\Delta_m)$ on deltoid. All other curves: interpolation on triangle, from top: uniform points; Hesthaven electrostatic points; $x(\Delta_m)$ straightened to triangle (37)–(38); Fekete points.

sphere is used for nodal based spectral element discretizations of shallow water equations in Giraldo and Warburton (2005).

The quality of a set of interpolation points $\mathcal{I}$ can be measured by the *Lebesgue* constant, defined as $L = \|I\|_\infty$, where I is the (multivariate) interpolation operator in the given nodes. Slow growth of the Lebesgue constant is necessary for spectral convergence. Uniform points typically show exponential growth. Points with the minimal Lebesgue constant are called Lebesgue points, but there are no known algorithm for computing these. It is known that the Lebesgue constant for the optimal Lebesgue points grow logarithmically in the number of points. For the 1D Chebyshev–Lobatto points, it is known that the Lebesgue constant grows logarithmically. The proof can be generalized to our points $x(\Delta_m) \subset \delta$, so probably these points have near optimal interpolation properties. It is not known if the same property holds for the interpolation points in the straightened deltoid.

Numerically, we can compute the Lebesgue constant by computing the *Lebesgue function*

$$\lambda(x) = \sum_{i\in\mathcal{I}} |\ell_i(x)|,$$

where $\ell_i(x)$ is the Lagrangian cardinal polynominal at node i. After computing $\lambda(x)$ on a very fine lattice, we find the Lebesgue constant taking the maximum: $L = \|\lambda(x)\|_\infty$. Figure 7 shows the Lebesgue constants on the deltoid and straightened triangle. In figure 8, we see Lebesgue constants for various choices of interpolation points.

The interpolation points on the deltoid show excellent behaviour. Even when $m = 60$, yielding 631 nodal points and polynomials of degree 35, the Lebesgue constant is 9.1, and the condition number of the Chebyshev Vandermonde matrix is just 3.6.

The Lebesgue constant for the nodal points on the straightened triangle are also good. The growth of these seems to be faster than logarithmic, but they are better then the Hesthaven points and not much worse than the Fekete points, which requires optimization algorithms to be found. We believe that the Chebyshev-based nodal points are suitable for constructing high-order spectral element bases.

A final remark on triangular interpolation. The nodal-based triangular spectral elements used in Giraldo and Warburton (2005), Hesthaven (1998) are based on a number of interpolation points given as $(q+1)(q+2)/2$. This corresponds to the number of monomials in the *triangular-truncated* monomial basis $\{x^r y^s : r + s \leqslant q\}$. The number of nodal points in Δ_m is instead given as the *centred triangular numbers*

$$|\Delta_m| = \tfrac{1}{2}m(m/3 + 1) + 1.$$

The linear space in which we do our interpolation and computation of Lebesgue constants is the space spanned by the Chebyshev polynomials $T_k(x)$ for $k \in \mathcal{S}_m$. In this space, the lower monomials $x^r y^s$ are linearly independent, while the highest monomials appear only in certain linear combinations. We cannot see that this fact introduces any practical problems for the construction of spectral element bases.

4. Concluding remarks

A recurring theme in this paper has been applications of (finite) symmetry groups in the discretization and solution of PDEs. Group theory provides us with a unified framework for developing discretizations, fast algorithms and software. For triangle-based spectral elements, we believe that methods based on the non-separable multivariate Chebyshev polynomials type A_2 are very promising because of both the excellent approximation properties of these polynomials and the availability of fast transforms and Gaussian quadrature rules. Similarly, we believe that the A_3 family and the $A_2 \times A_1$ families are useful for 3D computation. Furthermore, we hope that a combination of equivariant spectral element discretizations in the space, and exponential integrators in time will yield competitive algorithms for important classes of large scale computational problems.

However, there are still obstacles to overcome in order to make such group-based tools available in the toolbox of computational scientists. One problem is the lack of the literature focused on applications of group theory in computations. The other problem is the lack of software. It is our conviction that the group theoretical framework enables us to produce general software packages for dealing with discrete versions of Chebyshev polynomials related to any Dynkin diagram. These are issues to be addressed in future work.

Acknowledgments

I would like to thank Krister Åhlander for discussions on the topics of the paper, and for suggesting a number of corrections and improvements of the manuscript.

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