and references therein) but the technique limits the results to a few particular orders and degrees. An attempt to construct grids invariant under the icosahedral group may be found in [23, 22] (with some negative weights in the early construction). We also refer to [7, 42] for a review and further references.

In this paper we develop a systematic numerical approach for constructing nearly optimal quadratures invariant under the icosahe

As a replacement for spherical harmonics, such "cubed sphere" represen-

computed and some implementations of the DVR method [17] use quadratures developed by Lebedev [26, 27]. Our quadratures should extend such methods by allowing e ectively an arbitrary order and degree.

We start by reviewing necessary mathematics, outline a general method for constructing nodes invariant under the icosahedral group and illustrate resulting quadratures through several examples. Based on these new quadra-

The spherical harmonics Y_n^m are linearly independent and, hence, the dimension of $\mathcal{H}_n$ is $2n + 1$. The subspace of maximum degree N is then the direct sum

(2.5) $$\mathcal{P}_N = \bigoplus_{n=0}^{N} \mathcal{H}_n = \mathrm{span}\left\{Y_n^m(\ ,\ ),\ |m| \leq n,\ 0 \leq n \leq N\right\}$$

and has dimension $(N + 1)^2$. We make use of the addition theorem (see e.g. [13]), which states that for $\omega, \omega' \in \mathbb{S}^2$

(2.6) $$\frac{2n + 1}{4}P_n\left(\omega \cdot \omega'\right) = \sum_{m=-n}^{n} Y_n^m(\omega)\, Y_n^{*m}(\omega')\,,$$

where P_n is the Legendre o N

where $\lfloor \rfloor$ denotes the integer part .

This result may also be obtained using a theorem of Molien (circa 1897) [33]. In his approach the number of invariants for a finite group may be obtained as coefficients of a generating function. In our case we have (see [32])

Theorem For a given degree **n**, the number of functions invariant under the icosahedral rotation group in a subspace of spherical harmonics $\mathcal{H}_n$ is given by coefficients **S(n)** of the series expansion of the generating function,

$$\frac{1 + t^{15}}{(1 - t^6)(1 - t^{10})} = \sum_{n=0}^{\infty} S(n) t^n.$$

It is not difficult to see that both Theorems 2.2 and 2.3 yield the same result. We use theorems of this section to determine the number of equations contributed by each subspace $\mathcal{H}_n$ to the nonlinear system of equations determining the quadrature nodes and weights.

3. Quadratures for the sphere

The main difficulty in constructing quadratures comes from the need to solve a large system of nonlinear equations. Without using special structure of these equations, general root finding or optimization methods typically fail. The essence of our approach is to develop and use such structure within a root finding method.

We start by noting four different types of orbits of the icosahedral rotation group. In general, with three exceptions described below, a point on the sphere under the action of the group generates a total of 60

where $\{\,_i^v,\,_i^v\}_{i=1}^{12}$ are coordinates of the vertices of an icosahedron inscribed in the unit sphere, w_v their associated weight, N_g is the number of generators with coordinates $\{\,^{(j)},\,^{(j)}\}_{j=1}^{N_g}$ and weights $\{w_j\}_{j=1}^{N_g}$. For each $g_i \in G$, we denote $\left(\,_i^{(j)},\,_i^{(j)}\right) = \left(g_i^{-1}\,^{(j)}, g_i^{-1}\,^{(j)}\right)$

For this quadrature we have $3N_g + 3$ unknown generator coordinates and weights, with the total of $60N_g + 62$ nodes.

Using Theorem 2.2 or 2.3, we determine the number of invariant functions in the subspace $\mathcal{H}_n$. Theorem 2.1 allows us to limit the number of equations to not exceed the number of invariant functions. Ideally, when constructing a system of equations for the generator coordinates and weights, we would like to match the number of equations to the number of unknowns. For example, to construct a quadrature that integrates exactly the subspace $\mathcal{P}_{23}$, we must integrate the 10 invariant functions in $\mathcal{P}_{23}$. Therefore, we have 10 equations and, using quadrature (3.1), we have $3N_g + 1$ unknowns, where N_g is the number of generators. Setting $3N_g + 1 = 10$ gives $N_g = 3$ and, thus, we look for a quadrature with $192 = 3 \times 60 + 12$ nodes. We solve the corresponding system (see Section 3.2) and obtain a solution, thus verifying its existence directly. We illustrate a set of 7212 nodes that exactly integrates $\mathcal{P}_{145}$ in Figure 3.2. This set of nodes was found using the quadrature Q_v in (3.1).

However, it appears that in some cases so constructed system of equations may not have a solution. Our conclusion is based on the behavior of Newton's iteration and, so far, has not been verified analytically. In such cases, we reduce the number of equations by removing those from the subspace of the highest degree and solve a formally under determined system. We note that in this situation Newton's iteration may not converge quadratically and
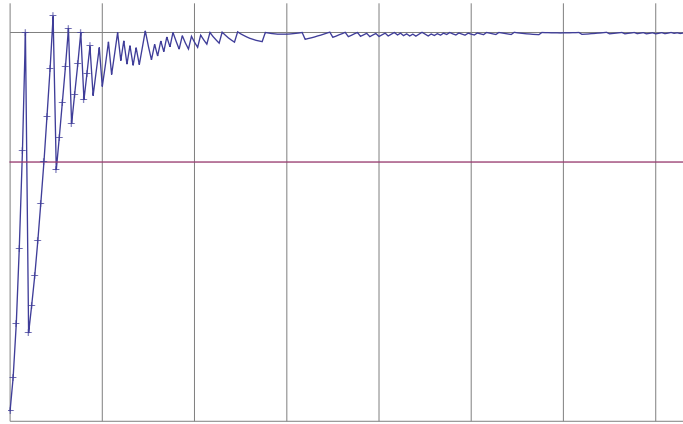
the case since any missing invariant functions would have been discovered during a posteriori verification of quadratures.

Recall that Newton's method for solving the system of nonlinear equations
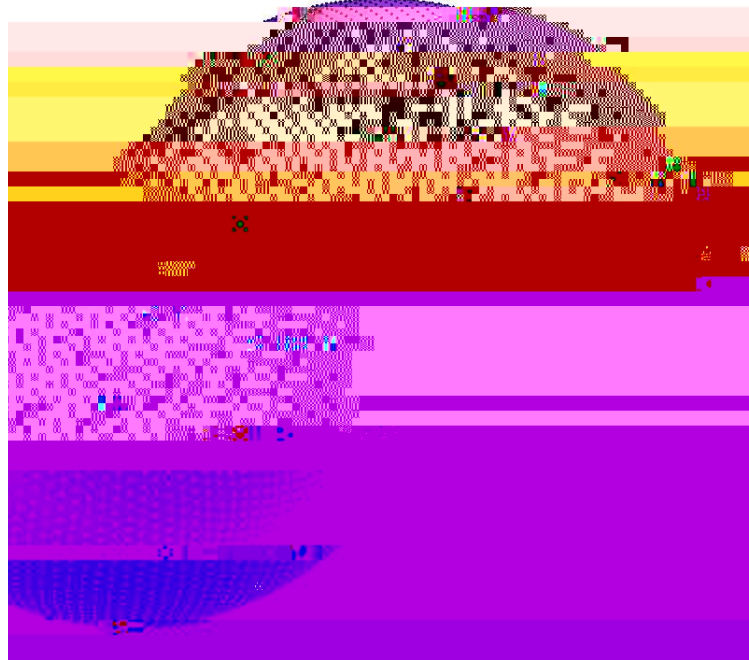
F

Figure 3.2. **Positions of 7212 quadrature nodes of a quadrature integrating exactly all spherical harmonics in the subspace of maximal order and degree 145. This quadrature has efficiency $\varepsilon = 0.98521....$**

uniquely determine the number and type of generators for which the triangle $P_0 P_1 P_2$ serves as a template. Thus, t and s uniquely determine the total number of unknown parameters in the nonlinear system (3.7). We illustrate this construction in Figure 3.3.

The center of the triangle $P_0 P_1 P_2$ is at the point

$$P_c = (t - s)/3\ _1 + (t + 2s)/3\ _2 = \left(t/2, (t + 2s)/(2\sqrt{3}) \right),$$

which may or may not be a point of the lattice. If the center coincides with a lattice point, then the type of quadrature is one with a face-centered node. In the same manner, for some choices of parameters t and s, there might beh
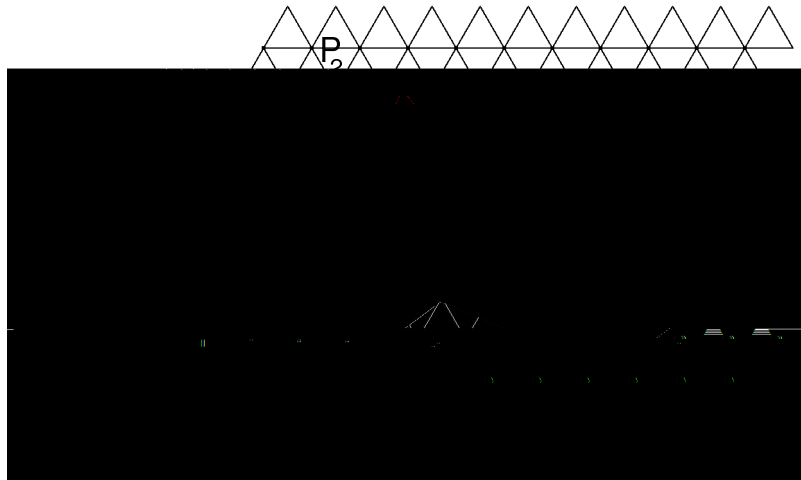
Figure 3.3. **A grid template on a face of the icosahedron. Here there are 9 generators with orbits of length 60 and 1 node at the face center with orbit length 20, yielding 28 nodes in the interior of the triangle and 572 total nodes on the sphere. The resulting quadrature found using Newton's method integrates the subspace of maximum order and degree N = 40. One of the possible 3 fundamental region is shown shaded.**

to position the generators onto the sphere, we first map the points from the

on this further below and note that an attempt to use the same number of functions $K(\omega \cdot \omega_j)$ as the dimension of $\mathcal{P}_N$ leads to ill-conditioned systems [38, 10].

Let us now consider $\mathbf{f} \in \mathcal{P}_N$ and evaluate (4.1) at the quadrature nodes $\{\omega_i\}_{i=1}^M$. We obtain

$$\sqrt{\mathbf{w}_i}\mathbf{f}\ (\omega$$

5. Algorithms associated with icosahedral grids

For e cient use of the quadratures developed in this paper, we need fast algorithms for evaluation of sums on these grids. Currently we only have $\mathcal{O}$

in [21] is the standard quadrature with $\mathcal{O}(N)$ Gauss-Legendre nodes in the polar direction (and thus $N_{planes} \sim N$) and $\mathcal{O}(N)$ equally spaced nodes in the azimuthal direction. Using the Fast Fourier transform to evaluate along the azimuthal direction and FMM to evaluate in the polar direction yields the overall complexity of $\mathcal{O}(N^2 \log N)$. Unfortunately, in our case the number of planes $N_{planes} \sim$

If we were to measure the decay of a function on the sphere using variance defined as

$$\text{(6.1)} \qquad \text{Var}(\mathbf{f}) \equiv \frac{\int_{\mathbb{S}^2} \|\xi - \langle\xi\rangle\|^2 \mathbf{f}(\xi)^2 \, \mathbf{d}}{\int_{\mathbb{S}^2} \mathbf{f}(\xi)^2 \, \mathbf{d}},$$

where the mean is defined as

$$\text{(6.2)} \qquad \langle\xi\rangle \equiv \frac{\int_{\mathbb{S}^2} \xi \, \mathbf{f}(\xi)^2 \, \mathbf{d}}{\int_{\mathbb{S}^2} \mathbf{f}(\xi)^2 \, \mathbf{d}},$$

then we can show that for large $\mathbf{N}$ the variance of the kernel $\mathbf{K}$ decays only as $\mathcal{O}(1/\mathbf{N})$.

To improve localization of the kernel, let us consider

$$\text{(6.3)} \qquad \tilde{\mathbf{K}}(\omega \cdot \omega') = \mathbf{K}(\omega \cdot \omega') + \sum_{n=N+1}^{pN} \frac{2\mathbf{n}+1}{4} a_n \mathbf{P}_n(\omega \cdot \omega'),$$

where $\mathbf{p}$ is the over-sampling factor and the coe cients a_n are chosen to improve localization. Substituting (6.3) into (6.1) and minimizing the result with respect to a_n, we find that the resulting coe cients a_n decrease linearly with a particular (optimal) slope. Using these optimal coe cients, we achieve $\text{Var}(\tilde{\mathbf{K}}) \sim \mathcal{O}(1/(\mathbf{pN})^2)$. Since the total number of nodes is also proportional to $\mathbf{N}^2$, this indicates that for a given node the number of neighbors needed to be taken into account to achieve a given accuracy remains constant as $\mathbf{N}$ becomes large.

We now show that $\tilde{\mathbf{K}}$ may be used as a projector onto $\mathcal{P}_N$. For fixed ω, we have $\tilde{\mathbf{K}} \in \mathcal{P}_{pN}$, while $\tilde{\mathbf{K}} - \mathbf{K} \notin \mathcal{P}_N$. Thus, we obtain

$$\mathbf{K}(\omega \cdot \omega') = \int_{\mathbb{S}^2} \tilde{\mathbf{K}}(\omega \cdot \nu) \mathbf{K}(\nu \cdot \omega') \, \mathbf{d}\nu.$$

Now for $\mathbf{f} \in \mathcal{P}_N$, we write

$$\mathbf{f}(\omega) = \int_{\mathbb{S}^2} \mathbf{K}(\omega \cdot \omega') \mathbf{f}(\omega') \, \mathbf{d}\omega'$$

resulting in

$$\begin{aligned}
\int_{\mathbb{S}^2} \tilde{\mathbf{K}}(\omega \cdot \nu) \mathbf{f}(\nu) \, \mathbf{d}\nu &= \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} \tilde{\mathbf{K}}(\omega \cdot \nu) \mathbf{K}(\nu \cdot \omega') \mathbf{f}(\omega') \, \mathbf{d}\omega' \mathbf{d}\nu \\
&= \int_{\mathbb{S}^2} \mathbf{K}(\omega \cdot \omega') \mathbf{f}(\omega') \, \mathbf{d}\omega' \\
&= \mathbf{f}(\omega),
\end{aligned}$$

so that $\tilde{\mathbf{K}}$ is a projector onto $\mathcal{P}_N$. One of the benefits of using $\tilde{\mathbf{K}}$ over $\mathbf{K}$ is that we may consider fast algorithms exploiting the local nature of $\tilde{\mathbf{K}}$. We leave it as a subject for future research.

7.

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where C_n^m is a normalization constant. We now compute the partial derivatives of (8.1) with respect to and . We obtain

ROTATIONALLY INVARIANT QUADRATURES FOR THE SPHERE

CORY AHRENS AND GREGORY BEYLKIN

Online supplement

Coordinates of vertices of an icosahedron. $\alpha = \left(1 - \sqrt{5}\right)/2$

	oo n
v_1	$(0, \alpha, 1)/\sqrt{1+\alpha^2}$
v_2	$(0, \alpha, -1)/\sqrt{1+\alpha^2}$
v_3	$(1, 0, \alpha)/\sqrt{1+\alpha^2}$
v_4	$(1, 0, -\alpha)/\sqrt{1+\alpha^2}$
v_5	$(\alpha, 1, 0)/\sqrt{1+\alpha^2}$
v_6	$(\alpha, -1, 0)/\sqrt{1+\alpha^2}$
v_{i+6}	$-v_i \quad i = 1 \dots 6$

Table 1.   n coo   n   o   n co   on $\alpha = \left(1 - \sqrt{5}\right)/2$

Elements of the icosahedral rotation group as quaternions.

1

$\mathbf{q}_1 = -\frac{1}{2} - \mathbf{i}\frac{1}{2} + \mathbf{j}\frac{1}{2} - \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{21} = \mathbf{i}$	$\mathbf{q}_{41} = -\beta + \mathbf{i}\frac{1}{2} + \mathbf{k}\gamma$
$\mathbf{q}_2 = -\frac{1}{2} - \mathbf{i}\frac{1}{2} + \mathbf{j}\frac{1}{2} + \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{22} = -\mathbf{i}\beta - \mathbf{j}\frac{1}{2} - \mathbf{k}\gamma$	$\mathbf{q}_{42} = -\beta + \mathbf{i}\frac{1}{2} - \mathbf{k}\gamma$
$\mathbf{q}_3 = -\frac{1}{2} - \mathbf{j}\beta + \mathbf{k}\gamma$	$\mathbf{q}_{23} = -\mathbf{i}\beta + \mathbf{j}\frac{1}{2} + \mathbf{k}\gamma$	$\mathbf{q}_{43} = -\beta + \mathbf{i}\gamma - \mathbf{j}\frac{1}{2}$
$\mathbf{q}_4 = -\frac{1}{2} + \mathbf{j}\beta + \mathbf{k}\gamma$	$\mathbf{q}_{24} = -\mathbf{i}\beta + \mathbf{j}\frac{1}{2} - \mathbf{k}\gamma$	$\mathbf{q}_{44} = -\beta + \mathbf{i}\gamma + \mathbf{j}\frac{1}{2}$
$\mathbf{q}_5 = -\frac{1}{2} + \mathbf{i}\frac{1}{2} - \mathbf{j}\frac{1}{2} - \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{25} = \mathbf{i}\gamma - \mathbf{j}\beta - \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{45} = -\beta - \mathbf{i}\gamma - \mathbf{j}\frac{1}{2}$
$\mathbf{q}_6 = -\frac{1}{2} + \mathbf{i}\frac{1}{2} - \mathbf{j}\frac{1}{2} + \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{26} = \mathbf{i}\gamma - \mathbf{j}\beta + \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{46} = -\beta - \mathbf{i}\gamma + \mathbf{j}\frac{1}{2}$
$\mathbf{q}_7 = -\frac{1}{2} - \mathbf{i}\beta + \mathbf{j}\gamma$	$\mathbf{q}_{27} = \mathbf{i}\gamma + \mathbf{j}\beta + \mathbf{k}\frac{1}{2}$	$\mathbf{q}_{47} = \gamma -$