Sparse spectral methods for partial differential equations on spherical caps and bands

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Abstract

In recent years, sparse spectral methods for solving partial differential equations have been derived using hierarchies of classical orthogonal polynomials on intervals, disks, and triangles. In this work we extend the methodology to a hierarchy of non-classical multivariate orthogonal polynomials on spherical caps and bands. The entries of discretisations of partial differential operators can be effectively computed using formulae in terms of (non-classical) univariate orthogonal polynomials. We demonstrate the results on partial differential equations involving the spherical Laplacian and Biharmonic operators, showing spectral convergence.

1 Introduction

This paper develops sparse spectral methods for solving linear partial differential equations on certain subsets of the sphere: spherical bands and spherical caps. More precisely, we consider the solution of partial differential equations on the domain Ω given by

$$\Omega := \{(x, y, z) \in \mathbb{R}^3 \quad | \quad \alpha < z < \beta,\ ||(x, y)|| := \sqrt{x^2 + y^2} = \rho(z)\}$$

and consider the case where $\alpha \in (0, 1)$ and where $\rho(z) := \sqrt{1 - z^2}$, $\beta := 1$. This framework then yields that Ω is a spherical cap (the region of the surface of a sphere where the z-coordinate ranges from α to 1), i.e.

Why is α restricted to be positive?

$$\Omega := \{(x, y, z) \in \mathbb{R}^3 \quad | \quad \alpha < z < 1,\ x^2 + y^2 + z^2 = 1\}$$

Of course, there is a simple extension to a spherical band by taking $\beta \in (\alpha, 1)$. However for simplicity we focus on the spherical cap in this paper.

Don't we need $\beta \neq 1$ to get a band?

We advocate using a basis that is polynomial in cartesian coordinates, that is, polynomial in x, y, and z, and orthogonal with respect to a prescribed weight: that is, multivariate

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orthogonal polynomials, whose construction was considered in [13]. Equivalently, we can think of these as polynomials modulo the vanishing ideal $\{x^2 + y^2 + z^2 = 1\}$, or simply as a linear recombination of spherical harmonics that are orthogonalised on a subset of the sphere. This is in contrast to more standard approaches based on mapping the geometry to a simpler one (e.g., a rectangle or disk) and using orthogonal polynomials in the mapped coordinates (e.g., a basis that is polynomial in the spherical coordinates φ and θ). The benefit of the new approach is that we do not need to resolve Jacobians, and thereby we can achieve sparse discretisations for partial differential operators, including those with polynomial variable coefficients. On the spherical cap, the family of weights we consider are of the form

$$W^{(a)}(x, y, z) := (z - \alpha)^a, \quad \text{for} \quad (x, y, z) \in \Omega,$$

noting that $W^{(a)}(x, y, z) = 0$ for $(x, y, z) \in \partial\,\Omega$. The corresponding OPs denoted $Q^{(a)}_{n,k,i}(x, y, z)$, where n denotes the polynomial degree, $0 \le k \le n$ and $i \in \{0, \min(1, k)\}$. We define these to be orthogonalised lexicographically, that is,

I don't understand this ordering. Shouldn't it either be $x^k y^j z^{n-k-j}$ or $x^k y^{j-k} z^{n-j}$? PS I prefer j to i

$$Q^{(a)}_{n,k,i}(x, y, z) = C_{n,k,i}\, x^{k-\tilde{k}_i}\, y^{\tilde{k}_i}\, z^{n-k} + (\text{lower order terms})$$

How can I write down what the ordering is? Is this necessary?

where $C_{n,k,i} \ne 0$ and "lower order terms" includes degree n polynomials of the form $x^{j-\tilde{j}_i}\, y^{\tilde{j}_i}\, z^{n-j}$ where $j < k$. The precise normalization arises from their definition in terms of one-dimensional OPs in Definition 2.

We consider partial differential operators involving the spherical Laplacian (the Laplace–Beltrami operator): in spherical coordinates

$$\begin{aligned} z &= \cos\varphi, \\ x &= \sin\varphi\cos\theta = \rho(z)\cos\theta, \\ y &= \sin\varphi\sin\theta = \rho(z)\sin\theta. \end{aligned}$$

we have

Double check

$$\Delta_{\mathrm{S}} = \frac{1}{\sin\varphi}\frac{\partial}{\partial\varphi}\sin\varphi\frac{\partial}{\partial\varphi} + \frac{1}{\sin^2\varphi}\frac{\partial^2}{\partial\theta^2} = \frac{1}{\rho}\frac{\partial}{\partial\varphi}\rho\frac{\partial}{\partial\varphi} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}$$

We do so by considering the component operators $\rho\frac{\partial}{\partial\varphi}$ and $\frac{\partial}{\partial\theta}$ applied to OPs with a specific choices of weight so that their discretisation is sparse, see Theorem 1. Sparsity comes from expanding the domain and range of an operator using different choices of the parameter a, a la the ultraspherical spectral method for intervals [10], triangles [12] and disk-slices and trapeziums [15], and the related work on sparse discretisations on disks [17] and spheres [18, 6]. As in the disk-slice case in 2D [15], we use an integration-by-parts argument to deduce the sparsity structure.

The three-dimensional orthogonal polynomials defined here involve the same non-classical (in fact, semi-classical) 1D OPs as those outlined for the disk-slice, and so methods for calculating these 1D OP recurrence coefficients and integrals has already been outlined [15]. In particular, by exploiting the connection with these 1D OPs we can construct discretizations of general partial differential operators of size $(p+1)^2 \times (p+1)^2$ in $O(p^3)$ operations, where p is the total polynomial degree. This clearly compares favourably to proceeding in a naïve approach where one would require $O(p^6)$ operations. Furthermore, we can use this framework to derive sparse p-finite element methods, which we introduce as an Appendix here. The methods are analogous to those of Beuchler and Schöberl on tetrahedra [2], see also work by Li and Shen [7].

Add citation

Note that we consider partial differential operators that are not necessarily rotational invariant: for example, one can use these techniques for Schrödinger operators $\Delta_{\mathrm{S}} + V(x, y, z)$ where V is first approximated by a polynomial. A nice feature though is that if the partial differential operator is invariant with respect to rotation around the z axes (e.g., a Schrödinger operator with potential $V(z)$) the discretisation decouples, and can be reordered as a block-diagonal matrix. This improves the complexity further to an optimal $O(p^2)$.

Adding a complexity plot showing this would be great

An overview of the paper is as follows:

Section 2: We present our definition of a (one-parameter) family of 3D orthogonal polynomials (OPs) on the spherical cap domain Ω, by combining 1D OPs on the interval $(\alpha, 1)$ with Chebyshev polynomials, to form 3D OPs on the spherical cap surface. We show that these families will lead to sparse Jacobi operators for multiplication by x, y, z and demonstrate how to obtain the 3D OPs.

Section 3: We define useful partial differential operators and further show that these will also be sparse. We can exactly calculate the non-zero entries of these sparse operators using the quadrature rule associated with the non-classical 1D OPs.

Section 4: We derive a quadrature rule on the spherical cap that can be used to expand a function in the OP basis up to a given order N, and demonstrate how to evaluate a function using the Clenshaw algorithm using the coefficients of its expansion.

Section 5: We demonstrate the proposed technique for solving differential equations on the spherical cap such as the Poisson equation, variable coefficient Helmholtz equation, and Biharmonic equation.

Appendix A: We outline how our framework can allow us to construct sparse hp-finite element method on the sphere, using spherical band and cap elements that would capture spherical geometry precisely. We lay the groundwork by simply presenting a sparse p-finite element method using a single spherical cap element.

2 Orthogonal polynomials on spherical caps

In this section we outline the construction and some basic properties of $Q^{(a)}_{n,k,i}(x, y, z)$.

2.1 Explicit construction

We can construct the 3D orthogonal polynomials on Ω from 1D orthogonal polynomials on the interval $[\alpha, \beta]$, and from Chebyshev polynomials. We do so in terms of Fourier series, which, following [13], we write here as orthogonal polynomials in x and y:

Definition 1. *Define the unit circle $\omega := \{\mathbf{x} = (x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 1\}$, and define the parameter θ for each $(x, y) \in \omega$ by $x = \cos\theta$, $y = \sin\theta$. Define the polynomials $\{Y_{k,i}\}$ for $k = 0, 1, \ldots,$ $i = 0, 1$ on $(x, y) \in \omega$ by*

$$\begin{aligned} Y_{0,0}(\mathbf{x}) \equiv Y_{0,0}(x,y) &:= Y_0 =: Y_{0,0}(\theta) \\ Y_{k,0}(\mathbf{x}) \equiv Y_{k,0}(x,y) &:= T_k(x) = \cos k\theta =: Y_{k,0}(\theta), \quad k = 1,2,3,\ldots \\ Y_{k,1}(\mathbf{x}) \equiv Y_{k,1}(x,y) &:= y\, U_{k-1}(x) = \sin k\theta =: Y_{k,1}(\theta), \quad k = 1,2,3,\ldots \end{aligned} \tag{1}$$

where $Y_0 := \frac{\sqrt{2}}{2}$ and T_k, U_{k-1} are the standard Chebyshev polynomials on the interval $[-1, 1]$. The $\{Y_{k,i}\}$ are orthonormal with respect to the inner product

The σ notation needs explanation

$$\langle p,\, q\rangle_Y := \frac{1}{\pi}\int_{||\mathbf{x}||=1} p(\mathbf{x})\, q(\mathbf{x})\, \mathrm{d}\sigma(\mathbf{x}) = \frac{1}{\pi}\int_0^{2\pi} p(\mathbf{x}(\theta))\, q(\mathbf{x}(\theta))\, \mathrm{d}\theta. \tag{2}$$

Note that we have defined Y_0 so as to ensure orthonormality.

Isn't the following from [13]? We then don't need to repeat the proof

Proposition 1. *Let $w : (\alpha, \beta) \to \mathbb{R}$ be a weight function. $\forall$, $n = 0, 1, 2, \ldots,$ let $\{r_{n,k}\}$ be polynomials orthogonal with respect to the weight $\rho(x)^{2k} w(x)$ where $0 \le k \le n$. Then the 3D polynomials defined on Ω*

$$Q_{n,k,i}(x,y,z) \equiv Q_{n,k,i}(\mathbf{x}, z) := r_{n-k,k}(z)\, \rho(z)^k\, Y_{k,i}\left(\frac{\mathbf{x}}{\rho(z)}\right)$$

for $i \in 0, 1$, $0 \le k \le n$, $n = 0, 1, 2, \ldots$ are orthogonal polynomials with respect to the inner *product*

$$\begin{aligned}\langle p,\, q\rangle &:= \int_\Omega p(\mathbf{x},z)\, q(\mathbf{x},z)\, w(z)\, \mathrm{d}\sigma(\mathbf{x},z)\\ &= \int_\alpha^1 \int_0^{2\pi} p(\rho(z)\cos\theta, \rho(z)\sin\theta, z)\, q(\rho(z)\cos\theta, \rho(z)\sin\theta, z)\, \mathrm{d}\theta\, w(z)\, \mathrm{d}z\end{aligned}$$

on Ω.

Proof.

$$\begin{aligned}\langle Q_{n,k,i},\, Q_{m,j,h}\rangle &= \int_\alpha^1 \int_0^{2\pi} r_{n-k,k}(z)\, \rho(z)^k\, Y_{k,i}(\theta)\, r_{m-j,j}(z)\, \rho(z)^j\, Y_{j,h}(\theta)\, \mathrm{d}\theta\, w(z)\, \mathrm{d}z\\ &= \Big(\int_0^{2\pi} Y_{k,i}(\theta)\;\, Y_{j,h}(\theta)\, \mathrm{d}\theta\Big)\Big(\int_\alpha^1 r_{n-k,k}(z)\, \rho(z)^k\, r_{m-j,j}(z)\, \rho(z)^j\, w(z)\, \mathrm{d}z\Big)\\ &= \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 r_{n-k,k}(z)\, r_{m-k,k}(z)\, \rho(z)^{2k}\, w(z)\, \mathrm{d}z\\ &= C\, \pi\, \delta_{k,j}\, \delta_{i,h}\end{aligned}$$

for some constant C. □

For the spherical cap, we can use Proposition 1 to create our one-parameter family of OPs. We first introduce notation for our family of non-classical univariate OPs that will be used as the r_n polynomials above.

Definition 2 ([15])**.** *Let* $w_R^{(a,b)}(x)$ *be a weight function on the interval* $(\alpha, 1)$ *given by:*

$$w_R^{(a,b)}(x) := (x-\alpha)^a\, \rho(x)^b$$

and define the associated inner product by:

$$\langle p,\, q\rangle_{w_R^{(a,b)}} := \frac{1}{\omega_R^{(a,b)}} \int_\alpha^1 p(x)\, q(x)\, w_R^{(a,b)}(x)\, \mathrm{d}x \tag{3}$$

where

$$\omega_R^{(a,b)} := \int_\alpha^1 w_R^{(a,b)}(x)\, \mathrm{d}x \tag{4}$$

is a normalising constant. Denote the two-parameter family of orthonormal polynomials on $[\alpha, \beta]$ *by* $\{R_n^{(a,b)}\}$*, orthonormal with respect to the inner product defined in (3).*

We can now define the 3D OPs for the spherical cap.

Definition 3. *Define the one-parameter 3D orthogonal polynomials via:*

$$Q^{(a)}_{n,k,i}(x,y,z) := R^{(a,2k)}_{n-k}(z)\,\rho(z)^k\,Y_{k,i}\left(\frac{x}{\rho(z)},\frac{y}{\rho(z)}\right), \quad (x,y,z)\in\Omega, \tag{5}$$

By construction, $\{Q^{(a)}_{n,k,i}\}$ are orthogonal with respect to the inner product

$$\langle p,\, q\rangle_{Q^{(a)}} := \int_\Omega p(\mathbf{x},z)\,q(\mathbf{x},z)\,w_R^{(a,0)}(z)\,\mathrm{d}\sigma(\mathbf{x},z) \tag{6}$$

$$= \int_\alpha^1 \int_0^{2\pi} p(\rho(z)\cos\theta,\rho(z)\sin\theta,z)\,q(\rho(z)\cos\theta,\rho(z)\sin\theta,z)\,\mathrm{d}\theta\,w_R^{(a,0)}(z)\,\mathrm{d}z, \tag{7}$$

with

$$\left\|Q^{(a)}_{n,k,i}\right\|^2_{Q^{(a)}} := \left\langle Q^{(a)}_{n,k,i},\, Q^{(a)}_{n,k,i}\right\rangle_{Q^{(a)}} = \pi\,\omega_R^{(a,2k)} \tag{8}$$

We note that the weight $w_R^{(a,b)}(z)$ has been used in the construction of 2D orthogonal polynomials on disk-slices and trapeziums [15], where a method for obtaining recurrence coefficients and evaluating integrals was established (the weight is in fact semi-classical, and is equivalent to a generalized Jacobi weight [8, §5]).

2.2 Jacobi matrices

We can express the three-term recurrences associated with $R_n^{(a,b)}$ as

$$xR_n^{(a,b)}(x) = \beta_n^{(a,b)}R_{n+1}^{(a,b)}(x) + \alpha_n^{(a,b)}R_n^{(a,b)}(x) + \beta_{n-1}^{(a,b)}R_{n-1}^{(a,b)}(x) \tag{9}$$

where the coefficients are calculatable (see [15]). We can use (9) to determine the 3D recurrences for $Q^{(a)}_{n,k,i}(x,y,z)$. Importantly, we can deduce sparsity in the recurrence relationships. We first require the following Lemma.

Lemma 1. *The following identities hold for $k = 2, 3, \ldots,\ j = 0, 1, \ldots$ and $i, h \in \{0, 1\}$:*

$$
\begin{array}{ll}
1) & \displaystyle\int_0^{2\pi} Y_0\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = Y_0\, \pi\, \delta_{0,h}\, \delta_{1,j} \\
2) & \displaystyle\int_0^{2\pi} Y_0\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = Y_0\, \pi\, \delta_{1,h}\, \delta_{1,j} \\
3) & \displaystyle\int_0^{2\pi} Y_{1,i}(\theta)\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = \pi\, \delta_{i,h}\, (Y_0\, \delta_{0,j} + \frac{1}{2}\delta_{2,j}) \\
4) & \displaystyle\int_0^{2\pi} Y_{1,i}(\theta)\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = \pi\, \delta_{|i-1|,h}\, ((-1)^{i+1}\, Y_0\, \delta_{0,j} + (-1)^i\, \frac{1}{2}\, \delta_{2,j}) \\
5) & \displaystyle\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = \frac{1}{2}\, \pi\, \delta_{i,h}\, (\delta_{k-1,j} + \delta_{k+1,j}) \\
6) & \displaystyle\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = \frac{1}{2}\, \pi\, \delta_{|i-1|,h}\, ((-1)^{i+1}\, \delta_{k-1,j} + (-1)^i\, \delta_{k+1,j}).
\end{array}
$$

Proof. Each follows from the definitions of $Y_{k,i}$ and Y_0, as well as the relationships:

$$
\begin{aligned}
2\cos k\theta \cos\theta &= \cos(k-1)\theta + \cos(k+1)\theta \\
2\sin k\theta \cos\theta &= \sin(k-1)\theta + \sin(k+1)\theta \\
2\cos k\theta \sin\theta &= -\sin(k-1)\theta + \sin(k+1)\theta \\
2\sin k\theta \sin\theta &= \cos(k-1)\theta - \cos(k+1)\theta.
\end{aligned}
$$

□

Lemma 2. *Define*

$$
\eta_k := \begin{cases} 0 & \text{if } k < 0 \\ Y_0 & \text{if } k = 0 \\ \frac{1}{2} & \text{otherwise} \end{cases} \tag{10}
$$

$Q^{(a)}_{n,k,i}(x,y,z)$ *satisfy the following recurrences:*

$$\begin{aligned} x\,Q^{(a)}_{n,k,i}(x,y,z) &= \alpha^{(a)}_{n,k,1}\,Q^{(a)}_{n-1,k-1,i}(x,y,z) + \alpha^{(a)}_{n,k,2}\,Q^{(a)}_{n-1,k+1,i}(x,y,z) \\ &\quad + \alpha^{(a)}_{n,k,3}\,Q^{(a)}_{n,k-1,i}(x,y,z) + \alpha^{(a)}_{n,k,4}\,Q^{(a)}_{n,k+1,i}(x,y,z) \\ &\quad + \alpha^{(a)}_{n,k,5}\,Q^{(a)}_{n+1,k-1,i}(x,y,z) + \alpha^{(a)}_{n,k,6}\,Q^{(a)}_{n+1,k+1,i}(x,y,z), \end{aligned}$$

$$\begin{aligned} y\,Q^{(a)}_{n,k,i}(x,y,z) &= \beta^{(a)}_{n,k,i,1}\,Q^{(a)}_{n-1,k-1,|i-1|}(x,y,z) + \beta^{(a)}_{n,k,i,2}\,Q^{(a)}_{n-1,k+1,|i-1|}(x,y,z) \\ &\quad + \beta^{(a)}_{n,k,i,3}\,Q^{(a)}_{n,k-1,|i-1|}(x,y,z) + \beta^{(a)}_{n,k,i,4}\,Q^{(a)}_{n,k+1,|i-1|}(x,y,z) \\ &\quad + \beta^{(a)}_{n,k,i,5}\,Q^{(a)}_{n+1,k-1,|i-1|}(x,y,z) + \beta^{(a)}_{n,k,i,6}\,Q^{(a)}_{n+1,k+1,|i-1|}(x,y,z), \end{aligned}$$

$$z\,Q^{(a)}_{n,k,i}(x,y,z) = \gamma^{(a)}_{n,k,1}\,Q^{(a)}_{n-1,k,i}(x,y,z) + \gamma^{(a)}_{n,k,2}\,Q^{(a)}_{n,k,i}(x,y,z) + \gamma^{(a)}_{n,k,3}\,Q^{(a)}_{n+1,k,i}(x,y,z),$$

for $(x,y,z) \in \Omega$*, where*

$$\begin{aligned} \alpha^{(a)}_{n,k,1} &:= \eta_{k-1}\,\left\langle R^{(a,2k)}_{n-k},\, R^{(a,2(k-1))}_{n-k} \right\rangle_{w_R^{(a,2k)}} \\ \alpha^{(a)}_{n,k,2} &:= \eta_k\,\left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k-2} \right\rangle_{w_R^{(a,2(k+1))}} \\ \alpha^{(a)}_{n,k,3} &:= \eta_{k-1}\,\left\langle R^{(a,2k)}_{n-k},\, R^{(a,2(k-1))}_{n-k+1} \right\rangle_{w_R^{(a,2k)}} \\ \alpha^{(a)}_{n,k,4} &:= \eta_k\,\left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k-1} \right\rangle_{w_R^{(a,2(k+1))}} \\ \alpha^{(a)}_{n,k,5} &:= \eta_{k-1}\,\left\langle R^{(a,2k)}_{n-k},\, R^{(a,2(k-1))}_{n-k+2} \right\rangle_{w_R^{(a,2k)}} \\ \alpha^{(a)}_{n,k,6} &:= \eta_k\,\left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k} \right\rangle_{w_R^{(a,2(k+1))}} \\ \beta^{(a)}_{n,k,i,j} &:= \begin{cases} -\alpha^{(a)}_{n,k,j} & \textit{if } (i=0 \textit{ and } j \textit{ is odd}) \textit{ or } (i=1 \textit{ and } j \textit{ is even}) \\ \alpha^{(a)}_{n,k,j} & \textit{otherwise} \end{cases} \\ \gamma^{(a)}_{n,k,1} &:= \beta^{(a,2k)}_{n-k-1}, \qquad \gamma^{(a)}_{n,k,2} := \alpha^{(a,2k)}_{n-k}, \qquad \gamma^{(a)}_{n,k,3} := \beta^{(a,2k)}_{n-k} \end{aligned}$$

Proof. The 3-term recurrence for multiplication by z follows from (9). For the recurrence for multiplication by x, since $\{Q^{(a)}_{m,j,h}\}$ for $m = 0,\dots,n+1$, $j = 0,\dots,m$, $h = 0,1$ is an orthogonal basis for any degree $n+1$ polynomial on Ω, we can expand

$$x\,Q^{(a)}_{n,k,i}(x,y,z) = \sum_{m=0}^{n+1}\sum_{j=0}^{m}\sum_{h=0}^{1} c_{m,j}\,Q^{(a)}_{m,j,h}(x,y,z).$$

These coefficients are given by

$$c_{m,j} = \left\langle x\, Q^{(a)}_{n,k,i}, Q^{(a)}_{m,j,h} \right\rangle_{Q^{(a)}} \left\| Q^{(a)}_{m,j,h} \right\|^{-2}_{Q^{(a)}}$$

where we show the non-zero coefficients that result are the $\alpha^{(a)}_{n,k,1}, \ldots, \alpha^{(a)}_{n,k,6}$ in the Lemma. Recall from equation (8) that $\left\| Q^{(a)}_{m,j,h} \right\|^{2}_{Q^{(a)}} = \pi\, \omega^{(a,2j)}_{R}$. Then for $m = 0, \ldots, n+1$, $j = 0, \ldots, m$, using a change of variables $(\cos(\theta)\sin(\varphi),\ \sin\theta\sin(\varphi),\ \cos(\varphi)) = (x, y, z)$:

$$\begin{aligned}
&\left\langle x\, Q^{(a)}_{n,k,i}, Q^{(a)}_{m,j,h} \right\rangle_{Q^{(a)}} \\
&= \int_{\Omega} Q^{(a)}_{n,k,i}(\mathbf{x}, z)\, Q^{(a)}_{m,j,h}(\mathbf{x}, z)\, x\, w^{(a,0)}_{R}(z)\, \mathrm{d}\sigma(\mathbf{x}, z) \\
&= \Big(\int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, \rho(z)^{k+j+1}\, w^{(a,0)}_{R}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_{0}^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \cos\theta\, \mathrm{d}\theta \Big) \\
&= \Big(\int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w^{(a,k+j+1)}_{R}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_{0}^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \cos\theta\, \mathrm{d}\theta \Big) \\
&= \frac{1}{2}\, \pi\, \delta_{i,h}\, (\eta_{k-1}\, \delta_{k-1,j} + \eta_k\, \delta_{k+1,j}) \int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w^{(a,k+j+1)}_{R}(z)\, \mathrm{d}z.
\end{aligned}$$

where $\delta_{k,j}$ is the standard Kronecker delta function, using Lemma 1. Similarly, for the recurrence for multiplication by y, we can expand

$$y\, Q^{(a)}_{n,k,i}(x, y, z) = \sum_{m=0}^{n+1} \sum_{j=0}^{m} \sum_{h=0}^{1} d_{m,j}\, Q^{(a)}_{m,j,h}(x, y, z).$$

These coefficients are given by

$$d_{m,j} = \left\langle y\, Q^{(a)}_{n,k,i}, Q^{(a)}_{m,j,h} \right\rangle_{Q^{(a)}} \left\| Q^{(a)}_{m,j,h} \right\|^{-2}_{Q^{(a)}}$$

where we show the non-zero coefficients that result are the $\beta^{(a)}_{n,k,1}, \ldots, \beta^{(a)}_{n,k,6}$ in the Lemma:

$$\begin{aligned}
&\left\langle y\, Q^{(a)}_{n,k,i}, Q^{(a)}_{m,j,h} \right\rangle_{Q^{(a)}} \\
&= \int_{\Omega} Q^{(a)}_{n,k,i}(\mathbf{x}, z)\, Q^{(a)}_{m,j,h}(\mathbf{x}, z)\, y\, w^{(a,0)}_{R}(z)\, \mathrm{d}\sigma(\mathbf{x}, z) \\
&= \Big(\int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, \rho(z)^{k+j+1}\, w^{(a,0)}_{R}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_{0}^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \sin\theta\, \mathrm{d}\theta \Big) \\
&= \Big(\int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w^{(a,k+j+1)}_{R}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_{0}^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \sin\theta\, \mathrm{d}\theta \Big) \\
&= \frac{1}{2}\, \pi\, \delta_{|i-1|,h} \left[(-1)^{i+1}\, \eta_{k-1}\, \delta_{k-1,j} + (-1)^{i}\, \eta_k\, \delta_{k+1,j} \right] \int_{\alpha}^{1} R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w^{(a,k+j+1)}_{R}(z)\, \mathrm{d}z.
\end{aligned}$$

where again $\delta_{k,j}$ is the standard Kronecker delta function, and we have used Lemma 1.

$\square$

The recurrences in Lemma 2 lead to Jacobi operators that correspond to multiplication by x, y and z. Let $N \in \mathbb{N}$ and define:

$$\mathbb{Q}_{N,k}^{(a)} := \begin{pmatrix} Q_{k,k,0}^{(a)}(x,y,z) \\ Q_{k,k,1}^{(a)}(x,y,z) \\ \vdots \\ Q_{N,k,0}^{(a)}(x,y,z) \\ Q_{N,k,1}^{(a)}(x,y,z) \end{pmatrix} \in \mathbb{R}^{2(N-k+1)}, \quad k = 1, \ldots, N, \tag{11}$$

$$\mathbb{Q}_{N,0}^{(a)} := \begin{pmatrix} Q_{0,0,0}^{(a)}(x,y,z) \\ \vdots \\ Q_{N,0,0}^{(a)}(x,y,z) \end{pmatrix} \in \mathbb{R}^{N+1}, \tag{12}$$

$$\mathbb{Q}_{N}^{(a)} := \begin{pmatrix} \mathbb{Q}_{N,0}^{(a)} \\ \vdots \\ \mathbb{Q}_{N,N}^{(a)} \end{pmatrix} \in \mathbb{R}^{(N+1)^2} \tag{13}$$

and set $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ as the Jacobi matrices corresponding to

$$\begin{aligned} J_x^{(a,b,c,d)}\, \mathbb{Q}_N^{(a)}(x,y,z) &= x\, \mathbb{Q}_N^{(a)}(x,y,z), \\ J_y^{(a,b,c,d)}\, \mathbb{Q}_N^{(a)}(x,y,z) &= y\, \mathbb{Q}_N^{(a)}(x,y,z), \\ J_z^{(a,b,c,d)}\, \mathbb{Q}_N^{(a)}(x,y,z) &= z\, \mathbb{Q}_N^{(a)}(x,y,z). \end{aligned} \tag{14}$$

The matrices $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ act on the coefficients vector of a function's expansion in the $\{Q_{n,k,i}^{(a)}\}$ basis. For example, let a be a general parameter and let a function $f(x,y,z)$ defined on Ω be approximated up to order $N \in \mathbb{N}$ by its expansion $f(x,y,z) = \mathbb{Q}_N^{(a)}(x,y,z)^\top \mathbf{f}$. Then $x\, f(x,y,z)$ is approximated by $\mathbb{Q}_N^{(a)}(x,y,z)^\top J_x^{(a)\top} \mathbf{f}$. In other words, $J_x^{(a,b,c,d)\top} \mathbf{f}$ is the coefficients vector for the expansion of the function $(x,y,z) \mapsto x\, f(x,y,z)$ in the $\{Q_{n,k,i}^{(a)}\}$ basis. Note that $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ are banded-block-banded matrices:

Definition 4. *A block matrix A with blocks $A_{i,j}$ has block-bandwidths (L, U) if $A_{i,j} = 0$ for $-L \le j - i \le U$, and sub-block-bandwidths (λ, μ) if all blocks $A_{i,j}$ are banded with bandwidths (λ, μ). A matrix where the block-bandwidths and sub-block-bandwidths are small compared to the dimensions is referred to as a banded-block-banded matrix.*

For example, $J_x^{(a)}, J_y^{(a)}$ are block-tridiagonal (block-bandwidths $(1,1)$) while $J_z^{(a)}$ is block-diagonal (block-bandwidths $(0,0)$):

$$J_{x/y/z}^{(a)} = \begin{pmatrix} B_{x/y/z,0}^{(a)} & A_{x/y/z,0}^{(a)} & & & \\ C_{x/y/z,1}^{(a)} & B_{x/y/z,1}^{(a)} & A_{x/y/z,1}^{(a)} & & \\ & C_{x/y/z,2}^{(a)} & B_{x/y/z,2}^{(a)} & A_{x/y/z,2}^{(a)} & \\ & & C_{x/y/z,3}^{(a)} & \ddots & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

For $J_x^{(a)}$, the sub-blocks $A_{x,k}^{(a)}, C_{x,k}^{(a)}$ have sub-block-bandwidths $(4,4)$ while the sub-blocks $B_{x,k}^{(a)}$ are zero matrices:

$$B_{x,0}^{(a)} = 0 \in \mathbb{R}^{(N+1)\times 2N}, \quad B_{x,k}^{(a)} = 0 \in \mathbb{R}^{2(N-k+1)\times 2(N-k)} \text{ for } k = 1,2,\ldots,N$$

$$A_{x,k}^{(a)} := \begin{pmatrix} A_{k,k,6}^{(a)} & & & \\ A_{k+1,k,4}^{(a)} & \ddots & & \\ A_{k+2,k,2}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & A_{N-1,k,6}^{(a)} \\ & & A_{N,k,2}^{(a)} & A_{N,k,4}^{(a)} \end{pmatrix}, \quad k = 0,1,2,\ldots,N$$

$$A_{x,0}^{(a)} \in \mathbb{R}^{(N+1)\times 2N}, \quad A_{x,k}^{(a)} \in \mathbb{R}^{2(N-k+1)\times 2(N-k)} \text{ for } k = 1,2,\ldots,N$$

$$C_{x,k}^{(a)} := \begin{pmatrix} A_{k,k,1}^{(a)} & A_{k,k,3}^{(a)} & A_{k,k,5}^{(a)} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & A_{N-1,k,5}^{(a)} \\ & & & A_{N,k,1}^{(a)} & A_{N,k,3}^{(a)} \end{pmatrix} \in \mathbb{R}^{2(N-k+1)\times 2(N-k+2)}, \quad k = 1,2,\ldots$$

$$C_{x,1}^{(a)} \in \mathbb{R}^{2N\times(N+1)}, \quad C_{x,k}^{(a)} \in \mathbb{R}^{2(N-k+1)\times 2(N-k+3)} \text{ for } k = 2,3,\ldots,N$$

where for $k = 1,\ldots,N$, $n = k,\ldots,N$

$$A_{n,k,j}^{(a)} := \begin{pmatrix} \alpha_{n,k,j}^{(a)} & 0 \\ 0 & \alpha_{n,k,j}^{(a)} \end{pmatrix} \in \mathbb{R}^{2\times 2}, (k \neq 1 \text{ for } j \text{ odd}) \tag{15}$$

$$A_{n,0,j}^{(a)} := \begin{pmatrix} \alpha_{n,0,j}^{(a)} & 0 \end{pmatrix} \in \mathbb{R}^{1\times 2}, j \text{ odd} \tag{16}$$

$$A_{n,1,j}^{(a)} := \begin{pmatrix} \alpha_{n,1,j}^{(a)} \\ 0 \end{pmatrix} \in \mathbb{R}^{2\times 1}, j \text{ odd} \tag{17}$$

$$\tag{18}$$

For $J_y^{(a)}$, the sub-blocks have sub-block-bandwidths $(5,5)$ while the sub-blocks $B_{y,k}^{(a)}$ are zero matrices:

$$B_{y,0}^{(a)} = 0 \in \mathbb{R}^{(N+1)\times 2N}, \quad B_{y,k}^{(a)} = 0 \in \mathbb{R}^{2(N-k+1)\times 2(N-k)} \text{ for } k = 1,2,\dots,N$$

$$A_{y,k}^{(a)} := \begin{pmatrix} B_{k,k,6}^{(a)} & & & \\ B_{k+1,k,4}^{(a)} & \ddots & & \\ B_{k+2,k,2}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & B_{N-1,k,6}^{(a)} \\ & & B_{N,k,2}^{(a)} & B_{N,k,4}^{(a)} \end{pmatrix}, \quad k = 0,1,2,\dots,N$$

$$A_{y,0}^{(a)} \in \mathbb{R}^{(N+1)\times 2N}, \quad A_{y,k}^{(a)} \in \mathbb{R}^{2(N-k+1)\times 2(N-k)} \text{ for } k = 1,2,\dots,N$$

$$C_{y,k}^{(a)} := \begin{pmatrix} B_{k,k,1}^{(a)} & B_{k,k,3}^{(a)} & B_{k,k,5}^{(a)} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & B_{N-1,k,5}^{(a)} \\ & & & B_{N,k,1}^{(a)} & B_{N,k,3}^{(a)} \end{pmatrix} \in \mathbb{R}^{2(N-k+1)\times 2(N-k+2)}, \quad k = 1,2,\dots$$

$$C_{y,1}^{(a)} \in \mathbb{R}^{2N\times(N+1)}, \quad C_{y,k}^{(a)} \in \mathbb{R}^{2(N-k+1)\times 2(N-k+3)} \text{ for } k = 2,3,\dots,N$$

where for $k = 1,\dots,N$, $n = k,\dots,N$

$$B_{n,k,j}^{(a)} := \begin{pmatrix} 0 & \beta_{n,k,0,j}^{(a)} \\ \beta_{n,k,1,j}^{(a)} & 0 \end{pmatrix} \in \mathbb{R}^{2\times 2}, (k \neq 1 \text{ for } j \text{ odd}) \tag{19}$$

$$B_{n,0,j}^{(a)} := \begin{pmatrix} 0 & \beta_{n,0,0,j}^{(a)} \end{pmatrix} \in \mathbb{R}^{1\times 2}, j \text{ odd} \tag{20}$$

$$B_{n,1,j}^{(a)} := \begin{pmatrix} 0 \\ \beta_{n,1,1,j}^{(a)} \end{pmatrix} \in \mathbb{R}^{2\times 1}, j \text{ odd} \tag{21}$$

$$\tag{22}$$

For $J_z^{(a)}$, the sub-blocks $B_{z,k}^{(a)}$ have sub-block-bandwidths $(2,2)$, while the sub-blocks $A_{z,k}^{(a)}, C_{z,k}^{(a)}$

are zero matrices:

$$
\begin{aligned}
&A^{(a)}_{z,0} = 0 \in \mathbb{R}^{(N+1)\times 2N}, \quad A^{(a)}_{z,k} = 0 \in \mathbb{R}^{2(N-k+1)\times 2(N-k)} \text{ for } k = 1,2,\dots,N \\
&C^{(a)}_{z,1} = 0 \in \mathbb{R}^{2N\times (N+1)}, \quad C^{(a)}_{z,k} = 0 \in \mathbb{R}^{2(N-k+1)\times 2(N-k+3)} \text{ for } k = 2,3,\dots,N \\
&B^{(a)}_{z,k} := \begin{pmatrix} \Gamma^{(a)}_{k,k,2} & \Gamma^{(a)}_{k,k,3} & & \\ \Gamma^{(a)}_{k+1,k,1} & \ddots & \ddots & \\ & \ddots & \ddots & \Gamma^{(a)}_{N-1,k,3} \\ & & \Gamma^{(a)}_{N,k,1} & \Gamma^{(a)}_{N,k,2} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)} \quad n = 0,1,2,\dots \\
&B^{(a)}_{z,0} \in \mathbb{R}^{(N+1)\times(N+1)}, \quad B^{(a)}_{z,k} \in \mathbb{R}^{2(N-k+1)\times 2(N-k+1)} \text{ for } k = 1,2,\dots,N
\end{aligned}
$$

where for $k = 1,\dots,N$, $n = k,\dots,N$

$$
\Gamma^{(a)}_{n,k,j} := \begin{pmatrix} \gamma_{n,k,j} & 0 \\ 0 & \gamma_{n,k,j} \end{pmatrix} \in \mathbb{R}^{2\times 2}, \tag{23}
$$

$$
\Gamma^{(a)}_{n,0,j} := \gamma^{(a)}_{n,0,j}. \tag{24}
$$

Note that the sparsity of the Jacobi matrices (in particular the sparsity of the sub-blocks) comes from the natural sparsity of the three-term recurrences of the 1D OPs and the circular harmonics, meaning that the sparsity is not limited to the specific spherical cap, and would extend to the spherical band.

2.3 Building the OPs

In this section, we introduce new notation for a different ordering of the OP vector, in order to demonstrate how we can obtain a recurrence for the OPs in matrix-vector form, and derive the associated "Clenshaw matrices". While in Section 2.2 the ordering used is convenient for the application of Jacobi and differential operators to the vector of coefficients of a given function's expansion, the ordering we will use in this section is convenient for building the OPs and more importantly obtaining the "Clenshaw matrices" necessary for efficient function evaluation using the Clenshaw algorithm. In practice, it is simply a matter of converting coefficients between the two orderings.

Explain what a Clenshaw matrix is

Define, for $n = 0, 1, 2, \ldots$:

$$\tilde{\mathbb{Q}}_n^{(a)} := \begin{pmatrix} Q_{n,0,0}^{(a)}(x,y,z) \\ Q_{n,1,0}^{(a)}(x,y,z) \\ Q_{n,1,1}^{(a)}(x,y,z) \\ \vdots \\ Q_{n,n,0}^{(a)}(x,y,z) \\ Q_{n,n,1}^{(a)}(x,y,z) \end{pmatrix} \in \mathbb{R}^{2n+1}, \qquad \tilde{\mathbb{Q}}^{(a)} := \begin{pmatrix} \tilde{\mathbb{Q}}_0^{(a)} \\ \tilde{\mathbb{Q}}_1^{(a)} \\ \tilde{\mathbb{Q}}_2^{(a)} \\ \vdots \end{pmatrix}$$

and set $\tilde{J}_x^{(a)}, \tilde{J}_y^{(a)}, \tilde{J}_z^{(a)}$ as the Jacobi matrices corresponding to

$$\begin{aligned} \tilde{J}_x^{(a,b,c,d)}\, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= x\, \tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ \tilde{J}_y^{(a,b,c,d)}\, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= y\, \tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ \tilde{J}_z^{(a,b,c,d)}\, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= z\, \tilde{\mathbb{Q}}^{(a)}(x,y,z). \end{aligned} \tag{25}$$

where

$$\tilde{J}_{x/y/z}^{(a)} = \begin{pmatrix} \tilde{B}_{x/y/z,0}^{(a)} & \tilde{A}_{x/y/z,0}^{(a)} & & & & \\ \tilde{C}_{x/y/z,1}^{(a)} & \tilde{B}_{x/y/z,1}^{(a)} & \tilde{A}_{x/y/z,1}^{(a)} & & & \\ & \tilde{C}_{x/y/z,2}^{(a)} & \tilde{B}_{x/y/z,2}^{(a)} & \tilde{A}_{x/y/z,2}^{(a)} & & \\ & & \tilde{C}_{x/y/z,3}^{(a)} & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

These matrices are then block-tridiagonal (block-bandwidths $(1,1)$).

For $\tilde{J}_x^{(a)}$, the sub-blocks have sub-block-bandwidths $(2,2)$:

$$\tilde{A}_{x,n}^{(a)} := \begin{pmatrix} 0 & A_{n,0,6}^{(a)} & 0 & & \\ A_{n,1,5}^{(a)} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & A_{n,n,5}^{(a)} & 0 & A_{n,n,6}^{(a)} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+3)}, \quad n = 0,1,2,\ldots$$

$$\tilde{B}_{x,n}^{(a)} := \begin{pmatrix} 0 & A_{n,0,4}^{(a)} & & \\ A_{n,1,3}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & \tilde{A}_{n,n-1,4}^{(a)} \\ & & A_{n,n,3}^{(a)} & 0 \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)} \quad n = 0,1,2,\ldots$$

$$\tilde{C}_{x,n}^{(a)} := \begin{pmatrix} 0 & A_{n,0,2}^{(a)} & & \\ A_{n,1,1}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & A_{n,n-2,2}^{(a)} \\ & & \ddots & 0 \\ & & & A_{n,n,1}^{(a)} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n-1)}, \quad n = 1,2,\ldots$$

where $A_{n,k,j}^{(a)}$ are defined in equations (15, 16, 17). For $\tilde{J}_y^{(a)}$, the sub-blocks have sub-block-bandwidths $(3,3)$:

$$\tilde{A}_{y,n}^{(a)} := \begin{pmatrix} 0 & B_{n,0,6}^{(a)} & 0 & & \\ B_{n,1,5}^{(a)} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & B_{n,n,5}^{(a)} & 0 & B_{n,n,6}^{(a)} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+3)}, \quad n = 0,1,2,\ldots$$

$$\tilde{B}_{y,n}^{(a)} := \begin{pmatrix} 0 & B_{n,0,4}^{(a)} & & \\ B_{n,1,3}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & B_{n,n-1,4}^{(a)} \\ & & B_{n,n,3}^{(a)} & 0 \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)} \quad n = 0,1,2,\ldots$$

$$\tilde{C}_{y,n}^{(a)} := \begin{pmatrix} 0 & B_{n,0,2}^{(a)} & & \\ B_{n,1,1}^{(a)} & \ddots & \ddots & \\ & \ddots & \ddots & B_{n,n-2,2}^{(a)} \\ & & \ddots & 0 \\ & & & B_{n,n,1}^{(a)} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n-1)}, \quad n = 1,2,\ldots$$

where $B^{(a)}_{n,k,j}$ are defined equations (19, 20, 21). For $\tilde{J}^{(a)}_z$, the sub-blocks are diagonal, i.e. have sub-block-bandwidths $(0,0)$:

$$\tilde{A}^{(a)}_{z,n} := \begin{pmatrix} \Gamma^{(a)}_{n,0,3} & 0 & & & \\ 0 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & \Gamma^{(a)}_{n,n,3} & 0 \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+3)}, \quad n = 0,1,2,\dots$$

$$\tilde{B}^{(a)}_{z,n} := \begin{pmatrix} \Gamma^{(a)}_{n,0,2} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \Gamma^{(a)}_{n,n,2} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)} \quad n = 0,1,2,\dots$$

$$\tilde{C}^{(a)}_{z,n} := \begin{pmatrix} \Gamma^{(a)}_{n,0,1} & 0 & & \\ 0 & \ddots & \ddots & \\ & \ddots & \ddots & 0 \\ & & \ddots & \Gamma^{(a)}_{n,n-1,1} \\ & & & 0 \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n-1)}, \quad n = 1,2,\dots$$

where $\Gamma^{(a)}_{n,k,j}$ are defined in equations (23, 24).

We can combine each system in (25) into a block-tridiagonal system, for any $(x,y,z) \in \Omega$:

$$\begin{pmatrix} 1 & & & \\ B_0 - G_0(x,y,z) & A_0 & & \\ C_1 & B_1 - G_1(x,y,z) & A_1 & \\ & C_2 & B_2 - G_2(x,y,z) & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tilde{\mathbb{Q}}^{(a)}(x,y,z) = \begin{pmatrix} Q^{(a)}_0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

where we note $Q^{(a)}_0 := Q^{(a)}_{0,0,0}(x,y,z) \equiv R^{(a,0)}_0 \, Y_0$, and for each $n = 0,1,2\dots,$

$$A_n := \begin{pmatrix} A^{(a)}_{x,n} \\ A^{(a)}_{y,n} \\ A^{(a)}_{z,n} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n+3)}, \quad C_n := \begin{pmatrix} C^{(a)}_{x,n} \\ C^{(a)}_{y,n} \\ C^{(a)}_{z,n} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n-1)} \quad (n \neq 0),$$

$$B_n := \begin{pmatrix} B^{(a)}_{x,n} \\ B^{(a)}_{y,n} \\ B^{(a)}_{z,n} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n+1)}, \quad G_n(x,y,z) := \begin{pmatrix} xI_{2n+1} \\ yI_{2n+1} \\ zI_{2n+1} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(n+1)}.$$

For each $n = 0, 1, 2\dots$ let $D_n^\top$ be any matrix that is a left inverse of A_n, i.e. such that $D_n^\top A_n = I_{2n+3}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the $D_n^\top$'s, we obtain a lower triangular system [5, p78], which can be expanded to obtain the recurrence:

$$\begin{cases} \tilde{\mathbb{Q}}_{-1}^{(a)}(x,y,z) := 0 \\ \tilde{\mathbb{Q}}_{0}^{(a)}(x,y) := Q_0^{(a)} \\ \tilde{\mathbb{Q}}_{n+1}^{(a)}(x,y) = -D_n^\top(B_n - G_n(x,y,z))\tilde{\mathbb{Q}}_{n}^{(a)}(x,y,z) - D_n^\top C_n\,\tilde{\mathbb{Q}}_{n-1}^{(a)}(x,y,z), \quad n = 0,1,2,\dots. \end{cases}$$

Note that we can define an explicit $D_n^\top$ as follows:

Improve following notation, say, by adding notation to the top part

$$D_n^\top := \begin{pmatrix} 0 & & 0 & & 1/\gamma_{n,0,3}^{(a)} & & \\ & \ddots & & \ddots & & \ddots & \\ & & 0 & & 0 & & 1/\gamma_{n,n,3}^{(a)} \\ & & & & \boldsymbol{\eta}_0^\top & & \\ & & & & \boldsymbol{\eta}_1^\top & & \end{pmatrix} \in \mathbb{R}^{(2n+3)\times 3(2n+1)},$$

for $n = 1, 2, \dots$ where $\boldsymbol{\eta}_0, \boldsymbol{\eta}_1 \in \mathbb{R}^{3(2n+1)}$ with entries given by

$$(\boldsymbol{\eta}_0)_j = \begin{cases} \frac{1}{\beta_{n,n,1,6}^{(a)}} & j = 2(2n+1) \\ \frac{-\beta_{n,n,1,5}^{(a)}}{\beta_{n,n,1,6}^{(a)}\,\gamma_{n,n-1,3}^{(a)}} & j = 3(2n+1) - 3 \\ 0 & o/w \end{cases}$$

$$(\boldsymbol{\eta}_1)_j = \begin{cases} \frac{1}{\alpha_{n,n,6}^{(a)}} & j = 2n+1 \\ \frac{-\alpha_{n,n,5}^{(a)}}{\alpha_{n,n,6}^{(a)}\,\gamma_{n,n-1,3}^{(a)}} & j = 3(2n+1) - 2 \text{ and } n > 1 \\ 0 & o/w \end{cases}$$

For $n = 0$, we can simply take

$$D_0^\top := \begin{pmatrix} 0 & 0 & \frac{1}{\gamma_{0,0,3}^{(a)}} \\ \frac{1}{\alpha_{0,0,6}^{(a)}} & 0 & 0 \\ 0 & \frac{1}{\beta_{0,0,6}^{(a)}} & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3}.$$

It follows that we can apply $D_n^\top$ in $O(n)$ complexity, and thereby calculate $\tilde{\mathbb{Q}}_0^{(a)}(x,y,z)$ through $\tilde{\mathbb{Q}}_n^{(a)}(x,y,z)$ in optimal $O(n^2)$ complexity.

I think this is correct for this case

Definition 5. *The Clenshaw matrices associated with the OPs* $\{Q^{(a)}_{n,k,i}\}$ *are given by the matrices* $A_n, B_n, C_n, D_n^\top$ *for* $n = 0, 1, 2, \ldots$ *defined above.*

3 Sparse partial differential operators

In this section, we will derive the entries of spherical partial differential operators applied to our basis, demonstrating their sparsity in the process. To this end, we will use a different ordering of the OPs and coefficients of a function's expansion, in order to exploit the orthogonality the circular harmonics will bring and thus the operators will be block-diagonal. Let $N \in \mathbb{N}$ and recall from equations (11, 12, 13) that:

I thought we would discuss this separately as a permutation of rows/columns?

$$\mathbb{Q}^{(a)}_{N,k} := \begin{pmatrix} Q^{(a)}_{k,k,0}(x,y,z) \\ Q^{(a)}_{k,k,1}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,k,0}(x,y,z) \\ Q^{(a)}_{N,k,1}(x,y,z) \end{pmatrix} \in \mathbb{R}^{2(N-k+1)}, \quad k = 1, \ldots, N,$$

$$\mathbb{Q}^{(a)}_{N,0} := \begin{pmatrix} Q^{(a)}_{0,0,0}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,0,0}(x,y,z) \end{pmatrix} \in \mathbb{R}^{N+1},$$

$$\mathbb{Q}^{(a)}_{N} := \begin{pmatrix} \mathbb{Q}^{(a)}_{N,0} \\ \vdots \\ \mathbb{Q}^{(a)}_{N,N} \end{pmatrix} \in \mathbb{R}^{(N+1)^2}.$$

We further denote the weighted set of OPs on Ω by

$$\mathbb{W}^{(a)}_N(x,y,z) := w_R^{(a,0)}(z)\, \mathbb{Q}^{(a)}_N(x,y,z),$$

and recall that a function $f(x,y,z)$ defined on Ω is approximated by its expansion $f(x,y,z) = \mathbb{Q}^{(a)}(x,y,z)^\top \mathbf{f}$.

Definition 6. *Define the operator matrices* $D^{(a)}_\varphi$, $W^{(a)}_\varphi$, D_θ, $\Delta^{(1)}_W$ *according to:*

$$\rho \frac{\partial f}{\partial \varphi}(x,y,z) = \mathbb{Q}^{(a+1)}_N(x,y,z)^\top\, D^{(a)}_\varphi\, \mathbf{f},$$

$$\rho \frac{\partial}{\partial \varphi}[w_R^{(a,0)}(z)\, f(x,y,z)] = \mathbb{W}^{(a-1)}_N(x,y)^\top\, W^{(a)}_\varphi\, \mathbf{f},$$

$$\frac{\partial f}{\partial \theta}(x,y,z) = \mathbb{Q}^{(a)}_N(x,y,z)^\top\, D_\theta\, \mathbf{f},$$

$$\Delta_{\mathrm{S}}\big(w_R^{(1,0)}(z)\, f(x,y,z)\big) = \mathbb{Q}^{(1)}_N(x,y,z)^\top\, \Delta^{(1)}_W\, \mathbf{f}, \qquad \textit{(for } a = 1 \textit{ only)}$$

The incrementing and decrementing of parameters as seen here is analogous to other well known orthogonal polynomial families' derivatives, for example the Jacobi polynomials on the interval, as seen in the DLMF [9, (18.9.3)], on the triangle [11], and on the disk-slice [15]. The operators we define here are for partial derivatives with respect to the spherical coordinates (φ, θ), so that we can more easily apply the operators to PDEs on the surface of a sphere (for example, surface Laplacian operator in the Poisson equation). With the OP ordering by Fourier mode k defined in equations (11, 12, 13) these rotationally invariant operators are block-diagonal, meaning simple and parallelisable practical application.

Theorem 1. *The operator matrices $D_\varphi^{(a)}$, $W_\varphi^{(a)}$, D_θ, $\Delta_W^{(1)}$ from Definition 6 are sparse, with banded-block-banded structure. More specifically:*

- $D_\varphi^{(a)}$ *has block-bandwidths* $(0,0)$*, and sub-block-bandwidths* $(2,4)$
- $W_\varphi^{(a)}$ *has block-bandwidths* $(0,0)$*, and sub-block-bandwidths* $(4,2)$
- D_θ *has block-bandwidths* $(0,0)$*, and sub-block-bandwidths* $(1,1)$
- $\Delta_W^{(1)}$ *has block-bandwidths* $(0,0)$*, and sub-block-bandwidths* $(1,1)$

In order to show the last part of Theorem 1, we require the following short Lemma.

Lemma 3. *For any general parameter a and any $n = 0, 1, \ldots,\ k = 0, \ldots, n$ we have that*

$$\begin{aligned}
&\frac{\partial}{\partial z}[w_R^{(a+1,2(k+1))}\, R_{n-k}^{(a,2k)\,\prime}] \\
&\quad = w_R^{(a+1,2(k+1))}\, R_{n-k}^{(a,2k)\,\prime\prime} - 2(k+1) z w_R^{(a+1,2k)}\, R_{n-k}^{(a,2k)\,\prime} + (a+1) w_R^{(a,2(k+1))}\, R_{n-k}^{(a,2k)\,\prime} \\
&\quad = \sum_{m=n-1}^{n+1} c_{m,k}\, w_R^{(a,2k)}\, R_{m-k}^{(a,2k)}
\end{aligned}$$

where

$$c_{m,k} = -\frac{1}{\omega_R^{(a,2k)}} \int_\alpha^1 R_{n-k}^{(a,2k)\,\prime}\, R_{m-k}^{(a,2k)\,\prime}\, w_R^{(a+1,2(k+1))}\, \mathrm{d}z$$

Proof of Lemma 3. Since $\frac{\partial}{\partial z}[w_R^{(a+1,2(k+1))} R_{n-k}^{(a,2k)\,\prime}] = w_R^{(a,2k)} r_{n-k+1}$ where r_{n-k+1} is a degree $n-k+1$ polynomial, we have that

$$\frac{\partial}{\partial z}[w_R^{(a+1,2(k+1))}\, R_{n-k}^{(a,2k)\,\prime}] = \sum_{m=0}^{n-k+1} \tilde{c}_{\{n,k\},m}\, w_R^{(a,2k)}\, R_m^{(a,2k)}$$

for some coefficients $\tilde{c}_{\{n,k\},m}$. These coefficients are given by

$$\begin{aligned}\tilde{c}_{\{n,k\},m} &= \frac{1}{\omega_R^{(a,2k)}} \left\langle \frac{\partial}{\partial z}[w_R^{(a+1,2(k+1))} \, R_{n-k}^{(a,2k)\,\prime}], R_m^{(a,2k)} \right\rangle_{w_R^{(0,0)}} \\ &= -\frac{1}{\omega_R^{(a,2k)}} \int_\alpha^1 R_{n-k}^{(a,2k)\,\prime} \, R_m^{(a,2k)\,\prime} \, w_R^{(a+1,2(k+1))} \, \mathrm{d}z\end{aligned}$$

We show that these are zero for $m < n-k-1$ by integrating twice by parts:

$$\begin{aligned}&\left\langle \frac{\partial}{\partial z}[w_R^{(a+1,2(k+1))} \, R_{n-k}^{(a,2k)\,\prime}], R_m^{(a,2k)} \right\rangle_{w_R^{(0,0)}} \\ &\quad= -\int_\alpha^1 R_{n-k}^{(a,2k)\,\prime} \, R_{m-k}^{(a,2k)\,\prime} \, w_R^{(a+1,2(k+1))} \, \mathrm{d}z \\ &\quad= \int_\alpha^1 R_{n-k}^{(a,2k)\,\prime} \, [(a+1) R_m^{(a,2k)\,\prime} \, w_R^{(0,2)} \\ &\qquad\qquad - 2(k+1) z R_m^{(a,2k)\,\prime} \, w_R^{(1,0)} + R_m^{(a,2k)\,\prime\prime} \, w_R^{(1,2)}] \, w_R^{(a,2k)} \, \mathrm{d}z\end{aligned}$$

which is indeed zero for $m < n-k-1$ by orthogonality. □

Proof of Theorem 1. First, note that :

$$w_R^{(a,b)\,\prime}(z) = a \, w_R^{(a-1,b)}(z) + c \, \rho(z) \, \rho'(z) \, w_R^{(a,b-2)}(z), \tag{26}$$

$$\rho(z) \, \rho'(z) = -z \tag{27}$$

$$\frac{\partial}{\partial \varphi} = -\rho \, \frac{\partial}{\partial z} \tag{28}$$

For the operator D_θ for partial differentiation by θ, we simply have that

$$\begin{aligned}\frac{\partial}{\partial \theta} Q_{n,k,i}^{(a)}(x,y,z) &= R_{n-k}^{(a,2k)}(z) \, \rho(z)^k \, \frac{\partial}{\partial \theta} Y_{k,i}(\theta) \\ &= \begin{cases} (-1)^{i+1} \, k \, Q_{n,k,|i-1|}^{(a)}(x,y,z) & k > 0 \\ 0 & k = 0 \end{cases}\end{aligned}$$

We now proceed with the case for the operator $D_\varphi^{(a)}$ for partial differentiation by φ. The entries of the operator are given by the coefficients in the expansion $\rho \frac{\partial}{\partial \varphi} Q_{n,k,i}^{(a)} = \sum_{m=0}^{n+1} \sum_{j=0}^{m} \sum_{h=0}^{1} c_{m,j,h} \, Q_{m,j,h}^{(a+1)}$, where the coefficients are

$$c_{m,j,h} = \left\| Q_{m,j,h}^{(a+1)} \right\|_{Q^{(a+1)}}^{-2} \left\langle \rho \frac{\partial}{\partial \varphi} Q_{n,k,i}^{(a)}, \; Q_{m,j,h}^{(a+1)} \right\rangle_{Q^{(a+1)}}.$$

Here and elsewhere: $\frac{\partial}{\partial z}$ is not well-defined as we are on the sphere. Though perhaps $\frac{\mathrm{d}}{\mathrm{d}z}$ works as we are differentiating the formula with respect to z?

Would it be better as $\frac{\mathrm{d}}{\mathrm{d}\theta}$?

Now,

$$\begin{aligned}
&\left\langle \rho \frac{\partial}{\partial \varphi} Q^{(a)}_{n,k,i},\ Q^{(a+1)}_{m,j,h} \right\rangle_{Q^{(a+1)}} \\
&\quad = -\int_\Omega \rho(z)^2 \frac{\partial}{\partial z} \left[R^{(a,2k)}_{n-k}(z)\, \rho(z)^k\right] R^{(a+1,2j)}_{m-j}(z)\, \rho(z)^j\, Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, w_R^{(a+1,0)}\, \mathrm{d}\Omega \\
&\quad = \Big(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \mathrm{d}\theta \Big) \Big(\int_\alpha^1 R^{(a+1,2j)}_{m-j} \left[kz R^{(a,2k)}_{n-k} - \rho^2 R^{(a,2k)}_{n-k}{}'\right] w_R^{(a+1,k+j)}\, \mathrm{d}z \Big) \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(a+1,2k)}_{m-k} \left[kz R^{(a,2k)}_{n-k} - \rho^2 R^{(a,2k)}_{n-k}{}'\right] w_R^{(a+1,2k)}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(a,2k)}_{n-k} \Big\{ kz\, R^{(a+1,2k)}_{m-k}\, w_R^{(1,0)} + R^{(a+1,2k)}_{m-k}{}'\, w_R^{(1,2)} \\
&\qquad\qquad + a\, \rho^2\, R^{(a+1,2k)}_{m-k} - (2k+2)z\, R^{(a+1,2k)}_{m-k}\, w_R^{(1,0)} \Big\}\, w_R^{(a,2k)}\, \mathrm{d}z
\end{aligned}$$

which is zero for $j \neq k$, $h \neq i$, and $m < n-2$ by orthogonality.

Similarly for the operator $W^{(a)}_\varphi$ for partial differentiation by φ on the weighted space, the entries of the operator are given by the coefficients in the expansion $\rho \frac{\partial}{\partial \varphi}(w_R^{(a,0)}\, Q^{(a)}_{n,k,i}) = \sum_{m=0}^{n+2} \sum_{j=0}^{m} \sum_{h=0}^{1} c_{m,j,h}\, w_R^{(a-1,0)}\, Q^{(a-1)}_{m,j,h}$, where the coefficients are

$$c_{m,j,h} = \left\| Q^{(a-1)}_{m,j,h} \right\|^{-2}_{Q^{(a-1)}} \left\langle \rho \frac{\partial}{\partial \varphi}(w_R^{(a,0)}\, Q^{(a)}_{n,k,i}),\ Q^{(a-1)}_{m,j,h} \right\rangle_{Q^{(0)}}.$$

Now,

$$
\begin{aligned}
&\left\langle \rho \frac{\partial}{\partial \varphi} (w_R^{(a,0)}\, Q^{(a)}_{n,k,i}),\ Q^{(a-1)}_{m,j,h} \right\rangle_{Q^{(0)}} \\
&\quad = - \int_\Omega \rho(z)^2 \frac{\partial}{\partial z} \, [R^{(a,2k)}_{n-k}(z)\, \rho(z)^k\, w_R^{(a,0)}(z)]\, R^{(a-1,2j)}_{m-j}(z)\, \rho(z)^j\, Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \mathrm{d}\Omega \\
&\quad = \Big(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \mathrm{d}\theta \Big) \\
&\qquad \cdot \Big(\int_\alpha^1 R^{(a-1,2j)}_{m-j}\, [kz R^{(a,2k)}_{n-k}\, w_R^{(1,0)} - R^{(a,2k)\,\prime}_{n-k}\, w_R^{(1,2)} - a\, R^{(a,2k)}_{n-k}\, \rho^2]\, w_R^{(a-1,k+j)}\, \mathrm{d}z \Big) \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(a-1,2k)}_{m-k}\, [kz R^{(a,2k)}_{n-k}\, w_R^{(1,0)} - R^{(a,2k)\,\prime}_{n-k}\, w_R^{(1,2)} - a\, R^{(a,2k)}_{n-k}\, \rho^2]\, w_R^{(a-1,2k)}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(a,2k)}_{n-k} \Big\{ kz\, R^{(a-1,2k)}_{m-k}\, w_R^{(1,0)} - a\, \rho^2\, R^{(a-1,2k)}_{m-k} + R^{(a-1,2k)\,\prime}_{m-k}\, w_R^{(1,2)} \\
&\qquad\qquad + a\, \rho^2\, R^{(a-1,2k)}_{m-k} - (2k+2) z\, R^{(a-1,2k)}_{m-k}\, w_R^{(1,0)} \Big\}\, w_R^{(a-1,2k)}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(a,2k)}_{n-k} \Big\{ kz\, R^{(a-1,2k)}_{m-k} + R^{(a-1,2k)\,\prime}_{m-k}\, \rho^2 - (2k+2) z\, R^{(a-1,2k)}_{m-k} \Big\}\, w_R^{(a,2k)}\, \mathrm{d}z
\end{aligned}
$$

which is zero for $j \neq k$, $h \neq i$, and $m < n-1$ by orthogonality.

Finally, fix $a = 1$. For the operator $\Delta_W^{(1)}$ for the Laplacian on the weighted space, the entries of the operator are given by the coefficients in the expansion $\Delta_{\mathrm{S}}\big(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\big) = \sum_{m=0}^{n+2} \sum_{j=0}^{m} \sum_{h=0}^{1} c_{m,j,h}\, Q^{(1)}_{m,j,h}$, where the coefficients are

$$
c_{m,j,h} = \left\| Q^{(1)}_{m,j,h} \right\|^{-2}_{Q^{(1)}} \left\langle \Delta_{\mathrm{S}}\big(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\big),\ Q^{(1)}_{m,j,h} \right\rangle_{Q^{(1)}} .
$$

Now, note that the Laplacian acting on the weighted spherical cap OP $Q^{(a)}_{n,k,i}$ yields

$$
\Delta_{\mathrm{S}}\big(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\big) =
$$

Hence,

$$
\begin{aligned}
&\Big\langle \Delta_{\mathrm{S}}\big(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\big),\, Q^{(1)}_{m,j,h} \Big\rangle_{Q^{(1)}} \\
&\quad = \Big(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\,\mathrm{d}\theta \Big) \\
&\qquad\quad \cdot \Big(\int_\alpha^1 R^{(1,2j)}_{m-j} \Big\{ R^{(a,2k)}_{n-k}\, [-k^2 w_R^{(1,k)} - w_R^{(1,k)} - 2(k+1) z w_R^{(0,k)}] \\
&\qquad\qquad\qquad\qquad + R^{(a,2k)\,\prime}_{n-k}\, [2 w_R^{(0,k+2)} - 2(k+1) z w_R^{(1,k)}] \\
&\qquad\qquad\qquad\qquad + R^{(a,2k)\,\prime\prime}_{n-k}\, w_R^{(1,k+2)} \Big\}\, w_R^{(1,j)}\,\mathrm{d}z \Big) \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(1,2k)}_{m-k} \Big\{ R^{(a,2k)}_{n-k} [-k(k+1) w_R^{(1,0)} - 2(k+1)z + c_{n,k}] \\
&\qquad\qquad\qquad\qquad + c_{n-1,k} R^{(a,2k)}_{n-k-1} + c_{n+1,k} R^{(a,2k)}_{n-k+1} \Big\}\, w_R^{(1,2k)}\,\mathrm{d}z \\
&\quad = -\pi\, \delta_{k,j}\, \delta_{i,h} (\delta_{m,n-1} + \delta_{m,n} + \delta_{m,n+1}) \int_\alpha^1 \Big\{ R^{(1,2k)}_{m-k}\, R^{(a,2k)}_{n-k} (k(k+1) w_R^{(1,0)} + 2(k+1)z) \\
&\qquad\qquad\qquad\qquad + R^{(a,2k)\,\prime}_{n-k}\, R^{(a,2k)\,\prime}_{m-k}\, w_R^{(a+1,2(k+1))} \Big\}\,\mathrm{d}z
\end{aligned}
$$

where the $c_{n-1,k}, c_{n,k}, c_{n+1,k}$ are those derived in Lemma 3. □

There exist conversion matrix operators that increment/decrement the parameters, transforming the OPs from one (weighted or non-weighted) parameter space to another.

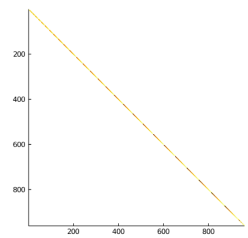
Definition 7. *Define the operator matrices $T^{(a)\to(a+\tilde{a})}$, $T^{(a)\to(a-\tilde{a})}$ for conversion between non-weighted spaces and weighted spaces respectively according to*

$$
\begin{aligned}
\mathbb{Q}^{(a)}_N(x,y,z) &= \Big(T^{(a)\to(a+\tilde{a})}\Big)^\top\, \mathbb{Q}^{(a+\tilde{a})}_N(x,y,z) \\
\mathbb{W}^{(a)}_N(x,y,z) &= \Big(T_W^{(a)\to(a-\tilde{a})}\Big)^\top\, \mathbb{W}^{(a-\tilde{a})}_N(x,y,z)
\end{aligned}
$$

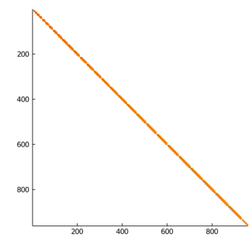
Lemma 4. *The operator matrices in Definition 7 are sparse, with banded-block-banded structure. More specifically:*

- $T^{(a)\to(a+\tilde{a})}$ *is block-diagonal with sub-block bandwidths* $(0, 2\tilde{a})$
- $T_W^{(a)\to(a-\tilde{a})}$ *is block-diagonal with sub-block bandwidths* $(2\tilde{a}, 0)$

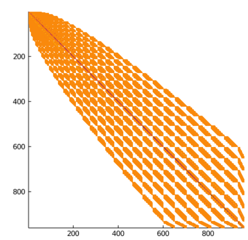
Proof. We proceed with the case for the non-weighted operators $T^{(a)\to(a+\tilde{a})}$. Since $\{Q^{(a+\tilde{a})}_{m,j,h}\}$ for $m = 0, \ldots, n$, $j = 0, \ldots, m$, $h = 0, 1$ is an orthogonal basis for any degree n polynomial, we can expand $Q^{(a)}_{n,k,i} = \sum_{m=0}^n \sum_{j=0}^m t_{m,j}\, Q^{(a+\tilde{a})}_{m,j,h}$. The coefficients of the expansion are then



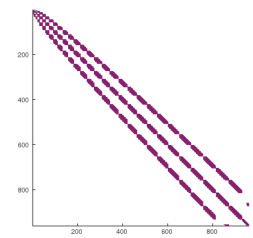
(a) The Laplace operator $\Delta_W^{(1)}$



(b) The ρ^2-factored Laplacian $L_W^{(1)}$



(c) A variable coefficient Helmholtz operator



(d) The Biharmonic operator $B_W^{(2)}$

This one is surprising as I was expecting rotational invariance to give us block-diagonal operators

Figure 1: "Spy" plots of (differential) operator matrices, showing their sparsity. For (c), the the weighted variable coefficient Helmholtz operator is $\Delta_W^{(1)} + k^2\, T^{(0)\to(1)}\, V({J_x^{(0)}}^\top, {J_y^{(0)}}^\top, {J_z^{(0)}}^\top)\, T_W^{(1)\to(0)}$ for $v(x,y,z) = 1 - (3(x-x_0)^2 + 5(y-y_0)^2 + 2(z-z_0)^2)$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{(x_0^2 + z_0^2)}$ and $k = 200$.

the entries of the operator matrix. We will show that the only non-zero coefficients are for $k = j$, $i = h$ and $m \geq n - \tilde{a}$. Note that

$$t_{m,j} = \left\| Q_{m,j,h}^{(a+\tilde{a})} \right\|_{Q^{(a+\tilde{a})}}^{-2} \left\langle Q_{n,k,i}^{(a)}, Q_{m,j,h}^{(a+\tilde{a})} \right\rangle_{Q^{(a+\tilde{a})}}.$$

where

$$\begin{aligned} \left\langle Q_{n,k,i}^{(a)}, Q_{m,j,h}^{(a+\tilde{a})} \right\rangle_{Q^{(a+\tilde{a})}} &= \left(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \mathrm{d}\theta \right) \cdot \left(\int_\alpha^1 R_{n-k}^{(a,2k)}\, R_{m-j}^{(a+\tilde{a},2j)}\, \rho^{k+j}\, w_R^{(a+\tilde{a},0)}\, \mathrm{d}z \right) \\ &= \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R_{n-k}^{(a,2k)}\, R_{m-k}^{(a+\tilde{a},2k)}\, w_R^{(a+\tilde{a},2k)}\, \mathrm{d}z \end{aligned}$$

which is zero for $n > m + \tilde{a} \iff m < n - \tilde{a}$. The sparsity argument for the weighted parameter transformation operator follows similarly. $\square$

General linear partial differential operators with polynomial variable coefficients can be constructed by composing the sparse representations for partial derivatives, conversion between bases, and Jacobi operators. As a canonical example, we can obtain the matrix operator for the ρ^2-factored surface Laplacian $\rho(z)^2\,\Delta_{\mathrm{S}}$, that will take us from coefficients for expansion in the weighted space $\mathbb{W}_N^{(1)}(x,y,z) = w_R^{(1,0)}(z)\,\mathbb{Q}_N^{(1)}(x,y,z)$ to coefficients in the non-weighted space $\mathbb{Q}_N^{(1)}(x,y,z)$. Note that this construction will ensure the imposition of the Dirichlet zero boundary conditions on Ω, similar to how the Dirichlet zero boundary conditions would be imposed for the operator $\Delta_W^{(1)}$ in Definition 6. The matrix operator for this ρ^2-factored Laplacian we denote $\mathcal{L}_W^{(1)}$ acting on the coefficients vector is then given by

$$\mathcal{L}_W^{(1)} := D_\varphi^{(0)}\,W_\varphi^{(1)} + T^{(0)\to(1)}\,T_W^{(1)\to(0)}\,(D_\theta)^2.$$

Importantly, this operator will have banded-block-banded structure, and hence will be sparse, as seen in Figure 1.

Another desirable operator is the Biharmonic operator Δ_{S}^2, for which we assume zero Dirichlet and Neumann conditions . To construct a matrix operator, we first note that we can obtain the matrix operator for the ρ^2-factored Laplacian $\rho(z)^2\Delta_{\mathrm{S}}$ that will take us from coefficients for expansion in the space $\mathbb{Q}_N^{(0)}(x,y,z)$ to coefficients in the space $\mathbb{Q}_N^{(2)}(x,y,z)$. We denote this matrix operator that acts on the coefficients vector as $\mathcal{L}^{(0)\to(2)}$, and it is given by

We need to explain Neumann conditions precisely, as the normal derivative is not so obvious

$$\mathcal{L}^{(0)\to(2)} := D_\varphi^{(2)}\,D_\varphi^{(0)} + T^{(0)\to(2)}\,D_\theta.$$

Further, we can represent this same Laplacian as a map from coefficients in the space $\mathbb{W}_N^{(2)}$ to coefficients in the space $\mathbb{W}_N^{(0)} \equiv \mathbb{Q}_N^{(0)}$. Note that a function expanded in the $\mathbb{W}_N^{(2)}$ basis will satisfy both zero Dirichlet and Neumann boundary conditions on Ω. We denote this matrix operator as $\mathcal{L}_W^{(2)\to(0)}$, and is given by

$$\mathcal{L}_W^{(2)\to(0)} := W_\varphi^{(1)}\,W_\varphi^{(2)} + T_W^{(2)\to(0,0,0)}\,D_\theta.$$

Since, for any scalar function $f : \Omega \to \mathbb{R}$,

The extra ρ^2 in front is weird to me

$$\rho^2(z)\,\Delta^2\,f(x,y,z) = \rho^2\,\Delta_{\mathrm{S}}(\rho^2\,\Delta_{\mathrm{S}} f) - z\,\rho\frac{\partial}{\partial\varphi}(\rho^2\,\Delta_{\mathrm{S}} f) - [2z^2 - 2\rho^2 + 3z]\,\rho^2\,\Delta_{\mathrm{S}} f$$

the matrix operator for the ρ^2-factored Biharmonic operator $\rho(z)^2\Delta_{\mathrm{S}}^2$ is then given by

$$\mathcal{B}_W^{(2)} := \mathcal{L}^{(0)\to(2)}\,\mathcal{L}_W^{(2)\to(0)} - (J_z^{(2)})^\top\,T^{(1)\to(2)}\,D_\varphi^{(0)}\,\mathcal{L}_W^{(2)\to(0)} - V^{(2)}\,T^{(0)\to(2)}\,\mathcal{L}_W^{(2)\to(0)},$$

where $V^{(a)}$ is an operator corresponding to multiplication by the scalar polynomial $v(z) := 2z^2 - 2\rho(z)^2 + 3z = 4z^2 + 3z - 2$ acting on coefficients in the $\mathbb{Q}_N^{(a)}$ space (see Section 4.6 for how to computationally obtain operators representing functional coefficients). The sparsity and structure of this biharmonic operator are seen in Figure 1.

4 Computational aspects

In this section we discuss how to expand and evaluate functions in our proposed basis, and take advantage of the sparsity structure in partial differential operators in practical computational applications.

4.1 Constructing $R_n^{(a,b)}(x)$

It is possible to recursively obtain the recurrence coefficients for the $\{R_n^{(a,b)}\}$ OPs in (9), see [15], by careful application of the Christoffel–Darboux formula [9, 18.2.12].

4.2 Quadrature rule on the spherical cap

In this section we construct a quadrature rule exact for polynomials on the spherical cap Ω that can be used to expand functions in the OPs $Q_{n,k,i}^{(a)}(x,y,z)$ for a given parameter a.

Theorem 2. *Let $M_1, M_2 \in \mathbb{N}$ and denote the M_1 Gauss quadrature nodes and weights on $[\alpha, 1]$ with weight $(t-\alpha)^a$ as $(t_j, w_j^{(t)})$. Further, denote the M_2 Gauss quadrature nodes and weights $[-1,1]$ with weight $(1-x^2)^{-\frac{1}{2}}$ as $(s_j, w_j^{(s)})$. Define for $j = 1, \dots, M_1$, $l = 1, \dots, M_2$:*

$$\begin{aligned}\left(x_{l+(j-1)M_2},\, y_{l+(j-1)M_2}\right) &:= \rho(t_j)\, \mathbf{s}_l, \\ z_{l+(j-1)M_2} &:= t_j, \\ w_{l+(j-1)M_2} &:= w_j^{(t)} w_l^{(s)}.\end{aligned}$$

Let $f(x,y,z)$ be a function on Ω, and $N \in \mathbb{N}$. The quadrature rule is then

$$\int_\Omega f(x,y,z)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z \approx \sum_{j=1}^{M} w_j \left[f(x_j, y_j, z_j) + f(-x_j, -y_j, z_j)\right],$$

where $M = M_1\, M_2$, and the quadrature rule is exact if $f(x,y,z)$ is a polynomial of degree $\le N$ with $M_1 \ge \frac{1}{2}(N+1), M_2 \ge N+1$.

Remark. *Note that the Gauss quadrature nodes and weights $(t_j, w_j^{(t)})$ will have to be calculated, however the Gauss quadrature nodes and weights $(s_j, w_j^{(s)})$ are simply the Chebyshev–Gauss quadrature nodes and weights given explicitly [9, 3.5.23] as $s_j := \cos\left(\frac{2j-1}{2M_2}\pi\right)$, $w_j^{(s)} := \frac{\pi}{M_2}$.*

Proof. Let $f : \Omega \to \mathbb{R}$. Define the functions $f_e, f_o : \Omega \to \mathbb{R}$ by

$$f_e(x,y,z) := \frac{1}{2}\Big(f(x,y,z) + f(-x,-y,z)\Big), \quad \forall (x,y,z) \in \Omega$$
$$f_o(x,y,z) := \frac{1}{2}\Big(f(x,y,z) - f(-x,-y,z)\Big), \quad \forall (x,y,z) \in \Omega$$

so that $\mathbf{x} \mapsto f_e(\mathbf{x}, z)$ for fixed z is an even function, and $\mathbf{x} \mapsto f_o(\mathbf{x}, z)$ for fixed z is an odd function. Note that if f is a polynomial, then $f_e(\rho(t)x, \rho(t)y, t)$ is a polynomial in $t \in [\alpha, 1]$ for fixed $(x, y) \in \mathbb{R}^2$.

Firstly, we note that

$$\int_0^{2\pi} g\big(\cos(\theta), \sin\theta\big)\, \mathrm{d}\theta = \int_{-1}^{1} \Big(g\big(x, \sqrt{1-x^2}\big) + g\big(x, -\sqrt{1-x^2}\big)\Big) \frac{\mathrm{d}x}{\sqrt{1-x^2}}$$

for some function g. Then, integrating the even function f_e we have

$$\begin{aligned}
&\int_\Omega f_e(x,y,z)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z \\
&\quad = \int_\alpha^1 w_R^{(a,0)}(z) \Big(\int_0^{2\pi} f_e\big(\rho(z)\cos(\theta), \rho(z)\sin\theta, z\big)\, \mathrm{d}\theta\Big)\, \mathrm{d}z \\
&\quad = 2\int_\alpha^1 w_R^{(a,0)}(z) \Big(\int_{-1}^{1} f_e\big(\rho(z)x, \rho(z)\sqrt{1-x^2}, z\big)\, \mathrm{d}x\Big)\, \mathrm{d}z \\
&\quad \approx \int_\alpha^1 w_R^{(a,0)}(z) \Big(\sum_{l=1}^{M_2} w_l^{(s)} f_e\big(\rho(z)s_l, \rho(z)\sqrt{1-s_l^2}, z\big)\Big)\, \mathrm{d}z \quad (\star) \\
&\quad \approx \sum_{j=1}^{M_1} w_j^{(t)} \sum_{l=1}^{M_2} w_l^{(s)} f_e\big(\rho(t_j)s_l, \rho(t_j)\sqrt{1-s_l^2}, t_j\big) \quad (\star\star) \\
&\quad = \sum_{k=1}^{M_1 M_2} w_j\, f_e(x_j, y_j, z_j).
\end{aligned}$$

Suppose f is a polynomial in x, y, z of degree N, and hence that f_e is a degree $\leq N$ polynomial. It follows that $s \mapsto f_e\big(\rho(z)s, \rho(z)\sqrt{1-s^2}, z\big)$ for fixed z is then a polynomial of degree $\leq N$. We therefore achieve equality at $(\star)$ if $2M_2 - 1 \geq N$ and we achieve equality at $(\star\star)$ if also $2M_1 - 1 \geq N$.

Integrating the odd function f_o results in

$$
\begin{aligned}
&\int_\Omega f_o(x,y,z)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z \\
&\qquad = \int_\alpha^1 w_R^{(a,0)}(z) \Big(\int_0^{2\pi} f_o\big(\rho(z)\cos(\theta), \rho(z)\sin\theta, z)\big)\, \mathrm{d}\theta \Big)\, \mathrm{d}z \\
&\qquad = \int_\alpha^1 w_R^{(a,0)}(z) \Big(\int_{-1}^1 \Big[f_o\big(\rho(z)x, \rho(z)\sqrt{1-x^2}, z\big) + f_o\big(\rho(z)x, -\rho(z)\sqrt{1-x^2}, z\big)\Big]\, \mathrm{d}x \Big)\, \mathrm{d}z \\
&\qquad = \int_\alpha^1 w_R^{(a,0)}(z) \Big(\int_{-1}^1 \Big[f_o\big(\rho(z)x, \rho(z)\sqrt{1-x^2}, z\big) - f_o\big(\rho(z)x, \rho(z)\sqrt{1-x^2}, z\big)\Big]\, \mathrm{d}x \Big)\, \mathrm{d}z \\
&\qquad = 0.
\end{aligned}
$$

since $f_o(x,y,z) = -f_o(-x,-y,z)$. Hence, for a polynomial f in x, y, z of degree N,

$$
\begin{aligned}
\int_\Omega f(x,y,z)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z &= \int_\Omega \Big(f_e(x,y,z) + f_o(x,y,z) \Big)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z \\
&= \int_\Omega f_e(x,y,z)\, w_R^{(a,0)}(z)\, \mathrm{d}\sigma(x,y)\, \mathrm{d}z \\
&= \sum_{j=1}^M w_j\, f_e(x_j, y_j, z_j),
\end{aligned}
$$

where $M = M_1 M_2$ and $2M_1 - 1 \geq N, 2M_2 - 1 \geq N$. $\square$

4.3 Obtaining the coefficients for expansion of a function on the spherical cap

Fix $a \in \mathbb{R}$. Then for any function $f : \Omega \to \mathbb{R}$ we can express f by

$$
f(x,y,z) \approx \sum_{k=0}^N \mathbb{Q}_{N,k}^{(a)}(x,y,z)^\top\, \boldsymbol{f}_k = \mathbb{Q}_N^{(a)}(x,y,z)^\top\, \boldsymbol{f}
$$

for N sufficiently large, where $\mathbb{Q}_{N,k}^{(a)}, \mathbb{Q}_N^{(a)}$ is defined in equations (11, 12, 13) and where

$$\boldsymbol{f}_k := \begin{pmatrix} f_{k,k,0} \\ f_{k,k,1} \\ \vdots \\ f_{N,k,0} \\ f_{N,k,1} \end{pmatrix} \in \mathbb{R}^{2(N-k+1)} \quad \text{for } n = 1, 2, \ldots, N, \quad \boldsymbol{f}_0 := \begin{pmatrix} f_{0,0,0} \\ \vdots \\ f_{N,0,0} \end{pmatrix} \in \mathbb{R}^{N+1},$$

$$\boldsymbol{f} := \begin{pmatrix} \boldsymbol{f}_0 \\ \vdots \\ \boldsymbol{f}_N \end{pmatrix} \in \mathbb{R}^{2(N+1)^2}, \qquad f_{n,k,i} := \left\langle f,\, Q^{(a)}_{n,k,i} \right\rangle_{Q^{(a)}} \left\| Q^{(a)}_{n,k,i} \right\|^{-2}_{Q^{(a)}}.$$

Recall from equation (8) that $\left\| Q^{(a)}_{n,k,i} \right\|^2_{Q^{(a)}} = \omega_R^{(a,2k)}\, \pi$. Using the quadrature rule detailed in Section 4.2 for the inner product, we can calculate the coefficients $f_{n,k,i}$ for each $n = 0, \ldots, N$, $k = 0, \ldots, n$, $i = 0, 1$:

$$\begin{aligned} f_{n,k,i} &= \frac{1}{2\, \omega_R^{(a,2k)}\, \pi} \sum_{j=1}^{M} w_j \big[f(x_j, y_j, z_j) Q^{(a)}_{n,k,i}(x_j, y_j, z_j) + f(-x_j, -y_j, z_j) Q^{(a)}_{n,k,i}(-x_j, -y_j, z_j) \big] \\ &= \frac{1}{M_2\, \omega_R^{(a,2k)}} \sum_{j=1}^{M} \big[f(x_j, y_j, z_j) Q^{(a)}_{n,k,i}(x_j, y_j, z_j) + f(-x_j, -y_j, z_j) Q^{(a)}_{n,k,i}(-x_j, -y_j, z_j) \big] \end{aligned}$$

where the quadrature nodes and weights are those from Theorem 2, and $M = M_1 M_2$ with $2M_1 - 1 \geq N, M_2 - 1 \geq N$ (i.e. we can choose $M_2 := N + 1$ and $M_1 := \lceil \frac{N+1}{2} \rceil$).

4.4 Function evaluation

For a function f, with coefficients vector $\boldsymbol{f}$ for expansion in the $\{Q_{n,k,i}\}$ basis as determined via the method in Section 4.3 up to order N, we can use the Clenshaw algorithm to evaluate the function at a point $(x, y, z) \in \Omega$ as follows. Let $A_n, B_n, D_n^\top, C_n$ be the Clenshaw matrices from Definition 5, and define the rearranged coefficients vector $\tilde{\boldsymbol{f}}$ via

$$\tilde{\boldsymbol{f}}_n := \begin{pmatrix} f_{n,0,0} \\ f_{n,1,0} \\ f_{n,1,1} \\ \vdots \\ f_{n,n,0} \\ f_{n,n,1} \end{pmatrix} \in \mathbb{R}^{2(N+1)} \quad \text{for } n = 1, 2, \ldots, N, \quad \tilde{\boldsymbol{f}}_0 = f_{0,0,0} \in \mathbb{R},$$

$$\tilde{\boldsymbol{f}} := \begin{pmatrix} \tilde{\boldsymbol{f}}_0 \\ \vdots \\ \tilde{\boldsymbol{f}}_N \end{pmatrix} \in \mathbb{R}^{(N+1)^2}.$$

The trivariate Clenshaw algorithm works similar to the bivariate Clenshaw algorithm introduced in [12]:

1) Set $\boldsymbol{\xi}_{N+2} = \mathbf{0}$, $\boldsymbol{\xi}_{N+2} = \mathbf{0}$.
2) For $n = N : -1 : 0$

   set $\boldsymbol{\xi}_n^T = \tilde{\boldsymbol{f}}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T (B_n - G_n(x, y, z)) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$
3) Output: $f(x, y, z) \approx \boldsymbol{\xi}_0 \, \tilde{\mathbb{Q}}_0^{(a)} = \xi_0 \, Q_0^{(a)}$

4.5 Calculating non-zero entries of the operator matrices

The proofs of Theorem 1 and Lemma 4 provide a way to calculate the non-zero entries of the operator matrices given in Definition 6 and Definition 7. We can simply use quadrature to calculate the 1D inner products, which has a complexity of $\mathcal{O}(N^3)$. This proves much cheaper computationally than using the 3D quadrature rule to calculate the 3D inner products, which has a complexity of $\mathcal{O}(N^4)$

correct the O(nd) complexity

.

4.6 Obtaining operator matrices for variable coefficients

The Clenshaw algorithm outlined in Section 4.4 can also be used with Jacobi matrices $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ replacing the point (x, y, z). Let $v : \Omega \to \mathbb{R}$ be the function that we wish to obtain an operator matrix V for v, so that

$$v(x, y, z) \, f(x, y, z) = v(x, y, z) \, \boldsymbol{f}^\top \, \mathbb{Q}_N^{(a)}(x, y, z) = (V \boldsymbol{f})^\top \, \mathbb{Q}_N^{(a)}(x, y, z),$$

i.e. $V\boldsymbol{f}$ is the coefficients vector for the function $v(x, y, z) \, f(x, y, z)$.

To this end, let $\tilde{\boldsymbol{v}}$ be the coefficients for expansion up to order N in the $\{Q_{n,k,i}\}$ basis of v (rearranged as in Section 4.4 so that $v(x, y, z) = \tilde{\boldsymbol{v}}^\top \, \tilde{\mathbb{Q}}^{(a)}(x, y, z)$). The operator V is then the result of the following:

1) Set $\boldsymbol{\xi}_{N+2} = \mathbf{0}$, $\boldsymbol{\xi}_{N+2} = \mathbf{0}$.
2) For $n = N : -1 : 0$

   set $\boldsymbol{\xi}_n^T = \tilde{\boldsymbol{v}}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T \big(B_n - G_n(J_x^{(a)}, J_y^{(a)}, J_z^{(a)})\big) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$
3) Output: $V(x, y, z) \approx \boldsymbol{\xi}_0 \, \tilde{\mathbb{Q}}_0^{(a)} = \xi_0 \, Q_0^{(a)}$

where at each iteration, $\boldsymbol{\xi}_n$ is a vector of matrices.

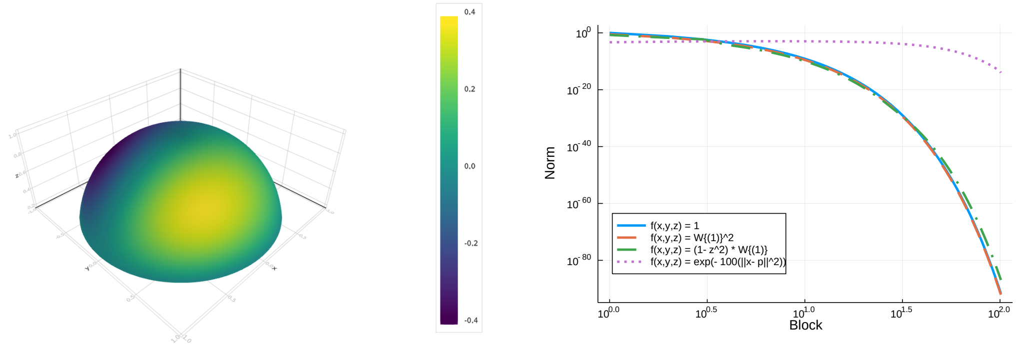


Figure 2: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y, z) = -2e^x yz(2 + x) + w_R^{(1,0)}(z)e^x(y^3 + z^2 y - 4xy - 2y)$. Right: The norms of each block of the computed solution of the Poisson equation with the given right hand side functions (here, $\mathbf{p}$ is simply a point on the spherical cap surface away from the pole and boundary). This demonstrates spectral convergence observed.

5 Examples on spherical caps with zero Dirichlet conditions

We now demonstrate how the sparse linear systems constructed as above can be used to efficiently solve PDEs with zero Dirichlet conditions on the spherical cap defined by Ω. We consider Poisson, inhomogeneous variable coefficient Helmholtz equation and the Biharmonic equation, as well as a time dependent heat equation, demonstrating the versatility of the approach.

5.1 Poisson

The Poisson equation is the classic problem of finding $u(x, y, z)$ given a function $f(x, y, z)$ such that:

$$\begin{cases} \Delta_{\mathbb{S}} u(x, y, z) = f(x, y, z) & \text{in } \Omega \\ u(x, y, z) = 0 & \text{on } \partial\Omega \end{cases} \tag{29}$$

noting the imposition of zero Dirichlet boundary conditions on u.

We can tackle the problem as follows. Choose an $N \in \mathbb{N}$ large enough for the problem, and denote the coefficient vector for expansion of u in the $\mathbb{W}_N^{(1)}$ OP basis up to degree N by $\mathbf{u}$, and the coefficient vector for expansion of f in the $\mathbb{Q}_N^{(1)}$ OP basis up to degree N by $\mathbf{f}$. Since f is known, we can obtain $\mathbf{f}$ using the quadrature rule in Section 4.3. In matrix-vector notation, our system hence becomes:

$$\Delta_W^{(1)} \mathbf{u} = \mathbf{f}$$

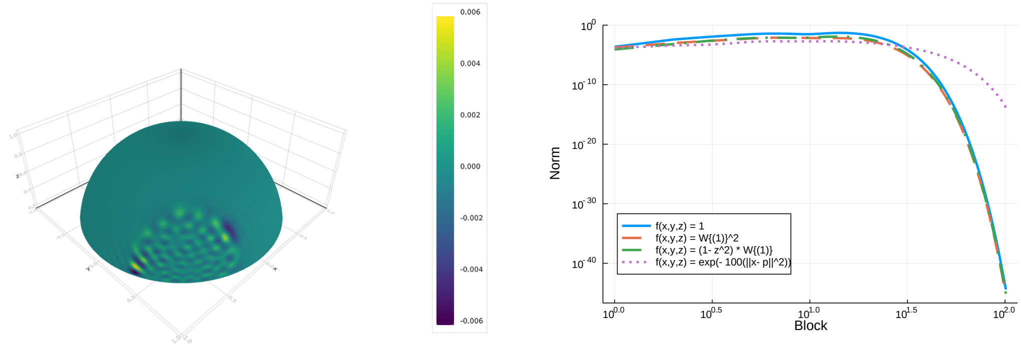


Figure 3: Left: The computed solution to $\Delta u + k^2\ v\ u = f$ with zero boundary conditions with $f(x, y, z) = y e^x w_R^{(1,0)}(z)$, $v(x, y, z) = 1-(3(x-x_0)^2+5(y-y_0)^2+2(z-z_0)^2)$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{(x_0^2 + z_0^2)}$ and $k = 100$. Right: The norms of each block of the computed solution of the Helmholtz equation with the given right hand side functions, with $k = 20$ and the same function v (again, $\mathbf{p}$ is simply a point on the spherical cap surface away from the pole and boundary). This demonstrates spectral convergence observed.

Change x-axis to use normal (not logarithmic) scaling: this will change exponential convergence to more readable straight lines. For examples, having nearby singularities (e.g. something like $f(\boldsymbol{x}) = \|\boldsymbol{x} - (1, 1, 1) * (1/\sqrt{3} + \epsilon)\|$) should give different exponential convergence rates.

Just write out W in terms of z

which can be solved to find $\mathbf{u}$. In Figure 2 we see the solution to the Poisson equation with zero boundary conditions given in (29) in the disk-slice Ω. In Figure 2 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the Poisson equation with $N = 100$, that is, $(N + 1)^2 = 10,201$ unknowns. In the plot, a "block" is simply the group of coefficients corresponding to OPs of the same degree, and so the plot shows how the norms of these blocks decay as the degree of the expansion increases. Thus, the rate of decay in the coefficients is a proxy for the rate of convergence of the computed solution: as typical of spectral methods, we expect the numerical scheme to converge at the same rate as the coefficients decay. We see that we achieve spectral convergence

Add to the comments here

Are there more suitable RHSs for the block norms plot that will demonstrate further properties? Or as there are no corners, we are pretty limited?

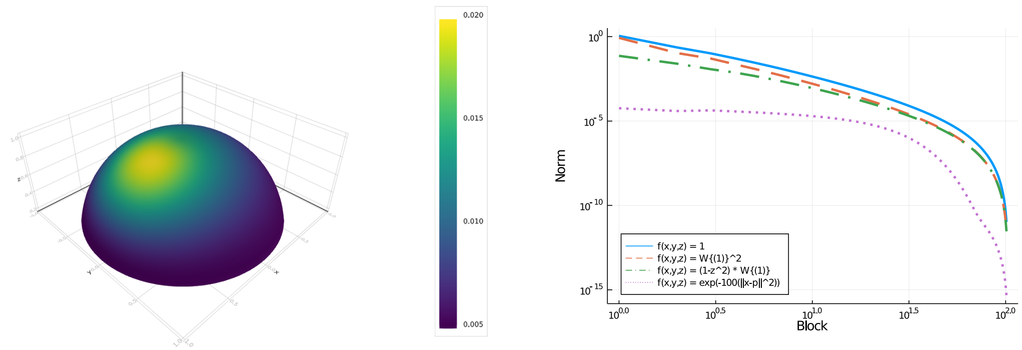


Figure 4: Left: The computed solution to $\Delta^2 u = f$ with zero Dirichlet and Neumann boundary conditions with $f(x, y, z) = (1 + \mathrm{erf}(5(1 - 10((x - 0.5)^2 + y^2))))\rho(z)^2$. Right: The norms of each block of the computed solution of the biharmonic equation with the given right hand side functions (again, $\mathbf{p}$ is simply a point on the spherical cap surface away from the pole and boundary). This demonstrates algebraic convergence observed.

5.2 Inhomogeneous variable-coefficient Helmholtz

Find $u(x, y)$ given functions $v,\ f : \Omega \to \mathbb{R}$ such that:

$$\begin{cases} \Delta_{\mathbb{S}} u(x, y, z) + k^2\, v(x, y, z)\, u(x, y, z) = f(x, y, z) & \text{in } \Omega \\ u(x, y, z) = 0 & \text{on } \partial\Omega \end{cases} \tag{30}$$

where $k \in \mathbb{R}$, noting the imposition of zero Dirichlet boundary conditions on u.

We can tackle the problem as follows. Denote the coefficient vector for expansion of u in the $\mathbb{W}_N^{(1)}$ OP basis up to degree N by $\mathbf{u}$, and the coefficient vector for expansion of f in the $\mathbb{Q}_N^{(1)}$ OP basis up to degree N by $\mathbf{f}$. Since f is known, we can obtain the coefficients $\mathbf{f}$ using the quadrature rule in Section 4.3. We can obtain the matrix operator for the variable-coefficient function $v(x, y, z)$ by using the Clenshaw algorithm with matrix inputs as the Jacobi matrices ${J_x^{(0)}}^\top, {J_y^{(0)}}^\top, {J_z^{(0)}}^\top$, yielding an operator matrix of the same dimension as the input Jacobi matrices a la the procedure introduced in [12]. We can denote the resulting operator acting on coefficients in the $\mathbb{Q}_N^{(0)}$ space by $V({J_x^{(0)}}^\top, {J_y^{(0)}}^\top, {J_z^{(0)}}^\top)$. In matrix-vector notation, our system hence becomes:

It would be cleaner defining $X := (J_x^{(0)})^\top$, $Y :=$ ..., $Z :=$ ...

$$(\Delta_W^{(1)} + k^2\, T^{(0)\to(1)}\, V\, T_W^{(1)\to(0)})\, \mathbf{u} = \mathbf{f}$$

which can be solved to find $\mathbf{u}$. We can see the sparsity and structure of this matrix system in Figure 1 with $v(x, y, z) = zxy^2$ as an example. In Figure 3 we see the solution to the inhomogeneous variable-coefficient Helmholtz equation with zero boundary conditions given in (30) in the spherical cap Ω, with $f(x, y, z) = ye^x w_R^{(1,0)}(z)$, $v(x, y, z) = 1 - (3(x - x_0)^2 + 5(y - y_0)^2 + 2(z - z_0)^2)$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{(x_0^2 + z_0^2)}$ and $k = 100$. In

Figure 3 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the inhomogeneous variable-coefficient Helmholtz equation with $k = 20$ using $N = 100$, that is, $(N+1)^2 = 10,201$ unknowns. Once again, the rate of decay in the coefficients is a proxy for the rate of convergence of the computed solution, and we see that we achieve spectral convergence.

Add to the comments here

We can extend this to constant non-zero boundary conditions by simply noting that the problem

$$\begin{cases} \Delta_{\mathrm{S}} u(x,y,z) + k^2\, v(x,y,z)\, u(x,y,z) = f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = c \in \mathbb{R} & \text{on } \partial\Omega \end{cases}$$

is equivalent to letting $u = \tilde{u} + c$ and solving

$$\begin{cases} \Delta_{\mathrm{S}} \tilde{u}(x,y,z) + k^2\, v(x,y,z)\, \tilde{u}(x,y,z) = f(x,y,z) - c\, k^2\, v(x,y,z) \ =: g(x,y,z) \quad \text{in } \Omega \\ \tilde{u}(x,y,z) = 0 \quad \text{on } \partial\Omega \end{cases}$$

and solving this zero boundary condition Helmholtz problem.

5.3 Biharmonic equation

Find $u(x,y,z)$ given a function $f(x,y,z)$ such that:

$$\begin{cases} \rho(z)^2\, \Delta^2 u(x,y,z) = \rho(z)^2\, f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = 0, \quad \frac{\partial u}{\partial n}(x,y,z) = 0 & \text{on } \partial\Omega \end{cases} \tag{31}$$

where Δ^2 is the Biharmonic operator, noting the imposition of zero Dirichlet and Neumann boundary conditions on u. In Figure 4 we see the solution to the Biharmonic equation (31) in the spherical cap Ω. In Figure 4 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the biharmonic equation with $N = 100$, that is, $(N+1)^2 = 10,201$ unknowns.

Add to the comments here

6 Conclusions

We have shown that trivariate orthogonal polynomials can lead to sparse discretizations of general linear PDEs on spherical cap domains, with Dirichlet boundary conditions on the $z = \alpha \in (0,1)$ boundary. We have provided a detailed practical framework for the application of the methods described for quadratic surfaces of revolution [13], by utilising the non-classical 1D OPs on the interval $[\alpha, 1]$ with the weight $(z-\alpha)^a \sqrt{(1-z^2)}^b$ defined for the disk-slice case [15]. This also forms a building block in developing an $hp-$finite element method to solve PDEs on the sphere by using spherical band and spherical cap shaped elements.

This work serves as a stepping stone to constructing similar methods to solve partial differential equations on other 3D sub-domains of the sphere – it is clear from the construction in this paper that discretizations of spherical gradients and Laplacian's are sparse on other suitable sub-components of the sphere. The resulting sparsity in high-polynomial degree discretizations presents an attractive alternative to methods based on bijective mappings (e.g., [3, 14, 4]). Constructing these sparse spectral methods for surface PDEs on spherical bands and spherical triangles is future work, and has applications in weather prediction [16].

The next stage is to develop an orthogonal basis for the tangent space of the spherical cap/band, and obtain sparse differential operators for gradient, divergence etc. On the complete sphere, the vector spherical harmonics that form the orthogonal basis are simply the gradients and perpendicular gradients of the scalar spherical harmonics [1] which has been used effectively for solving PDEs on the sphere [18, 6] – however, we do not have that luxury for the spherical cap or band, and hence the choice of basis will not be as straightforward.

A P-finite element methods using sparse operators

Is this worth including?

It's already a very long paper so probably better to skip this. But include it in your thesis

We follow the method of [2] to construct a sparse p-finite element method in terms of the operators constructed above, with the benefit of ensuring that the resulting discretisation is symmetric. Consider the 3D Dirichlet problem on a domain Ω:

$$\begin{cases} -\rho(z)^2\, \Delta_{\mathbb{S}} u(x,y,z) = \rho(z)^2\, f(x,y,z) \quad \text{in } \Omega \\ u = 0 \quad \text{on } \partial\Omega \end{cases}$$

This has the weak formulation

$$L(v) := \int_\Omega \rho^2\, f\, v \,\mathrm{d}\sigma(\boldsymbol{x}, z) = \int_\Omega \big(\rho\, \nabla u\big) \cdot \big(\rho\, \nabla v\big) \,\mathrm{d}\sigma(\boldsymbol{x}, z) =: a(u, v)$$

for any test function $v \in V := H_0^1(\Omega) = \{v \in H^1(\Omega) \quad | \quad v|_{\partial\Omega} = 0\}$.

In general, we would split a sphere domain into spherical band elements with spherical caps over the poles, and use a p-finite element method to solve PDEs on the sphere using these elements $\{\tau_n\}$. While spherical bands are an extension to this work, we note that we can still apply a p-FEM using two half-spheres ($\alpha = 0$). In this section, we limit our discretisation to a single element, that is we let $\tau = \Omega$ for a spherical cap domain.

We can choose our finite dimensional space $V_p = \{v_p \in V \quad | \quad \deg(v_p|_\tau) \leq p\}$ for some $p \in \mathbb{N}$.

We seek $u_p \in V_p$ s.t.

$$L(v_p) = a(u_p, v_p) \quad \forall\, v_p \in V_p. \tag{32}$$

Define

$$\Lambda^{(a)} := \left\langle \mathbb{Q}_p^{(a)},\, \mathbb{Q}_p^{(a)\top} \right\rangle_{Q^{(a)}} := \int_\tau \mathbb{Q}_p^{(a)}\, \mathbb{Q}_p^{(a)\top}\, w_R^{(a,0)}\, \mathrm{d}\sigma(\boldsymbol{x}, z) = \int_\tau \mathbb{W}_p^{(a)}\, \mathbb{Q}_p^{(a)\top}\, \mathrm{d}\sigma(\boldsymbol{x}, z)$$

for any a. Note that due to orthogonality this is a diagonal matrix. By choosing suitable bases for our FE spaces, we can rewrite (32) in matrix-vector form. We can choose a basis for V_p by using the weighted orthogonal polynomials on τ with parameter $a = 1$, the $\mathbb{W}_p^{(1)}$ OPs, and we can expand the function f in the $\mathbb{Q}_p^{(1)}$ basis.

Let $\mathbf{u}, \mathbf{v}$ be the coefficient vectors of the expansions of $u_p, v_p \in V_p$ respectively in the V_p basis ($\mathbb{W}^{(1,1,1)}$ OPs). Then,

$$\begin{aligned}
a(u_p, v_p) &= \int_\tau \big(\rho\, \nabla u\big) \cdot \big(\rho\, \nabla v\big)\, \mathrm{d}\sigma(\boldsymbol{x}, z) \\
&= \int_\tau \Big(\rho \frac{\partial}{\partial \varphi} u_p\, \rho \frac{\partial}{\partial \varphi} v_p + \frac{\partial}{\partial \theta} u_p\, \frac{\partial}{\partial \theta} v_p\Big)\, \mathrm{d}\sigma(\boldsymbol{x}, z) \\
&= \int_\tau \Big(\mathbf{v}^\top W_\varphi^{(1)\top} \mathbb{Q}_p^{(0)} \mathbb{Q}_p^{(0)\top} W_\varphi^{(1)} \mathbf{u} \\
&\qquad\qquad + \mathbf{v}^\top (T_W^{(1)\to(0)} D_\theta)^\top \mathbb{Q}_p^{(a)} \mathbb{Q}_p^{(a)\top} T_W^{(1)\to(0)} D_\theta \mathbf{u}\Big)\, \mathrm{d}\sigma(\boldsymbol{x}, z) \\
&= \mathbf{v}^\top \Big(W_\varphi^{(1)\top} \Lambda^{(0)} W_\varphi^{(1)} + (T_W^{(1)\to(0)} D_\theta)^\top \Lambda^{(0)} T_W^{(1)\to(0)} D_\theta\Big)\, \mathbf{u}.
\end{aligned}$$

Further, let $\mathbf{f}$ is the coefficient vector for the expansion of the function $f(x, y, z)$ in the $\mathbb{Q}_p^{(1)}$ OP basis and let P be the operator for multiplication by $\rho(z)^2$, that is the operator matrix defined by $P^\top \mathbb{Q}_p^{(1)}(x, y, z) = \rho(z)^2\, \mathbb{Q}_p^{(1)}(x, y, z)$. Then,

$$\begin{aligned}
L(v_p) &= \int_\tau v_p\, \rho^2\, f\, \mathrm{d}\sigma(\boldsymbol{x}, z) \\
&= \int_\tau \mathbf{v}^\top\, \mathbb{W}_p^{(1)}\, \mathbb{Q}_p^{(1)\top}\, P\, \mathbf{f}\, \mathrm{d}\sigma(\boldsymbol{x}, z) \\
&= \mathbf{v}^\top \Lambda^{(1)}\, P\, \mathbf{f}.
\end{aligned}$$

Since (32) is equivalent to stating that

$$L(w_R^{(1)} Q_{n,k,i}^{(1)}) = a(u_p, w_R^{(1)} Q_{n,k,i}^{(1)}) \quad \forall\, n = 0, \ldots, p,\ k = 0, \ldots, n,\ i = 0, 1$$

(i.e. holds for all basis functions of V_p) by choosing v_p as each basis function, we can equivalently write the linear system for our finite element problem as:

$$A\mathbf{u} = \tilde{\mathbf{f}}.$$

where the (element) stiffness matrix A is defined by

$$A = {W_\varphi^{(1)}}^\top \Lambda^{(0)} W_\varphi^{(1)} + (T_W^{(1)\to(0)} D_\theta)^\top \Lambda^{(0)} T_W^{(1)\to(0)} D_\theta$$

and the load vector $\tilde{\mathbf{f}}$ is given by

$$\tilde{\mathbf{f}} = \Lambda^{(1)}\, P\, \mathbf{f}.$$

Note that since we have sparse operator matrices for partial derivatives and basis-transform, we obtain a symmetric sparse (element) stiffness matrix, as well as a sparse operator matrix for calculating the load vector (rhs).

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