Imperial College of Science, Technology and Medicine
Department of Mathematics

Sparse Spectral Methods on Disk-Slices, Trapeziums and Spherical Caps

Ben Snowball

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Abstract

This thesis develops sparse spectral methods for solving partial differential equations (PDEs) on various multidimensional domains, with a specific focus on the disk-slice and trapezium in 2D, and the spherical cap as a surface in 3D.

We begin with an introduction to sparse spectral methods via the long established Spherical Harmonics on the whole sphere surface. We present a framework for how the spherical harmonics can be used to expand functions defined on the sphere as multidimensional polynomials in x, y, z, and how differential operators can be applied as banded-block-banded matrix operators to coefficient vectors for the function's expansion. Further, we demonstrate how the Vector Spherical Harmonics can be used as an orthogonal basis for vector valued functions lying in the tangent space of the sphere, and thus how one can additionally derive gradient and divergence operators.

Throughout this thesis we wish to utilise our understanding of the 3D spherical harmonics to build up to a new orthogonal polynomial basis for subdomains of the sphere surface. To this end, we move on working in 2D, where in recent years sparse spectral methods for solving PDEs have been derived using hierarchies of classical orthogonal polynomials on intervals, disks, and triangles. Presenting a new framework for choosing a suitable orthogonal polynomial basis for more general 2D domains defined via an algebraic curve as a boundary, this work builds on the observation that sparsity is guaranteed due to this definition of the boundary, and that the entries of partial differential operators can be determined using formulae in terms of (non-classical) univariate orthogonal polynomials. Triangles and the full disk are then special cases of our framework, which we formalise for the disk-slice and trapezium cases.

Finally, we adapt the tools developed in two dimensions to derive a similar OP basis complete with sparse differential operators.

Foreword

Text of the foreword.

Declaration

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I would like to express (whatever feelings I have) to:

- My supervisor

- My second supervisor

- Other researchers
- My family and friends

"If we hit that bullseye, the rest of the dominoes will fall like a house of cards. Checkmate."

Captain Zapp Brannigan

Contents

Chapter 1

Introduction

Univariate orthogonal polynomials (hereon also referred to as OPs) have been extensively involved in the development of multiple fields of computational and applied mathematics [**?**]. While there are many famous examples – such as the Jacobi polynomials, the Legendre polynomials and the Chebyshev polynomials but to name a few – the area of multivariate orthogonal polynomials has a smaller array of research. However, this branch of mathematics has an encouraging future [9], not least as a basis for sparse spectral methods for solving partial differential equations (PDEs) on multidimensional domains, such as on the triangle [22] with applications including solving Volterra integral equations [12].

One famous group of multidimensional orthogonal polynomials is of course the Spherical Harmonics. The European Centre for Medium-range Weather Forecasts (ECMWF) use a Spherical Harmonic spectral method in their weather and climate model [7]. Chapter 2 of this thesis provides an introduction to sparse spectral methods via the long established Spherical Harmonics on the whole sphere surface. We present a framework for how the spherical harmonics can be used to expand functions defined on the sphere as multidimensional polynomials in x, y, z, and how differential operators can be applied as banded-block-banded matrix operators to coefficient vectors for the function's expansion. Further, we demonstrate how the Vector Spherical Harmonics can be used as an orthogonal basis for vector valued functions lying in the tangent space of the sphere, and thus how one can additionally derive gradient and divergence operators.

While the whole sphere spectral method has been successful for numerous years [32], there is a drawback in the parallel scalability bottleneck that arises from the global spectral transform, which is expected to inhibit future performance of the ECMWF model [2]. This thesis serves to lay a foundation for addressing this while still utilising a spectral approach. More precisely, we develop a sparse spectral method for solving partial differential equations (PDEs) on the spherical cap as a surface in 3D, with a simple extension to a spherical band. Together, these frameworks can be pieced together to create a spectral element method for the whole sphere, or further developed to investigate spectral methods on other spherical subdomains.

To this end, in Chapter 3 we move on to working in 2D, where in recent years sparse spectral methods for solving PDEs have been derived using hierarchies of classical orthogonal polynomials on intervals, disks, and triangles. Presenting a new framework for choosing a suitable orthogonal polynomial basis for more general 2D domains defined via an algebraic curve as a boundary, this work builds on the observation that sparsity is guaranteed due to this definition of the boundary, and that the entries of partial differential operators can be determined using formulae in terms of (non-classical) univariate orthogonal polynomials, which we define. Triangles and the full disk are then special cases of our framework, which we formalise for the disk-slice and trapezium cases.

With a greater knowledge base in our quiver, we can adapt the techniques learnt from the founding of the disk-slice formulation to a surface in 3D in Chapter 4 – in particular the spherical cap, a subdomain of the surface of a unit sphere. Using the same family of (non-classical) 1D OPs, we present a suitable orthogonal polynomial basis once more, this time as polynomials in x, y, z complete with sparse differential operators.

Chapter 2

Spherical harmonics as orthogonal polynomials

To introduce ourselves to the world of multidimensional orthogonal polynomials for solving PDEs on the sphere, we can naturally choose to look at the famous spherical harmonics. Our aim here is to express the spherical harmonics as polynomials in three variables x, y, z to evaluate functions and solve PDEs on the whole sphere. More precisely, we desire the solution to partial differential equations on the domain

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

where

$$\rho(z) := \sqrt{1 - z^2}.$$

While it may seem somewhat odd, it should hopefully become apparent why this is a useful way to define our domain.

2.1 Defining the spherical harmonics in three variables

Before we proceed further, let's build up to our definition of the spherical harmonics. We first need to introduce a few classical orthogonal polynomials.

On the unit interval, $[-1, 1]$, we note that there is a hierarchy of orthogonal polynomials (OPs) in the sense that [19, table 18.3.1, eqn 18.9.15]:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x} P_l^{(a,b)}(x) &= \frac{1}{2}\,(l + a + b + 1)\, P_{l-1}^{(a+1,b+1)}(x) \\
\implies \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) &= \frac{(l+m)!}{2^m\, l!}\, P_{l-m}^{(m,m)}(x)
\end{aligned}$$

where $P_l^{(a,b)}(x)$ is the l degree *Jacobi polynomial*, and $P_l(x) := P_l^{(0,0)}(x)$ is simply the *Legendre polynomial* of degree l. Jacobi polynomials are orthogonal with weight $w(x) = (1-x)^a(1+x)^b$; that is for $l, l' \in \mathbb{N}_0$,

$$\int_{-1}^{1} {P_l^{(a,b)}(x)}^2 \, (1-x)^a(1+x)^b \,\mathrm{d}x =: \omega_{P,l}^{(a,b)}$$
$$\int_{-1}^{1} P_l^{(a,b)}(x)\, P_{l'}^{(a,b)}(x)\, (1-x)^a(1+x)^b \,\mathrm{d}x = \omega_{P,l}^{(a,b)}\, \delta_{l,l'}.$$

Further, the *associated Legendre polynomials* are a set of polynomials orthogonal with respect to unit weight on the unit interval, and are given by :

Add citation for associated legendre polys

$$P_l^m(x) := (-1)^m(1-x^2)^{\frac{m}{2}} \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) = \hat{c}_l^m (1-x^2)^{\frac{m}{2}} P_{l-m}^{(m,m)}(x)$$
$$P_l^{-m}(x) := \tilde{c}_l^m P_l^m(x),$$

for $m = 0, 1, 2, \ldots, l$ where

$$\hat{c}_l^m := \frac{(l+m)!}{(-2)^m \, l!}$$
$$\tilde{c}_l^m := \frac{(-1)^m \, (l-m)!}{(l+m)!}$$

and $n! := n\,(n-1)\,(n-2)\ldots 1$ for $n \in \mathbb{N}$ is the standard factorial. Further, define

$$c_l^m := \left(\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!} \right)^{\frac{1}{2}} \begin{cases} \hat{c}_l^m & \text{if } m \geq 0 \\ \hat{c}_l^{|m|} \tilde{c}_l^{|m|} & \text{if } m < 0 \end{cases} . \tag{2.1}$$

This allows us to explicitly see where the normalising constants that we shall be using for our definition of the spherical harmonics come from.

Let $(x, y, z) \in \Omega$. It is useful to be able to transform between these cartesian coordinates and the spherical coordinates (φ, θ). On this note, throughout we will use the convention that the spherical coordinate angles be defined by

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

We can now write down the spherical harmonics. We will use the standard definition – that is, the spherical harmonics, orthonormal on the unit sphere, are [19, 14.30.1]:

$$
\begin{aligned}
Y_l^m(\varphi, \theta) &:= \left(\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!} \right)^{\frac{1}{2}} e^{im\theta} P_l^m(\cos\varphi) \\
&= c_l^m (1 - (\cos\varphi)^2)^{\frac{|m|}{2}} e^{im\theta} P_{l-|m|}^{(|m|,|m|)}(\cos\varphi) \\
&= c_l^m P_{l-|m|}^{(|m|,|m|)}(z)\, \rho(z)^{|m|}\, e^{im\theta}
\end{aligned}
\tag{2.2}
$$

for $0 \leq |m| \leq l$, $l \in \mathbb{N}_0$ where c_l^m is defined in equation (2.1), and

$$
\begin{aligned}
&\int_0^{2\pi} \int_0^{\pi} Y_l^m(\varphi, \theta)\, Y_{l'}^{m'}(\varphi, \theta)^* \, \sin\varphi \, \mathrm{d}\varphi \, \mathrm{d}\theta \\
&\quad = 2\pi\, \delta_{m,m'}\, c_l^m\, c_{l'}^{m'} \int_{-1}^{1} P_{l-|m|}^{(|m|,|m|)}(z)\, P_{l'-|m|}^{(|m|,|m|)}(z)\, \rho(z)^{2|m|}\, \mathrm{d}z \\
&\quad = \delta_{l,l'}\, \delta_{m,m'}.
\end{aligned}
$$

where α^* denotes the complex conjugate of $\alpha \in \mathbb{C}$. Note how we can express the spherical harmonics Y_l^m in terms of x, y, z instead of φ, θ by noting that $\rho(z)^{|m|}e^{im\theta}$ can be expressed in terms of x, y, z for any $m \in \mathbb{Z}$. Indeed, they are polynomials in x, y, z which we denote $Y_l^m(x, y, z)$. They span all polynomials modulo the ideal generated by $x^2 + y^2 + z^2 - 1$.

2.2 Jacobi matrices

Jacobi operators that correspond to multiplication of the orthogonal polynomial basis, in this case the spherical harmonics, by our cartesian coordinates x, y, z. We start by expressing $x\,Y_l^m(x, y, z)$, $y\,Y_l^m(x, y, z)$, and $z\,Y_l^m(x, y, z)$ in terms of $Y_{l'}^{m'}(x, y, z)$ for any point (x, y, z) on the unit sphere.

Lemma 1. *For $l \in \mathbb{N}_0$, $m \in \mathbb{Z}$ s.t. $0 \leq |m| \leq l$, the spherical harmonics satisfy the relationships:*

$$
\begin{aligned}
x\,Y_l^m(x, y, z) &= \alpha_{l,m,1}Y_{l-1}^{m-1}(x, y, z) + \alpha_{l,m,2}Y_{l-1}^{m+1}(x, y, z)\\
&\qquad + \alpha_{l,m,3}Y_{l+1}^{m-1}(x, y, z) + \alpha_{l,m,4}Y_{l+1}^{m+1}(x, y, z), \qquad (2.3)\\
y\,Y_l^m(x, y, z) &= \beta_{l,m,1}Y_{l-1}^{m-1}(x, y, z) + \beta_{l,m,2}Y_{l-1}^{m+1}(x, y, z)\\
&\qquad + \beta_{l,m,3}Y_{l+1}^{m-1}(x, y, z) + \beta_{l,m,4}Y_{l+1}^{m+1}(x, y, z), \qquad (2.4)\\
z\,Y_l^m(x, y, z) &= \gamma_{l,m,1}Y_{l-1}^{m}(x, y, z) + \gamma_{l,m,2}Y_{l+1}^{m}(x, y, z), \qquad (2.5)
\end{aligned}
$$

where

$$\alpha_{l,m,1} := \begin{cases} \frac{c_l^m}{2c_{l-1}^{m-1}}\tilde{\alpha}_{l,m,1} & \textit{if } m > 0 \\ \frac{c_l^m}{2c_{l-1}^{m-1}}\tilde{\alpha}_{l,|m|,2} & \textit{if } m \leq 0,\ l-|m| \geq 2 \\ 0 & \textit{otherwise} \end{cases}$$

$$\alpha_{l,m,2} := \begin{cases} \frac{c_l^m}{2c_{l-1}^{m+1}}\tilde{\alpha}_{l,m,2} & \textit{if } m \geq 0,\ l-|m| \geq 2 \\ \frac{c_l^m}{2c_{l-1}^{m+1}}\tilde{\alpha}_{l,|m|,1} & \textit{if } m < 0 \\ 0 & \textit{otherwise} \end{cases}$$

$$\alpha_{l,m,3} := \begin{cases} \frac{c_l^m}{2c_{l+1}^{m-1}}\tilde{\alpha}_{l,m,3} & \textit{if } m > 0 \\ \frac{c_l^m}{2c_{l+1}^{m-1}}\tilde{\alpha}_{l,|m|,4} & \textit{if } m \leq 0 \end{cases}$$

$$\alpha_{l,m,4} := \begin{cases} \frac{c_l^m}{2c_{l+1}^{m+1}}\tilde{\alpha}_{l,m,4} & \textit{if } m \geq 0 \\ \frac{c_l^m}{2c_{l+1}^{m+1}}\tilde{\alpha}_{l,|m|,3} & \textit{if } m < 0 \end{cases}$$

$$\beta_{l,m,j} := (-1)^{j+1}\, i\, \alpha_{l,m,j}, \quad j = 1,2,3,4$$

$$\gamma_{l,m,1} := \frac{c_l^m}{c_{l-1}^m}\,\tilde{\gamma}_{l,m,1}$$

$$\gamma_{l,m,2} := \frac{c_l^m}{c_{l+1}^m}\,\tilde{\gamma}_{l,m,2}.$$

and

$$\begin{aligned}
\tilde{\alpha}_{l,m,1} &:= \frac{2l}{2l+1} \\
\tilde{\alpha}_{l,m,2} &:= \begin{cases} -\frac{l}{2(2l+1)} & \textit{if } l-m \geq 2 \\ 0 & \textit{otherwise} \end{cases} \\
\tilde{\alpha}_{l,m,3} &:= -\frac{2(l-m+2)(l-m+1)}{(2l+1)(l+1)} \\
\tilde{\alpha}_{l,m,4} &:= \frac{(l+m+2)(l+m+1)}{2(2l+1)(l+1)} \\
\tilde{\gamma}_{l,m,1} &:= \begin{cases} \frac{l}{2l+1} & \textit{if } l-m \geq 1 \\ 0 & \textit{otherwise} \end{cases} \\
\tilde{\gamma}_{l,m,2} &:= \frac{(l-m+1)(l+m+1)}{(2l+1)(l+1)}.
\end{aligned}$$

Proof. The recurrence relationship for the Jacobi polynomials satisfies [19, 18.9.1, 18.9.2]

$$zP_{l-m}^{(m,m)}(z) = \tilde{\gamma}_{l,m,1}P_{l-m-1}^{(m,m)}(z) + \tilde{\gamma}_{l,m,2}P_{l-m+1}^{(m,m)}(z),$$

for $k \geq 0$, $m \in \mathbb{Z}$. Hence, the expression for multiplication of the spherical harmonic Y_l^m by z is

$$\begin{aligned}
z\,Y_l^m(x,y,z) &= c_l^m e^{im\varphi}\rho(z)^{|m|} zP_{l-|m|}^{(|m|,|m|)}(z) \\
&= c_l^m e^{im\varphi}\rho(z)^{|m|} \left[\tilde{\gamma}_{l,m,1}P_{l-|m|-1}^{(|m|,|m|)}(z) + \tilde{\gamma}_{l,m,2}P_{l-|m|+1}^{(|m|,|m|)}(z)\right] \\
&= \gamma_{l,m,1}Y_{l-1}^m(x,y,z) + \gamma_{l,m,2}Y_{l+1}^m(x,y,z).
\end{aligned}$$

For multiplication by x and y, we require some further relations for the complex exponential and the Jacobi polynomials. First, recall that

$$\begin{aligned}
\cos\varphi\, e^{im\varphi} &= \frac{1}{2}(e^{i\varphi} + e^{-i\varphi})e^{im\varphi} = \frac{1}{2}(e^{i(m+1)\varphi} + e^{i(m-1)\varphi}) \\
\sin\varphi\, e^{im\varphi} &= \frac{1}{2i}(e^{i\varphi} - e^{-i\varphi})e^{im\varphi} = \frac{-i}{2}(e^{i(m+1)\varphi} - e^{i(m-1)\varphi})
\end{aligned}$$

Finally, we can express a Jacobi polynomial $P^{(a,b)}_{l-m}(z)$ in terms of an ultraspherical polynomial $C^{(\lambda)}_{l-m}(z)$ [19, 18.7.2]:

$$\frac{l!\,(2m)!}{(l+m)!\,m!}\, C^{(m+1/2)}_{l-m}(z) = P^{(m,m)}_{l-m}(z),$$

where the ultraspherical polynomials satisfy the relations [19, 18.9.7, 18.9.8]:

$$\begin{aligned}
C^{(\lambda)}_n(z) &= \frac{\lambda}{n+\lambda}\left[C^{(\lambda+1)}_n(z) - C^{(\lambda+1)}_{n-2}(z)\right] \\
(1-z^2)\, C^{(\lambda)}_n(z) &= \frac{1}{4(\lambda-1)(n+\lambda)}\left[(n+2\lambda-2)(n+2\lambda-1)\, C^{(\lambda-1)}_n(z)\right. \\
&\qquad\qquad \left. - (n+1)(n+2)\, C^{(\lambda-1)}_{n+2}(z)\right],
\end{aligned}$$

for $m \in \mathbb{N}_0$ where $\lambda > -\frac{1}{2}$ is some parameter. Thus, combining these, we can write three-term recurrences for the Jacobi polynomials as:

$$\begin{aligned}
P^{(m,m)}_{l-m}(z) &= \tilde{\alpha}_{l,m,4} P^{(m+1,m+1)}_{l-m}(z) + \tilde{\alpha}_{l,m,2} P^{(m+1,m+1)}_{l-m-2}(z) \\
(1-z^2)\, P^{(m,m)}_{l-m}(z) &= \tilde{\alpha}_{l,m,3} P^{(m-1,m-1)}_{l-m+2}(z) + \tilde{\alpha}_{l,m,1} P^{(m-1,m-1)}_{l-m}(z),
\end{aligned}$$

for $l, m \in \mathbb{N}_0$ s.t. $0 \le m \le l$. Hence, the expressions for multiplication of the spherical harmonic Y_l^m by x and y is then:

$$
\begin{aligned}
x\,Y_l^m(x,y,z) &= c_l^m \cos\varphi\, e^{im\varphi}\ \sin\theta\, \rho(z)^{|m|} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= \frac{1}{2} c_l^m (e^{i(m+1)\varphi} + e^{i(m-1)\varphi}) \rho(z)^{|m|+1} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= \frac{1}{2} c_l^m e^{i(m+1)\varphi} \rho(z)^{|m|+1} \left[\tilde{\alpha}_{l,m,4} P_{l-|m|}^{(|m|+1,|m|+1)}(z) + \tilde{\alpha}_{l,m,2} P_{l-|m|-2}^{(|m|+1,|m|+1)}(z)\right] \\
&\quad + \frac{1}{2} c_l^m e^{i(m-1)\varphi} \rho(z)^{|m|-1} \left[\tilde{\alpha}_{l,m,3} P_{l-|m|+2}^{(|m|-1,|m|-1)}(z) + \tilde{\alpha}_{l,m,1} P_{l-|m|}^{(|m|-1,|m|-1)}(z)\right] \\
&= \alpha_{l,m,1} Y_{l-1}^{m-1}(x,y,z) + \alpha_{l,m,2} Y_{l-1}^{m+1}(x,y,z) \\
&\quad + \alpha_{l,m,3} Y_{l+1}^{m-1}(x,y,z) + \alpha_{l,m,4} Y_{l+1}^{m+1}(x,y,z), \\
y\,Y_l^m(x,y,z) &= c_l^m \sin\varphi\, e^{im\varphi}\ \sin\theta\, \rho(z)^{|m|} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= -\frac{1}{2} i\, c_l^m (e^{i(m+1)\varphi} - e^{i(m-1)\varphi})\, \rho(z)^{|m|+1} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= -i\left[A_{l,m} Y_{l+1}^{m+1}(x,y,z) + B_{l,m} Y_{l-1}^{m+1}(x,y,z)\right] \\
&\qquad + i\left[D_{l,m} Y_{l+1}^{m-1}(x,y,z) + E_{l,m} Y_{l-1}^{m-1}(x,y,z)\right], \\
&= i\Big\{\alpha_{l,m,1} Y_{l-1}^{m-1}(x,y,z) - \alpha_{l,m,2} Y_{l-1}^{m+1}(x,y,z) \\
&\qquad + \alpha_{l,m,3} Y_{l+1}^{m-1}(x,y,z) - \alpha_{l,m,4} Y_{l+1}^{m+1}(x,y,z)\Big\}.
\end{aligned}
$$

$\square$

These recurrences lead to Jacobi operators that correspond to multiplication by

x, y, z. Define for $l \in \mathbb{N}_0$:

$$\mathbb{P}_l := \begin{pmatrix} Y_l^{-l} \\ \vdots \\ Y_l^l \end{pmatrix} \in \mathbb{C}^{2l+1}, \qquad \mathbb{P} := \left(\begin{array}{c} \mathbb{P}_0 \\ \hline \mathbb{P}_1 \\ \hline \mathbb{P}_2 \\ \vdots \end{array}\right).$$

and let the Jacobi matrices J^x, J^y, J^z be given by

$$J^x\mathbb{P} = x\mathbb{P}, \quad J^y\mathbb{P} = y\mathbb{P}, \quad J^z\mathbb{P} = z\mathbb{P}. \tag{2.6}$$

The Jacobi matrices act on the coefficients vector of a function's expansion in the spherical harmonic basis. For example, let the function $f(x, y, z) : \Omega \to \mathbb{C}$ be approximated by its expansion $f(x, y, z) = \mathbb{P}(x, y, z)^\top \boldsymbol{f}$ up to some degree order N. Then $xf(x, y, z)$ is approximated by $\mathbb{P}(x, y, z)^\top J^x \boldsymbol{f}$, i.e. $J^x \boldsymbol{f}$ is the coefficients vector for the expansion of the function $(x, y, z) \mapsto x\, f(x, y, z)$ in the spherical harmonics basis.

An important property of the Jacobi matrices is that they are sparse – specifically they are *banded-block-banded matrices.*

Definition 1. *A block matrix A with blocks $A_{i,j}$ has block-bandwidths (L, U) if $A_{i,j} = 0$ for $-L \leq j - i \leq U$, and subblock-bandwidths (λ, μ) if all blocks are banded with bandwidths (λ, μ). A matrix where the block-bandwidths and subblock-bandwidths are small compared to the dimensions is referred to as a banded-block-banded matrix.*

Using equations (2.3–2.5), we have that the Jacobi matrices take the following block-tridiagonal form (i.e. have block-bandwidths $(1,1)$):

$$J_x = \begin{pmatrix} B_{x,0} & A_{x,0} & & & & \\ C_{x,1} & B_{x,1} & A_{x,1} & & & \\ & C_{x,2} & B_{x,2} & A_{x,2} & & \\ & & C_{x,3} & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

$$J_y = \begin{pmatrix} B_{y,0} & A_{y,0} & & & & \\ C_{y,1} & B_{y,1} & A_{y,1} & & & \\ & C_{y,2} & B_{y,2} & A_{y,2} & & \\ & & C_{y,3} & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

$$J_z = \begin{pmatrix} B_{z,0} & A_{z,0} & & & & \\ C_{z,1} & B_{z,1} & A_{z,1} & & & \\ & C_{z,2} & B_{z,2} & A_{z,2} & & \\ & & C_{z,3} & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

J_x has subblock-bandwidths $(2,2)$, where the blocks for $l \in \mathbb{N}_0$ are given by:

$$A_{x,l} := \begin{pmatrix} \alpha_{l,-l,3} & 0 & \alpha_{l,-l,4} & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_{l,l,3} & 0 & \alpha_{l,l,4} \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l+3)},$$

$$B_{x,l} := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)}$$

$$C_{x,l} := \begin{pmatrix} \alpha_{l,-l,2} & & \\ 0 & \ddots & \\ \alpha_{l,-l+2,1} & \ddots & \alpha_{l,l-2,2} \\ & \ddots & 0 \\ & & \alpha_{l,l,1} \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l-1)} \quad (l \neq 0).$$

J_y also has subblock-bandwidths $(2,2)$, where the blocks for $l \in \mathbb{N}_0$ are given by:

$$A_{y,l} := \begin{pmatrix} \beta_{l,-l,3} & 0 & \beta_{l,-l,4} & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{l,l,3} & 0 & \beta_{l,l,4} \end{pmatrix} \in \mathbb{C}^{(2l+1)\times(2l+3)},$$

$$B_{y,l} := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)}$$

$$C_{y,l} := \begin{pmatrix} \beta_{l,-l,2} & & \\ 0 & \ddots & \\ \beta_{l,-l+2,1} & \ddots & \beta_{l,l-2,2} \\ & \ddots & 0 \\ & & \beta_{l,l,1} \end{pmatrix} \in \mathbb{C}^{(2l+1)\times(2l-1)} \quad (l \neq 0).$$

Finally, J_z has subblock-bandwidths $(1,1)$, where the blocks for $l \in \mathbb{N}_0$ are given by:

$$A_{z,l} := \begin{pmatrix} 0 & \gamma_{l,-l,2} & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & \gamma_{l,-l,2} & 0 \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l+3)},$$

$$B_{z,l} := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)}$$

$$C_{z,l} := \begin{pmatrix} 0 & & \\ \gamma_{l,-l+1,1} & \ddots & \\ 0 & \ddots & 0 \\ & \ddots & \gamma_{l,l-1,1} \\ & & 0 \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l-1)} \quad (l \neq 0).$$

2.3 Three-term recurrence relation for $\mathbb{P}$

Three-term recurrence relations for orthogonal polynomials are well established (e.g. [19, 18.9], [9]). In a similar vein, we can obtain a recurrence relation for the spherical harmonics by combining each system in (2.6).

$$\begin{pmatrix} 1 & & & \\ B_0 - G_0(x,y,z) & A_0 & & \\ C_1 & B_1 - G_1(x,y,z) & A_1 & \\ & C_2 & B_2 - G_2(x,y,z) & \ddots \\ & & \ddots & \ddots \end{pmatrix} \mathbb{P}(x,y,z) = \begin{pmatrix} Y_0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

where we note $Y_0^0(x,y,z) \equiv Y_0 := c_0^0 P_0^{(0,0)} \equiv \frac{1}{2}\frac{1}{\sqrt{\pi}}$, and for each $l = 0, 1, 2\dots$,

$$A_l := \begin{pmatrix} A_{x,l} \\ A_{y,l} \\ A_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+3)}, \quad C_l := \begin{pmatrix} C_{x,l} \\ C_{y,l} \\ C_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l-1)} \quad (n \neq 0), \tag{2.7}$$

$$B_l := \begin{pmatrix} B_{x,l} \\ B_{y,l} \\ B_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+1)}, \quad G_n(x,y) := \begin{pmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+1)}. \tag{2.8}$$

For each $l = 0, 1, 2\dots$ let $D_l^\top$ be any matrix that is a left inverse of A_l, i.e. such that $D_l^\top A_l = I_{2l+3}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the $D_l^\top$'s, we obtain a lower triangular system [9, p78], which can be expanded to obtain the recurrence:

$$\begin{cases} \mathbb{P}_{-1}(x,y,z) := 0 \\ \mathbb{P}_0(x,y,z) := Y_0 \\ \mathbb{P}_{l+1}(x,y,z) = -D_l^\top (B_l - G_l(x,y,z))\mathbb{P}_l(x,y,z) - D_l^\top C_l\, \mathbb{P}_{l-1}(x,y,z), \quad l = 0,1,2,\ldots. \end{cases}$$

Since the above holds for any $D_l^\top$ that is a left inverse of A_l, we are free to choose the $D_l^\top$ matrices in the following way. For $l \in \mathbb{N}$, we set

$$D_l^\top = \begin{pmatrix} \hat{A}_l^{x,y} & 0_{(2l+3)\times(2l+1)} \end{pmatrix} \in \mathbb{R}^{(2l+3)\times 3(2l+1)} \tag{2.9}$$

where $0_{(2l+3)\times(2l+1)}$ the zero matrix in $\mathbb{R}^{(2l+3)\times(2l+1)}$, and $\hat{A}_l^{x,y} \in \mathbb{R}^{(2l+3)\times 2(2l+1)}$ is the left inverse of the matrix $\begin{pmatrix} A_l^x \\ A_l^y \end{pmatrix}$, given by

$$\hat{A}_l^{x,y} = \begin{pmatrix} \frac{1}{2\alpha_{l,-l,3}} & 0 & \cdots & 0 & \frac{1}{2\beta_{l,-l,3}} & 0 & \cdots & 0 \\ & \ddots & & & & \ddots & & \\ & & \ddots & & & & \ddots & \\ & & & \frac{1}{2\alpha_{l,l,3}} & 0 & \cdots & 0 & \frac{1}{2\beta_{l,-l,3}} \\ 0 & \cdots & \frac{1}{2\alpha_{l,l-1,4}} & 0 & \cdots & 0 & \frac{1}{2\beta_{l,l-1,4}} & 0 \\ 0 & \cdots & 0 & \frac{1}{2\alpha_{l,l,4}} & 0 & \cdots & 0 & \frac{1}{2\beta_{l,l,4}} \end{pmatrix}.$$

For $l = 0$ we set

$$D_0^T = \begin{pmatrix} \frac{1}{2\alpha_{0,0,3}} & \frac{1}{2\beta_{0,0,3}} & 0 \\ 0 & 0 & \frac{1}{\gamma_{0,0,2}} \\ \frac{1}{2\alpha_{0,0,4}} & \frac{1}{2\beta_{0,0,4}} & 0 \end{pmatrix}. \tag{2.10}$$

It will be useful for us to give a formal name for these coefficient matrices above for a family of multidimensional orthogonal polynomials.

Definition 2. *The matrices* $-D_l^\top(B_l - G_l(x, y, z))$, $D_l^\top C_l$ *for* $l \in \mathbb{N}_0$ *defined via equations (2.7–2.10) are called the* ***recurrence coefficient matrices*** *for a given family of multidimensional orthogonal polynomials.*

2.4 Computational aspects

Once again, let $f(x, y, z)$ be a function on the unit sphere Ω be approximated by its expansion

$$f(x, y, z) \approx \mathbb{P}(x, y, z)^\top \boldsymbol{f} = \sum_{l=0}^{N} \mathbb{P}_l(x, y, z)^\top \boldsymbol{f}_l = \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m}\, Y_l^m(x, y, z),$$

where $\mathbb{P}_l(x, y, z), \boldsymbol{f}_l \in \mathbb{C}^{2l+1}$ for each $l \in \{0, \ldots, N\}$, for some coefficients vector $\boldsymbol{f} = (f_{l,m})$ up to degree order $N \in \mathbb{N}$.

2.4.1 Obtaining coefficients

obtaining coeffs/ transform

In spectral space, we wish to work only with vectors of coefficients for the expansion of a function, to which we can apply operator matrices to that represent differential or other operations. Naturally, we of course need a way to obtain the coefficients $f_{l,m}$. The coefficients can be calculated via the integral

$$f_{l,m} = \int_\Omega f(\cos\theta\sin\varphi, \sin\theta\sin\varphi, \cos\varphi)\, Y_l^m(\varphi,\theta)^* \, \sin\varphi \,\mathrm{d}\varphi\,\mathrm{d}\theta$$

using the orthonormality of the spherical harmonics. Methods to calculate these coefficients exist, known as spectral transforms, and are well established for the spherical harmonics (see e.g. [17, 28]).

2.4.2 Function evaluation

We can use the Clenshaw algorithm to evaluate this function at a given point (x, y, z) on Ω [24]. The *Clenshaw algorithm* is then as follows:

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

2) For $n = N : -1 : 0$

   set $\boldsymbol{\xi}_n^T = \boldsymbol{f}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T (B_n - G_n(x,y,z)) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$

3) Output: $f(x,y,z) \approx \boldsymbol{\xi}_0^T \mathbb{P}_0(x,y,z) \equiv \xi_0 Y_0$.

2.4.3 Obtaining operator matrices for variable coefficients

The Clenshaw algorithm presented in Section 2.4.2 can also be used with the Jacobi matrices replacing the point (x, y, z), to yield an operator matrix.

Let's explain what we mean. Suppose $v : \Omega \to \mathbb{C}$ is a function, and we encounter the problem of finding the coefficients of the expansion for $v(x, y, z)f(x, y, z)$. We wish to therefore find an operator V for v so that

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

i.e. $V\ \boldsymbol{f}$ is the coefficients vector for the expansion of the function $(x, y, z) \mapsto v(x, y, z)f(x, y, z)$ in the spherical harmonic basis.

Let $\boldsymbol{v}$ be the coefficients of the expansion of v up to order N. The operator V would then be the result of the following *operator Clenshaw algorithm*:

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

   set $\boldsymbol{\xi}_n^T = \boldsymbol{v}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T(B_n - G_n(J_x, J_y, J_z)) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$
3) Output: $f(x, y, z) \approx \boldsymbol{\xi}_0^T \mathbb{P}_0(x, y, z) \equiv \xi_0 Y_0$

where at each iteration, $\boldsymbol{\xi}_n$ is a vector of matrices (note that we are abusing notation here a bit, however it is the simplest way to present the algorithm without introducing yet more matrices!).

2.5 Vector spherical harmonics as orthogonal vectors in three variables

Since the spherical harmonics are a basis for the surface of the sphere, and the tangent space of the sphere is spanned by the gradient and perpendicular gradient of a scalar function, we have that the gradients and perpendicular gradients of the spherical harmonics

$$\nabla Y_l^m, \quad \nabla^{\perp} Y_l^m := \hat{\boldsymbol{r}} \times \nabla Y_l^m, \tag{2.11}$$

span the tangent space. Here, $\hat{\boldsymbol{r}}$ is simply the outward unit normal vector to the surface of the sphere at the point (x, y, z). Importantly, the set $\{\nabla Y_l^m, \nabla^{\perp} Y_l^m\}$ form a complete and orthogonal basis for vector valued functions in the tangent space of the sphere and are known as *vector spherical harmonics (VSHs)* [1], orthogonal with respect to the inner product $\langle \boldsymbol{A}, \boldsymbol{B} \rangle = \iint_{\Omega} \boldsymbol{A} \cdot \boldsymbol{B}^* \, \sin\varphi \, \mathrm{d}\varphi \, \mathrm{d}\theta$. Vector spherical harmonics have been widely used in electrostatics (e.g. [1]), electrodynamics (e.g. [6]), and of course fluid dynamics including weather and climate modelling (e.g. [18, 10, 30]). Other definitions for VSHs are used (e.g. [13]), however it is convenient for deriving explicit sparse relations and operators to use the one described here.

A simple calculation shows that such orthogonal vectors must still have block-tridiagonal Jacobi operators, as multiplication by x, y, or z remains inside the ideal.

2.5.1 Jacobi matrices

We start as before for the scalar case by finding $x\,\nabla Y_l^m(x,y,z)$, $x\,\nabla^\perp Y_l^m(x,y,z)$ etc. in terms of $\nabla Y_{l'}^{m'}(x,y,z)$, $\nabla^\perp Y_{l'}^{m'}(x,y,z)$. A lovely consequence of our definitions of the scalar and vector spherical harmonics is that we can once again find explicit expressions for the coefficients in the aforementioned relations. To this end, we recall and derive some important relations of the complex exponential and Jacobi polynomials that are a part of the spherical harmonics definitions. In particular we first note that:

$$\int_0^{2\pi} e^{im\theta}\, e^{-im'\theta}\, \cos(\theta)\mathrm{d}\theta = \pi(\delta_{m',m-1} + \delta_{m',m+1}) \tag{2.12}$$

$$\int_0^{2\pi} e^{im\theta}\, e^{-im'\theta}\, \sin(\theta)\mathrm{d}\theta = i\,\pi(\delta_{m',m-1} - \delta_{m',m+1}) \tag{2.13}$$

and

$$\int_{-1}^{1} P_{l-|m|}^{(|m|,|m|)}(z)\, P_{l'-|m|}^{(|m|,|m|)}(z)\, \rho(z)^{2|m|}\,\mathrm{d}z = \delta_{l',l}\,\frac{1}{2\pi(c_l^m)^2} \tag{2.14}$$

$$P_{l-|m|}^{(|m|,|m|)\,\prime}(z) = d_{l,m}\, P_{l-(|m|+1)}^{(|m|+1,|m|+1)} \quad \text{where } d_{l,m} := \frac{1}{2}(l+|m|+1),, \tag{2.15}$$

where equation (2.14) and equation (2.14) are consequences of the definition of the Jacobi polynomials, see [19, Table 18.3.1, 18.9.15]. One final relation we will need is that for incrementing the Jacobi parameters, which we will present in the following Lemma.

Lemma 2. *Let $\alpha, \beta \in \mathbb{R}$ be general parameters. Let $z \in [-1,1]$ and define*

$P_{-2}^{(\alpha+1,\beta+1)}(z) \equiv P_{-1}^{(\alpha+1,\beta+1)}(z) \equiv 0$. *Then, for any* $n \in \mathbb{N}_0$*:*

$$
\begin{aligned}
P_n^{(\alpha,\beta)}(z) = \frac{1}{2n+\alpha+\beta+1} \Big\{ & \frac{(n+\alpha+\beta+1)(n+\alpha+\beta+2)}{2n+\alpha+\beta+2} \, P_n^{(\alpha+1,\beta+1)}(z) \\
& + \Big[\frac{(n+\alpha+\beta+1)(n+\alpha)}{2n+\alpha+\beta} \\
& \qquad - \frac{(n+\alpha+\beta+1)(n+\beta+1)}{2n+\alpha+\beta+2} \Big] \, P_{n-1}^{(\alpha+1,\beta+1)}(z) \\
& + \frac{(n+\alpha)(n+\beta)}{2n+\alpha+\beta} \, P_{n-2}^{(\alpha+1,\beta+1)}(z) \Big\}.
\end{aligned}
$$

Proof. This is simply as consequence of the relationships established for incrementing the parameters of Jacobi polynomials detailed in [19, 18.9.5], along with the symmetry relation that $P_n^{(\alpha,\beta)}(-z) \equiv (-1)^n P_n^{(\beta,\alpha)}(z)$. □

We thus can present a useful corollary specific for our needs.

Corollary 1. *Let* $m \in \mathbb{N}_0$ *and* $z \in [-1, 1]$*. Then, for any* $n \in \mathbb{N}_0$*:*

$$
P_{l-m}^{(m,m)}(z) = \mu_{l,m,1} \, P_{l-m}^{(m+1,m+1)}(z) + \mu_{l,m,2} \, P_{l-m-2}^{(m+1,m+1)}(z) \Big],
$$

where

$$
\begin{aligned}
\mu_{l,m,1} &:= \frac{(l+m+\beta+1)(l+m+2)}{2(2l+1)(l+1)} \\
\mu_{l,m,2} &:= \frac{l}{2(2l+1)}.
\end{aligned}
$$

The expressions for the VSHs as given in equation (2.11) together with the above allow us to be able to find the coefficients for our desired expressions for $x\nabla Y_l^m$, $y\nabla Y_l^m$, $z\nabla Y_l^m$, $x\nabla^\perp Y_l^m$, $y\nabla^\perp Y_l^m$ and $z\nabla^\perp Y_l^m$.

Lemma 3. *For $l \in \mathbb{N}_0$, $-l \leq m \leq l$ the vector spherical harmonics satisfy the relationships:*

$$\begin{aligned}
x\nabla Y_l^m &= A_{l,m,1}\nabla Y_{l-1}^{m-1} + A_{l,m,2}\nabla Y_{l-1}^{m+1} + A_{l,m,3}\nabla Y_{l+1}^{m-1} + A_{l,m,4}\nabla Y_{l+1}^{m+1} \\
&\quad + A_{l,m,5}\nabla^\perp Y_l^{m-1} + A_{l,m,6}\nabla^\perp Y_l^{m+1}, \\
x\nabla^\perp Y_l^m &= A_{l,m,1}\nabla^\perp Y_{l-1}^{m-1} + A_{l,m,2}\nabla^\perp Y_{l-1}^{m+1} + A_{l,m,3}\nabla^\perp Y_{l+1}^{m-1} + A_{l,m,4}\nabla^\perp Y_{l+1}^{m+1} \\
&\quad - A_{l,m,5}\nabla Y_l^{m-1} - A_{l,m,6}\nabla Y_l^{m+1}, \\
y\nabla Y_l^m &= B_{l,m,1}\nabla Y_{l-1}^{m-1} + B_{l,m,2}\nabla Y_{l-1}^{m+1} + B_{l,m,3}\nabla Y_{l+1}^{m-1} + B_{l,m,4}\nabla Y_{l+1}^{m+1} \\
&\quad + B_{l,m,5}\nabla^\perp Y_l^{m-1} + B_{l,m,6}\nabla^\perp Y_l^{m+1}, \\
y\nabla^\perp Y_l^m &= B_{l,m,1}\nabla^\perp Y_{l-1}^{m-1} + B_{l,m,2}\nabla^\perp Y_{l-1}^{m+1} + B_{l,m,3}\nabla^\perp Y_{l+1}^{m-1} + B_{l,m,4}\nabla^\perp Y_{l+1}^{m+1} \\
&\quad - B_{l,m,5}\nabla Y_l^{m-1} - B_{l,m,6}\nabla Y_l^{m+1}, \\
z\nabla Y_l^m &= \Gamma_{l,m,1}\nabla Y_{l-1}^m + \Gamma_{l,m,2}\nabla Y_{l+1}^m + \Gamma_{l,m,3}\nabla^\perp Y_l^m, \\
z\nabla^\perp Y_l^m &= \Gamma_{l,m,1}\nabla^\perp Y_{l-1}^m + \Gamma_{l,m,2}\nabla^\perp Y_{l+1}^m - \Gamma_{l,m,3}\nabla Y_l^m
\end{aligned}$$

where,

finish typing up (will take a while as is quite fiddly to set out)

$$A_{l,m,1} := c_l^m \begin{cases} \tilde{A}_{l,m,1} & \textit{if } m > 1 \\ \textit{something} & \textit{if } m = 1 \\ \textit{something2} & \textit{if } m = 0 \\ \tilde{A}_{l,m,2} & \textit{if } m < 0 \end{cases}$$

$$A_{l,m,2} := c_l^m \begin{cases} \tilde{A}_{l,m,2} & \textit{if } m > 0 \\ \textit{something} & \textit{if } m = 0 \\ \textit{something2} & \textit{if } m = -1 \\ \tilde{A}_{l,m,1} & \textit{if } m < -1 \end{cases}$$

$$A_{l,m,3} := c_l^m \begin{cases} \tilde{A}_{l,m,3} & \textit{if } m > 1 \\ \textit{something} & \textit{if } m = 1 \\ \textit{something2} & \textit{if } m = 0 \\ \tilde{A}_{l,m,4} & \textit{if } m < 0 \end{cases}$$

$$A_{l,m,4} := c_l^m \begin{cases} \tilde{A}_{l,m,4} & \textit{if } m > 0 \\ \textit{something} & \textit{if } m = 0 \\ \textit{something2} & \textit{if } m = -1 \\ \tilde{A}_{l,m,3} & \textit{if } m < -1 \end{cases}$$

$$\begin{aligned} A_{l,m,5} := \frac{1}{\mu_{l,0}\, \mathcal{C}_{l,m-1}^{l,m_s}} \Big[& \mathcal{C}_{l,m}^{l-1,m_s}\, \mu_{l,-1}\, \alpha_{l-1,m-m_s,3} + \mathcal{C}_{l,m}^{l+1,m_s}\, \mu_{l,1}\, \alpha_{l-1,m-m_s,1} \\ & - A_{l,m,3}\, \mu_{l+1,-1}\, \mathcal{C}_{l+1,m-1}^{l,m_s} - A_{l,m,1}\, \mu_{l-1,1}\, \mathcal{C}_{l-1,m-1}^{l,m_s} \Big], \end{aligned}$$

$$\begin{aligned} A_{l,m,6} := \frac{1}{\mu_{l,0}\, \mathcal{C}_{l,m+1}^{l,m_s}} \Big[& \mathcal{C}_{l,m}^{l-1,m_s}\, \mu_{l,-1}\, \alpha_{l-1,m-m_s,4} + \mathcal{C}_{l,m}^{l+1,m_s}\, \mu_{l,1}\, \alpha_{l-1,m-m_s,2} \\ & - A_{l,m,4}\, \mu_{l+1,-1}\, \mathcal{C}_{l+1,m+1}^{l,m_s} - A_{l,m,2}\, \mu_{l-1,1}\, \mathcal{C}_{l-1,m+1}^{l,m_s} \Big], \end{aligned}$$

$$B_{l,m,j} := i(-1)^{j+1} A_{l,m,j} \quad \textit{for } j = 1, \ldots, 6,$$

$$E \ldots \quad \mu_{l,-1} \quad \mathcal{C}_{l,m}^{l-1,m_s}$$

Remark: We emphasise again that it is due to the unique relationships that the Jacobi polynomials possess that we are able to explicitly write down these coefficients.

Proof of Lemma 3. Fix $l \in \mathbb{N}, m \in \{-l, \dots, l\}$, and define $Y_{-1}^m := 0$ for any $m \in \mathbb{Z}$. We proceed first with the case for multiplication by z. Using the definitions given for $\Gamma_{l,m,1}, \Gamma_{l,m,2}, \Gamma_{l,m,3}$ in the Lemma, we have that

$$
\begin{aligned}
&\Gamma_{l,m,1} \nabla Y_{l-1}^m + \Gamma_{l,m,3} \nabla Y_{l+1}^m + \Gamma_{l,m,2}^* \nabla^\perp Y_l^m \\
&\quad = \sum_{m_s=-1}^{1} \chi_{1,m_s} \Big\{ \Gamma_{l,m,1} \mu_{l-1,-1} \mathcal{C}_{l-1,m}^{l-2,m_s} Y_{l-2}^{m-m_s} + \Gamma_{l,m,1} \mu_{l-1,1} \mathcal{C}_{l-1,m}^{l,m_s} Y_l^{m-m_s} \\
&\qquad\qquad + \Gamma_{l,m,3} \mu_{l+1,-1} \mathcal{C}_{l+1,m}^{l,m_s} Y_l^{m-m_s} + \Gamma_{l,m,3} \mu_{l+1,1} \mathcal{C}_{l+1,m}^{l+2,m_s} Y_{l+2}^{m-m_s} \\
&\qquad\qquad + \Gamma_{l,m,2} \mu_{l,0} \mathcal{C}_{l,m}^{l,m_s} Y_l^{m-m_s} \Big\} \\
&\quad = \sum_{m_s=-1}^{1} \chi_{1,m_s} \Big\{ Y_{l-2}^{m-m_s} \Gamma_{l,m,1} \mu_{l-1,-1} \mathcal{C}_{l-1,m}^{l-2,m_s} + Y_{l+2}^{m-m_s} \Gamma_{l,m,3} \mu_{l+1,1} \mathcal{C}_{l+1,m}^{l+2,m_s} \\
&\qquad\qquad + Y_l^{m-m_s} \Big[\Gamma_{l,m,1} \mu_{l-1,1} \mathcal{C}_{l-1,m}^{l,m_s} + \Gamma_{l,m,2} \mu_{l,0} \mathcal{C}_{l,m}^{l,m_s} + \Gamma_{l,m,3} \mu_{l+1,-1} \mathcal{C}_{l+1,m}^{l,m_s} \Big] \Big\} \\
&\quad = \sum_{m_s=-1}^{1} \chi_{1,m_s} \Big\{ \mathcal{C}_{l,m}^{l-1,m_s} \mu_{l,-1} \Big[\gamma_{l-1,m-m_s,1} \, Y_{l-2}^{m-m_s} + \gamma_{l-1,m-m_s,2} \, Y_l^{m-m_s} \Big] \\
&\qquad\qquad + \mathcal{C}_{l,m}^{l+1,m_s} \mu_{l,1} \Big[\gamma_{l+1,m-m_s,1} \, Y_l^{m-m_s} + \gamma_{l+1,m-m_s,2} \, Y_{l+2}^{m-m_s} \Big] \Big\} \\
&\quad = \sum_{m_s=-1}^{1} \chi_{1,m_s} \, z \Big\{ \mathcal{C}_{l-1,m}^{l,m_s} \mu_{l,-1} Y_{l-1}^{m-m_s} + \mathcal{C}_{l+1,m}^{l,m_s} \mu_{l,1} Y_{l+1}^{m-m_s} \Big\} \\
&\quad = z \nabla Y_l^m,
\end{aligned}
$$

demonstrating that the expression for $z \nabla Y_l^m(x, y, z)$ holds.

Firstly, reiterating the previous remark, the ratios of the CG coeffs are equal for each valid m_s value.

Now, we compare coeffs and we are done.

$\square$

As for the scalar case, these recurrences above lead us to Jacobi matrices for the tangent space basis. Define $\tilde{\mathbb{T}}$ by

$$\tilde{\mathbb{T}} = \begin{pmatrix} \tilde{\mathbb{T}}_0 \\ \tilde{\mathbb{T}}_1 \\ \vdots \end{pmatrix}, \quad \text{where} \quad \tilde{\mathbb{T}}_l = \begin{pmatrix} (\nabla Y_l^{-l})^\top \\ (\nabla^\perp Y_l^{-l})^\top \\ \vdots \\ (\nabla Y_l^{l})^\top \\ (\nabla^\perp Y_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{2(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0. \tag{2.16}$$

The Jacobi matrices are then defined according to the matrices ${}^TJ_x, {}^TJ_y, {}^TJ_z$ satisfying

$$\begin{aligned} {}^TJ_x \tilde{\mathbb{T}}(x,y,z) &= x\tilde{\mathbb{T}}(x,y,z) \\ {}^TJ_y \tilde{\mathbb{T}}(x,y,z) &= y\tilde{\mathbb{T}}(x,y,z) \\ {}^TJ_z \tilde{\mathbb{T}}(x,y,z) &= z\tilde{\mathbb{T}}(x,y,z) \end{aligned} \tag{2.17}$$

for each $(x, y, z) \in \Omega$. The tangent space Jacobi matrices are banded-block-banded due to the sparse relationships we obtain from Lemma 3. Specifically, they each have block-bandwidths $(1,1)$:

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

Let $0_2 \in \mathbb{R}^{2\times 2}$ be the 2x2 zero matrix. ${}^{T}J_x$ has subblock-bandwidths $(4,4)$ since for $l \in \mathbb{N}_0$:

$$
A_{x,l} := \begin{pmatrix}
\mathcal{A}_{l,-l,5} & 0_2 & \mathcal{A}_{l,-l,6} & & \\
 & \ddots & \ddots & \ddots & \\
 & & \mathcal{A}_{l,l,5} & 0_2 & \mathcal{A}_{l,l,6}
\end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)},
$$

$$
B_{x,l} := \begin{pmatrix}
0_2 & \mathcal{A}_{l,-l,4} & & \\
\mathcal{A}_{l,-l+1,3} & \ddots & \ddots & \\
 & \ddots & \ddots & \mathcal{A}_{l,l-1,4} \\
 & & \mathcal{A}_{l,l,3} & 0_2
\end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)},
$$

$$
C_{x,l} := \begin{pmatrix}
\mathcal{A}_{l,-l,2} & & \\
0_2 & \ddots & \\
\mathcal{A}_{l,-l+2,1} & \ddots & \ddots & \\
 & \ddots & \ddots & \mathcal{A}_{l,l-2,2} \\
 & & \ddots & 0_2 \\
 & & & \mathcal{A}_{l,l,1}
\end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l-1)} \quad (l \neq 0),
$$

where

$$\mathcal{A}_{l,m,j} := \begin{pmatrix} A_{l,m,j} & 0 \\ 0 & A^*_{l,m,j} \end{pmatrix} \text{ for } j = 1, 2, 5, 6, \quad \mathcal{A}_{l,m,j} := \begin{pmatrix} 0 & A_{l,m,j} \\ A^*_{l,m,j} & 0 \end{pmatrix} \text{ for } j = 3, 4.$$

Similarly, ${}^T J_y$ also has subblock-bandwidths $(4, 4)$ since for $l \in \mathbb{N}_0$:

$$A_{y,l} := \begin{pmatrix} \mathcal{B}_{l,-l,5} & 0_2 & \mathcal{B}_{l,-l,6} & & \\ & \ddots & \ddots & \ddots & \\ & & \mathcal{B}_{l,l,5} & 0_2 & \mathcal{B}_{l,l,6} \end{pmatrix} \in \mathbb{R}^{2(2l+1) \times 2(2l+3)},$$

$$B_{y,l} := \begin{pmatrix} 0_2 & \mathcal{B}_{l,-l,4} & & \\ \mathcal{B}_{l,-l+1,3} & \ddots & \ddots & \\ & \ddots & \ddots & \mathcal{B}_{l,l-1,4} \\ & & \mathcal{B}_{l,l,3} & 0_2 \end{pmatrix} \in \mathbb{R}^{2(2l+1) \times 2(2l+1)},$$

$$C_{y,l} := \begin{pmatrix} \mathcal{B}_{l,-l,2} & & \\ 0_2 & \ddots & \\ \mathcal{B}_{l,-l+2,1} & \ddots & \ddots & \\ & \ddots & \ddots & \mathcal{B}_{l,l-2,2} \\ & & \ddots & 0_2 \\ & & & \mathcal{B}_{l,l,1} \end{pmatrix} \in \mathbb{R}^{2(2l+1) \times 2(2l-1)} \quad (l \neq 0),$$

where

$$\mathcal{B}_{l,m,j} := \begin{pmatrix} B_{l,m,j} & 0 \\ 0 & B^*_{l,m,j} \end{pmatrix} \text{ for } j = 1, 2, 5, 6, \quad \mathcal{B}_{l,m,j} := \begin{pmatrix} 0 & B_{l,m,j} \\ B^*_{l,m,j} & 0 \end{pmatrix} \text{ for } j = 3, 4.$$

Finally, ${}^{T}J_z$ has subblock-bandwidths $(2,2)$, as for $l \in \mathbb{N}_0$:

$$A_l^z := \begin{pmatrix} 0 & 0 & \Gamma_{l,-l,3} & & & & & & \\ & & & \Gamma_{l,-l,3}^* & & & & & \\ & & & & \ddots & & & & \\ & & & & & \Gamma_{l,l,3} & & & \\ & & & & & & \Gamma_{l,l,3}^* & 0 & 0 \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)},$$

$$B_l^z := \begin{pmatrix} 0 & \Gamma_{l,-l,2} & & & \\ \Gamma_{l,-l,2}^* & 0 & & & \\ & & \ddots & & \\ & & & 0 & \Gamma_{l,l,2} \\ & & & \Gamma_{l,l,2}^* & 0 \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)},$$

$$C_l^z := \begin{pmatrix} 0 & & & & \\ 0 & & & & \\ \Gamma_{l,-l+1,1} & & & & \\ & \Gamma_{l,-l+1,1}^* & & & \\ & & \ddots & & \\ & & & \Gamma_{l,l-1,1} & \\ & & & & \Gamma_{l,l-1,1}^* \\ & & & & 0 \\ & & & & 0 \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l-1)} \quad (l \neq 0).$$

2.5.2 Three-term recurrence relation for $\tilde{\mathbb{T}}(x, y, z)$

We can combine each system in equation (2.17) into a block-tridiagonal system for any $(x, y, z) \in \Omega$:

$$\begin{pmatrix} I_6 & & & \\ B_1 - G_1(x,y,z) & A_1 & & \\ C_2 & B_2 - G_2(x,y,z) & A_3 & \\ & C_3 & B_3 - G_3(x,y,z) & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tilde{\mathbb{T}}(x,y,z) = \begin{pmatrix} \tilde{\mathbb{T}}_1(x,y,z) \\ \mathbf{0} \\ \mathbf{0} \\ \vdots \end{pmatrix},$$

where we note that

$$\tilde{\mathbb{T}}_1(x,y,z) := \begin{pmatrix} \nabla Y_1^{-1}(x,y,z) \\ \nabla^\perp Y_1^{-1}(x,y,z) \\ \nabla Y_1^{0}(x,y,z) \\ \nabla^\perp Y_1^{0}(x,y,z) \\ \nabla Y_1^{1}(x,y,z) \\ \nabla^\perp Y_1^{1}(x,y,z) \end{pmatrix},$$

can be calculated explicitly, and for each $l \in \mathbb{N}$,

$$A_l := \begin{pmatrix} A_{x,l} \\ A_{y,l} \\ A_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+3)}, \quad C_l := \begin{pmatrix} C_{x,l} \\ C_{y,l} \\ C_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l-1)} \quad (n \neq 0), \tag{2.18}$$

$$B_l := \begin{pmatrix} B_{x,l} \\ B_{y,l} \\ B_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+1)}, \quad G_n(x,y) := \begin{pmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+1)}. \tag{2.19}$$

For each $l \in \mathbb{N}$ let $D_l^\top$ be any matrix that is a left inverse of A_l, i.e. such that $D_l^\top A_l = I_{2(2l+3)}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the $D_l^\top$'s, we obtain a lower triangular system [9, p78] which can be expanded to obtain the three-term recurrence:

$$\tilde{\mathbb{T}}_{l+1}(x,y,z) = -D_l^\top [B_l - G_l(x,y,z)]\tilde{\mathbb{T}}_l(x,y,z) - D_l^\top C_l\, \tilde{\mathbb{T}}_{l-1}(x,y,z), \quad l \in \mathbb{N}$$

where of course we have that $\mathbb{T}(x,y,z) \equiv \mathbf{0}_{2\times 3}$.

We note that we can choose the matrices $D_l^\top$ in the following way. For $l \in \mathbb{N}$, we set

$$D_l^\top = \begin{pmatrix} \hat{A}_l^{x,y} & 0_{2(2l+3)\times 2(2l+1)} \end{pmatrix} \in \mathbb{R}^{2(2l+3)\times 6(2l+1)} \tag{2.20}$$

where $0_{2(2l+3)\times 2(2l+1)}$ the zero matrix in $\mathbb{R}^{2(2l+3)\times 2(2l+1)}$, and $\hat{A}_l^{x,y} \in \mathbb{R}^{2(2l+3)\times 4(2l+1)}$

is the left inverse of the matrix $\begin{pmatrix} A_l^x \\ A_l^y \end{pmatrix}$, given by

$$
\hat{A}_l^{x,y} = \begin{pmatrix}
\frac{1}{2d_{l,-l}} & 0 & \dots & 0 & -\frac{i}{2d_{l,-l}} & 0 & \dots & & & \\
0 & \frac{1}{2d^{\perp}_{l,-l}} & 0 & \dots & 0 & -\frac{i}{2d^{\perp}_{l,-l}} & 0 & \dots & & \\
 & & \ddots & & & & \ddots & & & \\
\vdots & & & \ddots & & & & \ddots & & \\
 & & & & \frac{1}{2d_{l,l}} & 0 & \dots & 0 & -\frac{i}{2d_{l,l}} & \\
 & & & & & \frac{1}{2d^{\perp}_{l,l}} & 0 & \dots & 0 & -\frac{i}{2d^{\perp}_{l,l}} \\
0 & \dots & \frac{1}{2a_{l,l-1}} & 0 & \dots & 0 & \frac{i}{2a_{l,l-1}} & 0 & 0 & 0 \\
0 & \dots & 0 & \frac{1}{2a^{\perp}_{l,l-1}} & 0 & \dots & 0 & \frac{i}{2a^{\perp}_{l,l-1}} & 0 & 0 \\
0 & \dots & \dots & 0 & \frac{1}{2a_{l,l}} & 0 & \dots & 0 & \frac{i}{2a_{l,l}} & 0 \\
0 & \dots & \dots & & 0 & \frac{1}{2a^{\perp}_{l,l}} & 0 & \dots & 0 & \frac{i}{2a^{\perp}_{l,l}}
\end{pmatrix}. \tag{2.21}
$$

Derive Dlts again

2.5.3 Computational aspects

Let $\boldsymbol{u}$ be a vector-valued function on Ω whose values are of the form

$$
\boldsymbol{u}(x,y,z) = u_{\varphi}(x,y,z)\,\hat{\boldsymbol{\phi}} + u_{\theta}(x,y,z)\,\hat{\boldsymbol{\theta}}, \quad (x,y,z) \in \Omega
$$

for some scalar functions u^{φ}, u^{θ} where $\hat{\boldsymbol{\phi}}, \hat{\boldsymbol{\theta}}$ are the standard non-radial unit basis vectors on the sphere defined by $\hat{\boldsymbol{\phi}} := (\cos\theta \sin\varphi, \sin\theta \sin\varphi, \cos\varphi)^{\top}$, $\hat{\boldsymbol{\theta}} := (-\sin\theta, \cos\theta, 0)^{\top}$. Such a function $\boldsymbol{u}$ we refer to as a *vector-valued function in the tangent space of* Ω. We can then approximate this function by its expansion in the VSH basis, i.e. for some large enough $N \in \mathbb{N}$:

$$\boldsymbol{u}(x,y,z) \approx \tilde{\mathbb{T}}(x,y,z)^{\top} \boldsymbol{u}^{c} := \sum_{l=0}^{N} \sum_{m=-l}^{l} \left[u_{l,m} \, \nabla Y_{l}^{m}(x,y,z) + u_{l,m}^{\perp} \, \nabla^{\perp} Y_{l}^{m}(x,y,z) \right].$$

Obtaining coefficients

The development of vector spherical harmonic transforms is well established [29], and continues today (see [11]).

VSH Transform

Function evaluation

The Clenshaw algorithm presented in Section 2.4.2 can also be used to evaluate a vector-valued function in the tangent space for a point $(x, y, z) \in \Omega$:

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

2) For $n = N : -1 : 1$

$$\text{set } \boldsymbol{\xi}_n^\top = (\mathbf{u}_n^c)^\top - \boldsymbol{\xi}_{n+1}^\top D_n^\top (B_n - G_n) - \boldsymbol{\xi}_{n+2}^\top D_{n+1}^\top C_{n+1}$$

3) Output: $\mathbf{u}(x, y, z) \approx \tilde{\mathbb{T}}_1(x, y, z)^\top \boldsymbol{\xi}_1$

$$\begin{aligned} &= (\boldsymbol{\xi}_1)_1 \nabla Y_1^{-1} + (\boldsymbol{\xi}_1)_2 \nabla^\perp Y_1^{-1} + (\boldsymbol{\xi}_1)_3 \nabla Y_1^0 \\ &\quad + (\boldsymbol{\xi}_1)_4 \nabla^\perp Y_1^0 + (\boldsymbol{\xi}_1)_5 \nabla Y_1^1 + (\boldsymbol{\xi}_1)_6 \nabla^\perp Y_1^1. \end{aligned}$$

2.5.4 Sparse partial differential operators

The framework we have outlined for the spherical harmonics and the vector spherical harmonics allows us to easily and explicitly derive sparse operator matrices for partial differential operators such as the spherical gradient, divergence and Laplacian, as well as other key operators useful in examples such as the linearised shallow water equations. These operators will take coefficients of a function's expansion in either the SSH or VSH basis, to coefficients in either basis.

In order to ensure we fully capitalise on the natural sparsity of the relationships so that we yield banded-block-banded operators, we will "split" coefficient vectors of a vector-valued function on the tangent space of Ω into two. On that note, define

$\mathbb{T}, \mathbb{T}^\perp$ by

$$\mathbb{T} := \begin{pmatrix} \mathbb{T}_0 \\ \mathbb{T}_1 \\ \vdots \end{pmatrix}, \quad \text{where} \quad \mathbb{T}_l := \begin{pmatrix} (\nabla Y_l^{-l})^\top \\ \vdots \\ (\nabla Y_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0, \tag{2.22}$$

$$\mathbb{T}^\perp := \begin{pmatrix} \mathbb{T}_0^\perp \\ \mathbb{T}_1^\perp \\ \vdots \end{pmatrix}, \quad \text{where} \quad \mathbb{T}_l^\perp := \begin{pmatrix} (\nabla^\perp Y_l^{-l})^\top \\ \vdots \\ (\nabla^\perp Y_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0. \tag{2.23}$$

Let $\boldsymbol{u}$ be a vector-valued function on the tangent space of Ω with coefficients vectors $\boldsymbol{u}^c, \boldsymbol{u}^{\perp c}$ for its expansion in the VSH basis up to order $N \in \mathbb{N}$, and let f be a scalar function on Ω with coefficients vector $\boldsymbol{f}^c$ for its expansion in the SSH basis also up to order N, i.e.

$$\begin{aligned} \boldsymbol{u}(x,y,z) &\approx \mathbb{T}(x,y,z)^\top\, \boldsymbol{u}^c + \mathbb{T}^\perp(x,y,z)^\top\, \boldsymbol{u}^{\perp c} \\ &:= \sum_{l=0}^{N} \sum_{m=-l}^{l} \big[u_{l,m}\, \nabla Y_l^m(x,y,z) + u_{l,m}^\perp\, \nabla^\perp Y_l^m(x,y,z)\big], \\ f(x,y,z) &\approx \mathbb{P}(x,y,z)^\top\, \boldsymbol{f}^c := \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m}\, Y_l^m(x,y,z) \end{aligned}$$

We are now in a position to derive the sparse differential operators that can be applied to the functions $\boldsymbol{u}, f$.

Definition 3. *We define the operator matrices $\mathcal{D}, \mathcal{G}, \mathcal{L}$ according to:*

$$\nabla \cdot \boldsymbol{u}(x,y,z) = \mathbb{P}(x,y,z)^\top \, \mathcal{D} \, \boldsymbol{u}^c,$$

$$\nabla_{\mathrm{S}} f(x,y,z) = \mathbb{T}(x,y,z)^\top \, \mathcal{G} \, \boldsymbol{f}^c,$$

$$\Delta_{\mathrm{S}} f(x,y,z) = \mathbb{P}(x,y,z)^\top \, \mathcal{L} \, \boldsymbol{f}^c.$$

Theorem 1. *The operator matrices defined in Definition 3 are diagonal, and are given by:*

$$\mathcal{G} = I_{(N+1)^2}, \quad \mathcal{D} \equiv \mathcal{L} := \begin{pmatrix} \mathcal{L}_0 & & \\ & \ddots & \\ & & \mathcal{L}_N \end{pmatrix},$$

where

$$\mathcal{L}_l := \begin{pmatrix} -l(l+1) & & \\ & \ddots & \\ & & -l(l+1) \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l+1)}.$$

Proof. The argument for $\mathcal{G}$ is trivial by definition. Now, the spherical harmonics, as the name eludes to, satisfy a harmonic relationship $\Delta_{\mathrm{S}} Y_l^m = l(l+1) Y_l^m$. Thus,

cite

for the proof for $\mathcal{D}$, consider

$$\begin{aligned}
\nabla \cdot \boldsymbol{u} &= \nabla \cdot \Big(\sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m] \Big) \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} u_{l,m}\, \Delta_{\mathrm{S}} Y_l^m \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} -u_{l,m}\, l(l+1) Y_l^m,
\end{aligned}$$

using the fact that $\nabla \cdot (\nabla^{\perp} f) \equiv 0$ for any function f. We similarly have for $\mathcal{L}$:

$$\begin{aligned}
\Delta_{\mathrm{S}} f &= \Delta_{\mathrm{S}} \Big(\sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m} Y_l^m \Big) \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m}\, \Delta_{\mathrm{S}} Y_l^m \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} -f_{l,m}\, l(l+1) Y_l^m.
\end{aligned}$$

□

Now that we have our differential operators, let's apply them in an example.

2.6 Example: linear shallow water equations

The linearised shallow water equations allow us to showcase the differential operators that we defined in Definition 3 (namely the divergence and gradient operators) and demonstrate how the natural sparsity that our framework brings to the problem leads to a simple sparse linear system to solve.

Let $\boldsymbol{u}(x, y, z)$ be the tangential velocity of a flow and $h(x, y, z)$ be the height deviation of the flow from some constant reference height $\mathcal{H}$. Define $\hat{\boldsymbol{r}}$ as the unit outward normal vector at the point on the sphere (x, y, z), so that

$$\hat{\boldsymbol{r}} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

The linear SWEs are

$$\begin{cases} \frac{\partial \boldsymbol{u}}{\partial t} + f \hat{\boldsymbol{r}} \times \boldsymbol{u} - \nabla h = \boldsymbol{0} \\ \frac{\partial h}{\partial t} + \mathcal{H} \nabla \cdot \boldsymbol{u} = 0 \end{cases}$$

where $f = 2\tilde{\Omega}\cos(\varphi) = 2\tilde{\Omega}z$ is the Coriolis parameter, and $\tilde{\Omega} = 7.292110^{-5}$ rad s^{-1} is the rotation rate of the Earth (note that $\varphi = \frac{\pi}{2} -$ latitude).

A keen eye may notice that we require one more operator not yet defined – one for the Coriolis parameter cross product (i.e. $f\, \hat{\boldsymbol{r}} \times \boldsymbol{u}$).

Definition 4. *Define the operator matrices $\mathcal{F}, \mathcal{F}^{\perp}$ according to:*

$$f\, \hat{\boldsymbol{r}} \times \boldsymbol{u}(x, y, z) = \mathbb{T}(x, y, z)^{\top} \mathcal{F}\, \boldsymbol{u}^{\perp c} + \left(\mathbb{T}^{\perp}(x, y, z)\right)^{\top} \mathcal{F}^{\perp}\, \boldsymbol{u}^{c}$$

Lemma 4. *The operators $\mathcal{F}, \mathcal{F}^{\perp}$ defined in Definition 4 are sparse with banded-block-banded structure. More specifically,*

- $\mathcal{F}$ *has block-bandwidths* $(1,1)$*, and sub-block-bandwidths* $(1,1)$

- $\mathcal{F}^{\perp}$ *has block-bandwidths* $(1,1)$*, and sub-block-bandwidths* $(1,1)$

Proof. Using Lemma 3, we have that:

$$\begin{aligned}
f\,\hat{\boldsymbol{r}} \times \mathbf{u} &= f\,\hat{\boldsymbol{r}} \times \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m] \\
&= 2\,\tilde{\Omega}\,z \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m} \hat{\boldsymbol{r}} \times \nabla Y_l^m + u_{l,m}^{\perp} \hat{\boldsymbol{r}} \times (\hat{\boldsymbol{r}} \times \nabla Y_l^m)] \\
&= 2\,\tilde{\Omega} \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m} z\, \nabla^{\perp} Y_l^m - u_{l,m}^{\perp} z\, \nabla Y_l^m)] \\
&= 2\,\tilde{\Omega} \sum_{l=0}^{N} \sum_{m=-l}^{l} \Big[u_{l,m} \left(\Gamma_{l,m,1}^{*} \nabla^{\perp} Y_{l-1}^m + \Gamma_{l,m,3}^{*} \nabla^{\perp} Y_{l+1}^m + \Gamma_{l,m,2} \nabla Y_l^m \right) \\
&\qquad\qquad - u_{l,m}^{\perp} \left(\Gamma_{l,m,1} \nabla Y_{l-1}^m + \Gamma_{l,m,3} \nabla Y_{l+1}^m + \Gamma_{l,m,2}^{*} \nabla^{\perp} Y_l^m \right) \Big].
\end{aligned}$$

We can then write down the operators $\mathcal{F}, \mathcal{F}^{\perp}$ as follows:

$$\mathcal{F} = \bar{\mathcal{F}^{\perp}} = 2\,\tilde{\Omega} \begin{pmatrix} \mathcal{F}_{0,2} & \mathcal{F}_{1,1} & & & \\ \mathcal{F}_{0,3} & \mathcal{F}_{1,2} & \mathcal{F}_{2,1} & & \\ & \mathcal{F}_{1,3} & \mathcal{F}_{2,2} & \mathcal{F}_{3,1} & \\ & & \mathcal{F}_{2,3} & \ddots & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

where $\bar{A}$ denotes the conjugate matrix of A (i.e. where the entries of $\bar{A}$ are simply the complex conjugates of the entries of A) [8, p.10], and for $l = 0, \dots, N$

$$\mathcal{F}_{l,1} := \begin{pmatrix} 0 & \Gamma_{l,-l+1,1} & & & \\ & & \ddots & & \\ & & & \Gamma_{l,l-1,1} & 0 \end{pmatrix} \in \mathbb{R}^{(2l-1)\times(2l+1)}, \quad (l \neq 0),$$

$$\mathcal{F}_{l,2} := \begin{pmatrix} \Gamma_{l,-l,2} & & \\ & \ddots & \\ & & \Gamma_{l,l,2} \end{pmatrix} \in \mathbb{R}^{(2l+1)\times(2l+1)},$$

$$\mathcal{F}_{l,3} := \begin{pmatrix} 0 & & \\ \Gamma_{l,-l,3} & & \\ & \ddots & \\ & & \Gamma_{l,l,3} \\ & & 0 \end{pmatrix} \in \mathbb{R}^{(2l+3)\times(2l+1)}.$$

□

For simplicity, we implement a backward Euler timestepping method to solve the linear SWEs with timestep Δt:

$$\begin{aligned} \boldsymbol{u}_{n+1} &= \boldsymbol{u}_n + \Delta t \left(\nabla h_{n+1} - f \hat{\boldsymbol{r}} \times \boldsymbol{u}_{n+1} \right) \\ h_{n+1} &= h_n - \Delta t \, \mathcal{H} \nabla \cdot \boldsymbol{u}_{n+1} \end{aligned}$$

In coefficient space, this system becomes:

$$\begin{aligned}
\boldsymbol{u}_{n+1}^c &= \boldsymbol{u}_n^c + \Delta t\,(\mathcal{G}\boldsymbol{h}_{n+1}^c - \mathcal{F}\boldsymbol{u}_{n+1}^{\perp c}) \\
\boldsymbol{u}_{n+1}^{\perp c} &= -\Delta t\,\mathcal{F}^{\perp}\boldsymbol{u}_{n+1}^c \\
\boldsymbol{h}_{n+1}^c &= \boldsymbol{h}_n^c - \Delta t\,\mathcal{H}D\boldsymbol{u}_{n+1}^c
\end{aligned}$$

$\iff$

$$\begin{aligned}
\boldsymbol{u}_{n+1}^c &= \boldsymbol{u}_n^c + \Delta t\,(\mathcal{G}\boldsymbol{h}_n^c - \Delta t\,\mathcal{H}\mathcal{G}\mathcal{D}\boldsymbol{u}_{n+1}^c + \Delta t\mathcal{F}\mathcal{F}^{\perp}\boldsymbol{u}_{n+1}^c) \\
\boldsymbol{u}_{n+1}^{\perp c} &= -\Delta t\,\mathcal{F}^{\perp}\boldsymbol{u}_{n+1}^c \\
\boldsymbol{h}_{n+1}^c &= \boldsymbol{h}_n^c - \Delta t\,\mathcal{H}D\boldsymbol{u}_{n+1}^c
\end{aligned}$$

$\iff$

$$\begin{aligned}
\boldsymbol{u}_{n+1}^c &= (I + \Delta t^2\mathcal{H}\mathcal{G}\mathcal{D} - \Delta t^2\mathcal{F}\mathcal{F}^{\perp})^{-1}\,(\boldsymbol{u}_n^c + \Delta t\,\mathcal{G}\boldsymbol{h}_n^c) \\
\boldsymbol{u}_{n+1}^{\perp c} &= -\Delta t\,\mathcal{F}^{\perp}\boldsymbol{u}_{n+1}^c \\
\boldsymbol{h}_{n+1}^c &= \boldsymbol{h}_n^c - \Delta t\,\mathcal{H}\mathcal{D}\boldsymbol{u}_{n+1}^c.
\end{aligned}$$

Here, it is clear that the matrix $I + \Delta t^2\mathcal{H}\mathcal{G}\mathcal{D} - \Delta t^2\mathcal{F}\mathcal{F}^{\perp}$ is sparse with banded-block-banded structure, and hence this system will be efficient to solve. Doing so at each iteration provides us with the coefficients vectors $\boldsymbol{u}_{n+1}^c, \boldsymbol{u}_{n+1}^{\perp c}, \boldsymbol{h}_{n+1}^c$ if we know $\boldsymbol{u}_n^c, \boldsymbol{u}_n^{\perp c}, \boldsymbol{h}_n^c$.

Chapter 3

Disk slices and trapeziums

The contents of the previous chapter on spherical harmonics can allow us to use similar techniques for developing sparse spectral methods for solving linear partial differential equations on other domains. Before we can return to the 3D surface realm, let's first achieve a foundation in two-dimensions, by looking at a special class of geometries that includes disk slices and trapeziums.

More precisely, we will consider the solution of partial differential equations on the domain

$$\Omega := \{(x, y) \in \mathbb{R}^2 \quad | \quad \alpha < x < \beta,\ \gamma\rho(x) < y < \delta\rho(x)\}$$

where either of the following conditions hold:

Condition 1. *ρ is a degree 1 polynomial.*

Condition 2. *ρ is the square root of a non-negative degree $\leq$ 2 polynomial, $-\gamma =$*

$\delta > 0$.

For simplicity of presentation we focus on the disk-slice in this chapter, where $\rho(x) = \sqrt{1-x^2}$, $(\alpha, \beta) \subset (0, 1)$, and $(\gamma, \delta) = (-1, 1)$. However, we will discuss an extension to other geometries, including the half-disk and trapeziums.

We show that partial differential equations become sparse linear systems when viewed as acting on expansions involving a family of orthogonal polynomials (OPs) that generalise Jacobi polynomials, mirroring the ultraspherical spectral method for ordinary differential equations [20] and its analogue on the disk [31] and triangle [21, 22]. On the disk-slice the family of weights we consider are of the form

$$W^{(a,b,c)}(x, y) = (\beta - x)^a \, (x - \alpha)^b \, (1 - x^2 - y^2)^c, \quad \text{for} \quad \alpha \le x \le \beta, \quad -\rho(x) \le y \le \rho(x).$$

The corresponding OPs denoted $H^{(a,b,c)}_{n,k}(x, y)$, where n denotes the polynomial degree, and $0 \le k \le n$. We define these to be orthogonalised lexicographically, that is,

$$H^{(a,b,c)}_{n,k}(x, y) = C_{n,k} x^{n-k} y^k + \text{(lower order terms)}$$

where $C_{n,k} \neq 0$ and "lower order terms" includes degree n polynomials of the form $x^{n-j} y^j$ where $j < k$. The precise normalization arises from their definition in terms of one-dimensional OPs in Definition 11.

Sparsity comes from expanding the domain and range of an operator using different choices of the parameters a, b and c. Whereas the sparsity pattern and entries derived in [21, 22] for equations on the triangle and [31] for equations on the disk results from manipulations of Jacobi polynomials, in the present work we use a more general integration-by-parts argument to deduce the sparsity structure, alongside careful use of the Christoffel–Darboux formula [19, 18.2.2] and quadrature rules to determine the entries. In particular, by exploiting the connection with one-dimensional orthogonal polynomials we can construct discretizations of general partial differential operators of size $p(p-1)/2 \times p(p-1)/2$ in $O(p^3)$ operations, where p is the total polynomial degree. This compares favourably to $O(p^6)$ operations if one proceeds naïvely. Furthermore, we use this framework to derive sparse p-finite element methods that are analogous to those of Beuchler and Schöberl on tetrahedra [3], see also work by Li and Shen [15].

3.1 Orthogonal polynomials on the disk-slice and the trapezium

We can mirror the approach for the spherical harmonics, in that we will outline the construction and some basic properties of our 2D OPs on Ω that we denote by $H_{n,k}^{(a,b,c,d)}(x,y)$. The symmetry in the weight allows us to express the polynomials in terms of 1D OPs, and deduce certain properties such as recurrence relationships.

3.1.1 Explicit construction

We can construct 2D orthogonal polynomials on Ω from 1D orthogonal polynomials on the intervals $[\alpha, \beta]$ and $[\gamma, \delta]$.

Proposition 1 ([9, p55–56])**.** *Let $w_1 : (\alpha, \beta) \to \mathbb{R}$, $w_2 : (\gamma, \delta) \to \mathbb{R}$ be weight functions with $\alpha, \beta, \gamma, \delta \in \mathbb{R}$, and let $\rho : (\alpha, \beta) \to (0, \infty)$ be such that either Condition 1 or Condition 2 with w_2 being an even function hold. $\forall$, $n = 0, 1, 2, \ldots$, let $\{p_{n,k}\}$ be polynomials orthogonal with respect to the weight $\rho(x)^{2k+1} w_1(x)$ where $0 \le k \le n$, and $\{q_n\}$ be polynomials orthogonal with respect to the weight $w_2(x)$. Then the 2D polynomials defined on Ω*

$$H_{n,k}(x, y) := p_{n-k,k}(x)\, \rho(x)^k\, q_k\left(\frac{y}{\rho(x)}\right) \qquad \text{for} \qquad 0 \le k \le n,\ n = 0, 1, 2, \ldots$$

are orthogonal polynomials with respect to the weight $W(x, y) := w_1(x)\, w_2\left(\frac{y}{\rho(x)}\right)$ on Ω.

For disk slices and trapeziums, we specialise Proposition 4 in the following definitions. First we introduce notation for two families of univariate OPs.

Definition 5. *Let $w_R^{(a,b,c)}(x)$ and $w_P^{(a,b)}(x)$ be two weight functions on the intervals (α, β) and (γ, δ) respectively, given by:*

$$\begin{cases} w_R^{(a,b,c)}(x) & := (\beta - x)^a\, (x - \alpha)^b\, \rho(x)^c \\ w_P^{(a,b)}(x) & := (\delta - x)^a\, (x - \gamma)^b \end{cases}$$

and define the associated inner products by:

$$\langle p,\, q\rangle_{w_R^{(a,b,c)}} := \frac{1}{\omega_R^{(a,b,c)}} \int_\alpha^\beta p(x)\, q(x)\, w_R^{(a,b,c)}(x)\,\mathrm{d}x \tag{3.1}$$

$$\langle p, q\rangle_{w_P^{(a,b)}} := \frac{1}{\omega_P^{(a,b)}} \int_\gamma^\delta p(y)\, q(y)\, w_P^{(a,b)}(y)\,\mathrm{d}y \tag{3.2}$$

where

$$\omega_R^{(a,b,c)} := \int_\alpha^\beta w_R^{(a,b,c)}(x)\,\mathrm{d}x, \quad \omega_P^{(a,b)} := \int_\gamma^\delta w_P^{(a,b)}(y)\,\mathrm{d}y. \tag{3.3}$$

Denote the three-parameter family of orthonormal polynomials on $[\alpha, \beta]$ *by* $\{R_n^{(a,b,c)}\}$*, orthonormal with respect to the inner product defined in (4.1), and the two-parameter family of orthonormal polynomials on* $[\gamma, \delta]$ *by* $\{P_n^{(a,b)}\}$*, orthonormal with respect to the inner product defined in (3.2).*

We can now write down our 2D OP family.

Definition 6. *Define the four-parameter 2D orthogonal polynomials via:*

$$H_{n,k}^{(a,b,c,d)}(x,y) := R_{n-k}^{(a,b,c+d+2k+1)}(x)\, \rho(x)^k\, P_k^{(d,c)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega,$$

The comparison with the construction of the 3D spherical harmonics is evident here (the R OPs are in place of the Jacobi polynomials, and the P OPs are in place of the complex exponentials, which are just Chebyshev polynomials). By defining our OPs in this way, we will be able to yield sparse and banded relations for the necessary operators involved in PDEs, just as we did before.

$\{H_{n,k}^{(a,b,c,d)}\}$ are orthogonal with respect to the weight

$$W^{(a,b,c,d)}(x,y) := w_R^{(a,b,c+d)}(x)\, w_P^{(d,c)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega,$$

assuming that either Condition 1 or Condition 2 with $w_P^{(a,b)}$ being an even function (i.e. $a = b$, and we can hence denote the weight as $w_P^{(a)}(x) = w_P^{(a,a)}(x) = (\delta - x^2)^a$) hold. That is,

$$\left\langle H_{n,k}^{(a,b,c,d)},\ H_{m,j}^{(a,b,c,d)} \right\rangle_{W^{(a,b,c,d)}} = \omega_R^{(a,b,c+d+2k+1)}\, \omega_P^{(d,c)}\, \delta_{n,m}\, \delta_{k,j},$$

where for $f, g : \Omega \to \mathbb{R}$ the inner product is defined as

$$\langle f,\ g \rangle_{W^{(a,b,c,d)}} := \iint_\Omega f(x,y)\, g(x,y)\, W^{(a,b,c,d)}(x,y)\, \mathrm{d}y\, \mathrm{d}x.$$

We can see that they are indeed orthogonal using the change of variable $t = \frac{y}{\rho(x)}$, for the following normalisation:

$$\begin{aligned}
&\left\langle H_{n,k}^{(a,b,c,d)},\, H_{m,j}^{(a,b,c,d)} \right\rangle_{W^{(a,b,c,d)}} \qquad (3.4)\\
&\quad = \iint_{\Omega} \Big[R_{n-k}^{(a,b,c+d+2k+1)}(x)\, R_{m-j}^{(a,b,c+d+2j+1)}(x)\, \rho(x)^{k+j} \\
&\qquad\quad \cdot\, P_k^{(d,c)}\left(\frac{y}{\rho(x)}\right)\, P_j^{(d,c)}\left(\frac{y}{\rho(x)}\right)\, W^{(a,b,c,d)}(x,y) \Big]\, \mathrm{d}y\, \mathrm{d}x \\
&\quad = \left(\int_{\alpha}^{\beta} R_{n-k}^{(a,b,c+d+2k+1)}(x)\, R_{m-j}^{(a,b,c+d+2j+1)}(x)\, w_R^{(a,b,c+d+k+j+1)}(x)\, \mathrm{d}x \right) \\
&\qquad\quad \cdot \left(\int_{\gamma}^{\delta} P_k^{(d,c)}(t)\, P_j^{(d,c)}(t)\, w_P^{(d,)}(t)\, \mathrm{d}t \right) \\
&\quad = \omega_P^{(d,c)}\, \delta_{k,j} \int_{\alpha}^{\beta} R_{n-k}^{(a,b,c+d+2k+1)}(x)\, R_{m-k}^{(a,b,c+d+2k+1)}(x)\, w_R^{(a,b,c+d+2k+1)}(x)\, \mathrm{d}x \\
&\quad = \omega_R^{(a,b,c+d+2k+1)}\, \omega_P^{(d,c)}\, \delta_{n,m}\, \delta_{k,j}. \qquad (3.5)
\end{aligned}$$

For the disk-slice, the weight $W^{(a,b,c)}(x,y) = (\beta-x)^a\,(x-\alpha)^b\,(1-x^2-y^2)^c$ results from setting:

$$\begin{cases}
(\alpha,\beta) & \subset (0,1) \\
(\gamma,\delta) & := (-1,1) \\
\rho(x) & := (1-x^2)^{\frac{1}{2}}
\end{cases}$$

so that

$$\begin{cases}
w_R^{(a,b,c)}(x) := (\beta-x)^a\,(x-\alpha)^b\,\rho(x)^c \\
w_P^{(c)}(x) := (1-x)^c\,(1+x)^c = (1-x^2)^c.
\end{cases}$$

Note here we can simply remove the need for including a fourth parameter d. The 2D OPs orthogonal with respect to the weight above on the disk-slice Ω are then given by:

$$H_{n,k}^{(a,b,c)}(x,y) := R_{n-k}^{(a,b,2c+2k+1)}(x)\,\rho(x)^k\,P_k^{(c,c)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega \tag{3.6}$$

In this case the weight $w_P(x)$ is an ultraspherical weight, and the corresponding OPs are the normalized Jacobi polynomials $\{P_n^{(b,b)}\}$, while the weight $w_R(x)$ is non-classical (it is in fact semi-classical, and is equivalent to a generalized Jacobi weight [16, §5]).

3.1.2 Jacobi matrices

Recall that Jacobi matrices are an important piece of the puzzle for using these orthogonal polynomials to practically solve PDEs in a sparse spectral method. To obtain the entries for them, we first need to establish the three-term recurrences associated with $R_n^{(a,b,c)}$ and $P_n^{(d,c)}$. These can be expressed as:

$$xR_n^{(a,b,c)}(x) = \beta_n^{(a,b,c)} R_{n+1}^{(a,b,c)}(x) + \alpha_n^{(a,b,c)} R_n^{(a,b,c)}(x) + \beta_{n-1}^{(a,b,c)} R_{n-1}^{(a,b,c)}(x) \tag{3.7}$$

$$yP_n^{(d,c)}(y) = \delta_n^{(d,c)} P_{n+1}^{(d,c)}(y) + \gamma_n^{(d,c)} P_n^{(d,c)}(y) + \delta_{n-1}^{(d,c)} P_{n-1}^{(d,c)}(y). \tag{3.8}$$

Of course, for the disk-slice case, we have that $c = d$ and $\gamma_n^{(c,c)} = 0\ \forall n = 0, 1, 2, \ldots$. We can use (3.7) and (3.8) to determine the 2D recurrences for $H_{n,k}^{(a,b,c,d)}(x,y)$. Importantly, we can deduce sparsity in the recurrence relationships:

Lemma 5. *$H^{(a,b,c,d)}_{n,k}(x,y)$ satisfy the following 3-term recurrences:*

$$
\begin{aligned}
xH^{(a,b,c,d)}_{n,k}(x,y) &= \alpha^{(a,b,c,d)}_{n,k,1}\, H^{(a,b,c,d)}_{n-1,k}(x,y) + \alpha^{(a,b,c,d)}_{n,k,2}\, H^{(a,b,c,d)}_{n,k}(x,y) + \alpha^{(a,b,c,d)}_{n+1,k,1}\, H^{(a,b,c)}_{n+1,k}(x,y),\\
yH^{(a,b,c,d)}_{n,k}(x,y) &= \beta^{(a,b,c,d)}_{n,k,1}\, H^{(a,b,c,d)}_{n-1,k-1}(x,y) + \beta^{(a,b,c,d)}_{n,k,2}\, H^{(a,b,c,d)}_{n-1,k}(x,y) + \beta^{(a,b,c,d)}_{n,k,3}\, H^{(a,b,c,d)}_{n-1,k+1}(x,y)\\
&\quad + \beta^{(a,b,c,d)}_{n,k,4}\, H^{(a,b,c,d)}_{n,k-1}(x,y) + \beta^{(a,b,c,d)}_{n,k,5}\, H^{(a,b,c,d)}_{n,k}(x,y) + \beta^{(a,b,c,d)}_{n,k,6}\, H^{(a,b,c,d)}_{n,k+1}(x,y)\\
&\quad + \beta^{(a,b,c,d)}_{n,k,7}\, H^{(a,b,c,d)}_{n+1,k-1}(x,y) + \beta^{(a,b,c,d)}_{n,k,8}\, H^{(a,b,c,d)}_{n+1,k}(x,y) + \beta^{(a,b,c,d)}_{n,k,9}\, H^{(a,b,c,d)}_{n+1,k+1}(x,y),
\end{aligned}
$$

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

$$
\begin{aligned}
\alpha^{(a,b,c,d)}_{n,k,1} &:= \beta^{(a,b,c+d+2k+1)}_{n-k-1}, \qquad \alpha^{(a,b,c,d)}_{n,k,2} := \alpha^{(a,b,c+d+2k+1)}_{n-k}\\
\beta^{(a,b,c,d)}_{n,k,1} &:= \delta^{(d,c)}_{k-1}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ R^{(a,b,c+d+2k-1)}_{n-k} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,2} &:= \gamma^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ \rho(x)R^{(a,b,c+d+2k+1)}_{n-k-1} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,3} &:= \delta^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k}, R^{(a,b,c+d+2k+3)}_{n-k-2} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}\\
\beta^{(a,b,c,d)}_{n,k,4} &:= \delta^{(d,c)}_{k-1}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ R^{(a,b,c+d+2k-1)}_{n-k+1} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,5} &:= \gamma^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ \rho(x)R^{(a,b,c+d+2k+1)}_{n-k} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,6} &:= \delta^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k}, R^{(a,b,c+d+2k+3)}_{n-k-1} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}\\
\beta^{(a,b,c,d)}_{n,k,7} &:= \delta^{(d,c)}_{k-1}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ R^{(a,b,c+d+2k-1)}_{n-k+2} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,8} &:= \gamma^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ \rho(x)R^{(a,b,c+d+2k+1)}_{n-k+1} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}\\
\beta^{(a,b,c,d)}_{n,k,9} &:= \delta^{(d,c)}_{k}\, \left\langle R^{(a,b,c+d+2k+1)}_{n-k}, R^{(a,b,c+d+2k+3)}_{n-k} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}.
\end{aligned}
$$

Proof. The 3-term recurrence for multiplication by x follows from equation (3.7).

For the recurrence for multiplication by y, since $\{H_{m,j}^{(a,b,c,d)}\}$ for $m = 0, \ldots, n+1$, $j = 0, \ldots, m$ is an orthogonal basis for any degree $n+1$ polynomial, we can expand $y\, H_{n,k}^{(a,b,c,d)}(x, y) = \sum_{m=0}^{n+1} \sum_{j=0}^{m} c_{m,j}\, H_{m,j}^{(a,b,c,d)}(x, y)$. These coefficients are given by

$$c_{m,j} = \left\langle y\, H_{n,k}^{(a,b,c,d)}, H_{m,j}^{(a,b,c,d)} \right\rangle_{W^{(a,b,c,d)}} \left\| H_{m,j}^{(a,b,c,d)} \right\|_{W^{(a,b,c,d)}}^{-2}.$$

Recall from equation (3.5) that $\left\| H_{m,j}^{(a,b,c,d)} \right\|_{W^{(a,b,c,d)}}^{2} = \omega_R^{(a,b,c+d+2j+1)}\ \omega_P^{(d,c)}$. Then for $m = 0, \ldots, n+1$, $j = 0, \ldots, m$, using the change of variable $t = \frac{y}{\rho(x)}$:

$$\begin{aligned}
&\left\langle y H_{n,k}^{(a,b,c,d)}, H_{m,j}^{(a,b,c,d)} \right\rangle_{W^{(a,b,c,d)}} \\
&\quad = \iint_\Omega H_{n,k}^{(a,b,c,d)}(x, y)\, H_{m,j}^{(a,b,c,d)}(x, y)\, y\, W^{(a,b,c,d)}(x, y)\, dy\, dx \\
&\quad = \Big(\int_\alpha^\beta R_{n-k}^{(a,b,c+d+2k+1)}(x)\, R_{m-j}^{(a,b,c+d+2j+1)}(x)\, \rho(x)^{k+j+2}\, w_R^{(a,b,c+d)}(x)\, \mathrm{d}x \Big) \\
&\qquad\qquad \cdot \Big(\int_\gamma^\delta P_k^{(d,c)}(t)\, P_j^{(d,c)}(t)\, t\, w_P^{(d,c)}(t)\, \mathrm{d}t \Big) \\
&\quad = \Big(\int_\alpha^\beta R_{n-k}^{(a,b,c+d+2k+1)}(x)\, R_{m-j}^{(a,b,c+d+2j+1)}(x)\, w_R^{(a,b,c+d+k+j+2)}(x)\, \mathrm{d}x \Big) \\
&\qquad\qquad \cdot \Big(\int_\gamma^\delta P_k^{(d,c)}(t)\, P_j^{(d,c)}(t)\, t\, w_P^{(d,c)}(t)\, \mathrm{d}t \Big)
\end{aligned}$$

$$= \begin{cases}
\delta_k^{(d,c)}\ \omega_P^{(d,c)}\ \omega_R^{(a,b,c+d+2k+3)}\ \left\langle R_{n-k}^{(a,b,c+d+2k+1)}, R_{m-k-1}^{(a,b,c+d+2k+3)} \right\rangle_{w_R^{(a,b,c+d+2k+3)}} & \text{if } j = k+1 \\
\gamma_k^{(d,c)}\ \omega_P^{(d,c)}\ \omega_R^{(a,b,c+d+2k+1)}\ \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x) R_{m-k}^{(a,b,c+d+2k+1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}} & \text{if } j = k \\
\delta_{k-1}^{(d,c)}\ \omega_P^{(d,c)}\ \omega_R^{(a,b,c+d+2k-1)}\ \left\langle R_{n-k}^{(a,b,c+d+2k-1)},\ \rho(x)^2 R_{m-k+1}^{(a,b,c+d+2k-1)} \right\rangle_{w_R^{(a,b,c+d+2k-1)}} & \text{if } j = k-1 \\
0 & \text{otherwise}
\end{cases}$$

where, by orthogonality,

$$\left\langle R_{n-k}^{(a,b,c+d+2k+1)}, R_{m-k-1}^{(a,b,c+d+2k+3)} \right\rangle_{w_R^{(a,b,c+d+2k+3)}} = 0 \quad \text{for} \quad m < n-1,$$
$$\left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x)^2 R_{m-k+1}^{(a,b,c+d+2k-1)} \right\rangle_{w_R^{(a,b,c+d+2k-1)}} = 0 \quad \text{for} \quad m < n-1.$$

Finally, if Condition 1 holds we have that

$$\left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x) R_{m-k}^{(a,b,c+d+2k+1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}} = 0 \quad \text{for} \quad m < n-1.$$

If Condition 2 holds we have that $\gamma_k^{(d,c)} = \gamma_k^{(c,c)} \equiv 0$ for any k.

$\square$

Three-term recurrences lead to Jacobi operators that correspond to multiplication by x and y. Define, for $n = 0, 1, 2, \ldots$:

$$\mathbb{H}_n^{(a,b,c,d)} := \begin{pmatrix} H_{n,0}^{(a,b,c,d)}(x,y) \\ \vdots \\ H_{n,n}^{(a,b,c,d)}(x,y) \end{pmatrix} \in \mathbb{R}^{n+1}, \qquad \mathbb{H}^{(a,b,c,d)} := \begin{pmatrix} \mathbb{H}_0^{(a,b,c,d)} \\ \mathbb{H}_1^{(a,b,c,d)} \\ \mathbb{H}_2^{(a,b,c,d)} \\ \vdots \end{pmatrix}$$

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

$$J_x^{(a,b,c,d)}\, \mathbb{H}^{(a,b,c,d)}(x,y) = x\, \mathbb{H}^{(a,b,c,d)}(x,y), \quad J_y^{(a,b,c,d)}\, \mathbb{H}^{(a,b,c,d)}(x,y) = y\, \mathbb{H}^{(a,b,c,d)}(x,y). \tag{3.9}$$

The matrices $J_x^{(a,b,c,d)}, J_y^{(a,b,c,d)}$ act on the coefficients vector of a function's expansion in the $\{H_{n,k}^{(a,b,c,d)}\}$ basis. For example, let a, b be general parameters and a function $f(x, y)$ defined on Ω be approximated by its expansion $f(x, y) = \mathbb{H}^{(a,b,c,d)}(x, y)^\top \mathbf{f}$. Then $x\, f(x, y)$ is approximated by $\mathbb{H}^{(a,b,c,d)}(x, y)^\top J_x^{(a,b,c,d)\top} \mathbf{f}$. In other words, $J_x^{(a,b,c,d)\top} \mathbf{f}$ is the coefficients vector for the expansion of the function $(x, y) \mapsto x\, f(x, y)$ in the $\{H_{n,k}^{(a,b,c,d)}\}$ basis.

Further, note that $J_x^{(a,b,c,d)}, J_y^{(a,b,c,d)}$ are banded-block-banded matrices (see Definition 1). They are block-tridiagonal (block-bandwidths $(1, 1)$):

$$J_{x/y}^{(a,b,c,d)} = \begin{pmatrix} B_0^{x/y} & A_0^{x/y} & & & \\ C_1^{x/y} & B_1^{x/y} & A_1^{x/y} & & \\ & C_2^{x/y} & B_2^{x/y} & A_2^{x/y} & \\ & & C_3^{x/y} & \ddots & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

where the blocks themselves are diagonal for $J_x^{(a,b,c,d)}$ (sub-block-bandwidths $(0,0)$),

$$
\begin{aligned}
A_n^x &:= \begin{pmatrix} \alpha_{n+1,0,1}^{(a,b,c,d)} & 0 & \dots & 0 \\ & \ddots & & \vdots \\ & & \alpha_{n+1,n,1}^{(a,b,c,d)} & 0 \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+2)}, \quad n = 0,1,2,\dots \\
B_n^x &:= \begin{pmatrix} \alpha_{n,0,2}^{(a,b,c,d)} & & \\ & \ddots & \\ & & \alpha_{n,n,2}^{(a,b,c,d)} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)} \quad n = 0,1,2,\dots \\
C_n^x &:= \left(A_n^x\right)^\top \in \mathbb{R}^{(n+1)\times n}, \quad n = 1,2,\dots
\end{aligned}
$$

and tridiagonal for $J_y^{(a,b,c,d)}$ (sub-block-bandwidths $(1,1)$),

$$A_n^y := \begin{pmatrix} \beta_{n,0,8}^{(a,b,c,d)} & \beta_{n,0,9}^{(a,b,c,d)} & & & \\ \beta_{n,1,7}^{(a,b,c,d)} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n,n,7}^{(a,b,c,d)} & \beta_{n,n,8}^{(a,b,c,d)} & \beta_{n,n,9}^{(a,b,c,d)} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+2)}, \quad n = 0,1,2,\ldots$$

$$B_n^y := \begin{pmatrix} \beta_{n,0,5}^{(a,b,c,d)} & \beta_{n,0,6}^{(a,b,c,d)} & & \\ \beta_{n,1,4}^{(a,b,c,d)} & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{n,n-1,6}^{(a,b,c,d)} \\ & & \beta_{n,n,4}^{(a,b,c,d)} & \beta_{n,n,5}^{(a,b,c,d)} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)} \quad n = 0,1,2,\ldots$$

$$C_n^y := \begin{pmatrix} \beta_{n,0,2}^{(a,b,c,d)} & \beta_{n,0,3}^{(a,b,c,d)} & & \\ \beta_{n,1,1}^{(a,b,c,d)} & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{n,n-2,3}^{(a,b,c,d)} \\ & & \ddots & \beta_{n,n-1,2}^{(a,b,c,d)} \\ & & & \beta_{n,n,1}^{(a,b,c,d)} \end{pmatrix} \in \mathbb{R}^{(n+1)\times n}, \quad n = 1,2,\ldots$$

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, meaning that the sparsity is not limited to the specific disk-slice case.

3.1.3 Building the OPs

We can combine each system in (3.9) into a block-tridiagonal system:

$$\begin{pmatrix} 1 & & & & \\ B_0 - G_0(x,y) & A_0 & & & \\ C_1 & B_1 - G_1(x,y) & A_1 & & \\ & C_2 & B_2 - G_2(x,y) & \ddots & \\ & & \ddots & \ddots \end{pmatrix} \mathbb{H}^{(a,b,c,d)}(x,y) = \begin{pmatrix} H_{0,0}^{(a,b,c,d)} \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

where we note $H_{0,0}^{(a,b,c,d)}(x,y) \equiv R_0^{(a,b,c+d+1)} P_0^{(d,c)}$, and for each $n = 0, 1, 2 \ldots,$

$$A_n := \begin{pmatrix} A_n^x \\ A_n^y \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+2)}, \quad C_n := \begin{pmatrix} C_n^x \\ C_n^y \end{pmatrix} \in \mathbb{R}^{2(n+1)\times n} \quad (n \neq 0),$$
$$B_n := \begin{pmatrix} B_n^x \\ B_n^y \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+1)}, \quad G_n(x,y) := \begin{pmatrix} xI_{n+1} \\ yI_{n+1} \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+1)}.$$

For each $n = 0, 1, 2 \ldots$ let $D_n^\top$ be any matrix that is a left inverse of A_n, i.e. such that $D_n^\top A_n = I_{n+2}$. 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 [9, p78], which can be expanded to obtain the recurrence:

$$\begin{cases} \mathbb{H}_{-1}^{(a,b,c,d)}(x,y) := 0 \\ \mathbb{H}_{0}^{(a,b,c,d)}(x,y) := H_{0,0}^{(a,b,c,d)} \\ \mathbb{H}_{n+1}^{(a,b,c,d)}(x,y) = -D_n^\top (B_n - G_n(x,y))\mathbb{H}_{n}^{(a,b,c,d)}(x,y) - D_n^\top C_n \, \mathbb{H}_{n-1}^{(a,b,c,d)}(x,y), \quad n = 0,1,2,\dots. \end{cases}$$

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

$$D_n^\top := \begin{pmatrix} \frac{1}{\alpha_{n+1,0,1}^{(a,b,c,d)}} & & & & & & & \\ & \ddots & & & & & & \\ & & \ddots & & & & & \\ & & & \frac{1}{\alpha_{n+1,n,1}^{(a,b,c,d)}} & & & & \\ \eta_0 & 0 & \dots & 0 & \eta_1 & \dots & \dots & \eta_{n+1} \end{pmatrix},$$

where

$$\begin{aligned} \eta_{n+1} &= \frac{1}{\beta_{n,n,9}^{(a,b,c,d)}}, \\ \eta_n &= -\frac{1}{\beta_{n,n-1,9}^{(a,b,c,d)}} \big(\beta_{n,n,8}^{(a,b,c,d)} \, \eta_{n+1}\big), \\ \eta_j &= -\frac{1}{\beta_{n,j-1,9}^{(a,b,c,d)}} \big(\beta_{n,n+j+1,7}^{(a,b,c,d)} \, \eta_{j+2} + \beta_{n,n+j,8}^{(a,b,c,d)} \, \eta_{j+1}\big) \quad \text{for} \quad j = n-1, n-2, \dots, 1, \\ \eta_0 &= -\frac{1}{\alpha_{n+1,0,1}^{(a,b,c,d)}} \big(\beta_{n,1,7}^{(a,b,c,d)} \, \eta_2 + \beta_{n,0,8}^{(a,b,c,d)} \, \eta_1\big). \end{aligned}$$

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

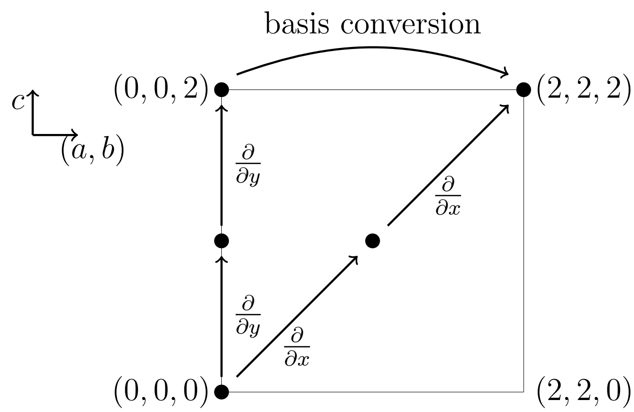


Figure 3.1: The Laplace operator acting on vectors of $H^{(0,0,0)}_{n,k}$ coefficients has a sparse matrix representation if the range is represented as vectors of $H^{(2,2,2)}_{n,k}$ coefficients. Here, the arrows indicate that the corresponding operation has a sparse matrix representation when the domain is $H^{(a,b,c)}_{n,k}$ coefficients, where (a, b, c) is at the tail of the arrow, and the range is $H^{(\tilde{a},\tilde{b},\tilde{c})}_{n,k}$ coefficients, where $(\tilde{a}, \tilde{b}, \tilde{c})$ is at the head of the arrow.

For the disk-slice, $\beta^{(a,b,c)}_{n,k,2} = \beta^{(a,b,c)}_{n,k,5} = \beta^{(a,b,c)}_{n,k,8} \equiv 0$ for any n, k.

3.2 Sparse partial differential operators

In this section, we concentrate on the disk-slice case, and simply note that similar arguments apply for the trapezium case. Recall that, for the disk-slice,

$$\Omega := \{(x, y) \in \mathbb{R}^2 \quad | \quad \alpha < x < \beta,\ \gamma\rho(x) < y < \delta\rho(x)\}$$

where

$$\begin{cases} (\alpha, \beta) & \subset (0, 1) \\ (\gamma, \delta) & := (-1, 1) \\ \rho(x) & := (1 - x^2)^{\frac{1}{2}} \end{cases}.$$

The 2D OPs on the disk-slice Ω, orthogonal with respect to the weight

$$\begin{aligned} W^{(a,b,c)}(x, y) &:= w_R^{(a,b,2c)}(x)\, w_P^{(c)}\left(\frac{y}{\rho(x)}\right) \\ &= (\beta - x)^a\, (x - \alpha)^b\, (1 - x^2 - y^2)^c, \quad (x, y) \in \Omega, \end{aligned}$$

are then given by:

$$H_{n,k}^{(a,b,c)}(x, y) := R_{n-k}^{(a,b,2c+2k+1)}(x)\, \rho(x)^k\, P_k^{(c,c)}\left(\frac{y}{\rho(x)}\right), \quad (x, y) \in \Omega$$

where the 1D OPs $\{R_n^{(a,b,c)}\}$ are orthogonal on the interval (α, β) with respect to the weight

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

and the 1D OPs $\{P_n^{(c,c)}\}$ are orthogonal on the interval $(\gamma, \delta) = (-1, 1)$ with respect to the weight

$$w_P^{(c)}(x) := (1 - x)^c\, (1 + x)^c = (1 - x^2)^c.$$

Denote the weighted OPs by

$$\mathbb{W}^{(a,b,c)}(x,y) := W^{(a,b,c)}(x,y)\,\mathbb{H}^{(a,b,c)}(x,y),$$

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

Definition 7. *Define the operator matrices $D_x^{(a,b,c)}$, $D_y^{(a,b,c)}$, $W_x^{(a,b,c)}$, $W_y^{(a,b,c)}$ according to:*

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \mathbb{H}^{(a+1,b+1,c+1)}(x,y)^\top\, D_x^{(a,b,c)}\,\mathbf{f},\\
\frac{\partial f}{\partial y} &= \mathbb{H}^{(a,b,c+1)}(x,y)^\top\, D_y^{(a,b,c)}\,\mathbf{f},\\
\frac{\partial}{\partial x}[W^{(a,b,c)}(x,y)\, f(x,y)] &= \mathbb{W}^{(a-1,b-1,c-1)}(x,y)^\top\, W_x^{(a,b,c)}\,\mathbf{f},\\
\frac{\partial}{\partial y}[W^{(a,b,c)}(x,y)\, f(x,y)] &= \mathbb{W}^{(a,b,c-1)}(x,y)^\top\, W_y^{(a,b,c)}\,\mathbf{f}.
\end{aligned}$$

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 [19, (18.9.3)], and on the triangle [21]. An illustration of how the non-weighted differential operators increment the parameters (a,b,c) is seen in Figure 3.1.

Theorem 2. *The operator matrices $D_x^{(a,b,c)}$, $D_y^{(a,b,c)}$, $W_x^{(a,b,c)}$, $W_y^{(a,b,c)}$ from Definition 15 are sparse, with banded-block-banded structure. More specifically:*

- $D_x^{(a,b,c)}$ *has block-bandwidths* $(-1,3)$*, and sub-block-bandwidths* $(0,2)$*.*
- $D_y^{(a,b,c)}$ *has block-bandwidths* $(-1,1)$*, and sub-block-bandwidths* $(-1,1)$*.*

- $W_x^{(a,b,c)}$ *has block-bandwidths* $(3,-1)$*, and sub-block-bandwidths* $(2,0)$*.*

- $W_y^{(a,b,c)}$ *has block-bandwidths* $(1,-1)$*, and sub-block-bandwidths* $(1,-1)$*.*

Proof. First, note that:

$$w_R^{(a,b,c)\,\prime}(x) = -a\, w_R^{(a-1,b,c)}(x) + b\, w_R^{(a,b-1,c)}(x) + c\,\rho(x)\,\rho'(x)\, w_R^{(a,b,c-2)}(x), \quad (3.10)$$

$$w_P^{(c)\,\prime}(y) = -2c\, y\, w_P^{(c-1)}(y), \quad (3.11)$$

$$\rho(x)\,\rho'(x) = -x. \quad (3.12)$$

We proceed with the case for the operator $D_y^{(a,b,c)}$ for partial differentiation by y. Since $\{H_{m,j}^{(a,b,c+1)}\}$ for $m = 0,\dots,n-1$, $j = 0,\dots,m$ is an orthogonal basis for any degree $n-1$ polynomial, we can expand $\frac{\partial}{\partial y} H_{n,k}^{(a,b,c)} = \sum_{m=0}^{n-1}\sum_{j=0}^{m} c_{m,j}^{y}\, H_{m,j}^{(a,b,c+1)}$. The coefficients of the expansion are then the entries of the relevant operator matrix. We can use an integration-by-parts argument to show that the only non-zero coefficient of this expansion is when $m = n-1$, $j = k-1$. First, note that

$$c_{m,j}^{y} = \left\langle \frac{\partial}{\partial y} H_{n,k}^{(a,b,c)}, H_{m,j}^{(a,b,c+1)} \right\rangle_{W^{(a,b,c+1)}} \left\| H_{m,j}^{(a,b,c+1)} \right\|_{W^{(a,b+1)}}^{-2}.$$

Then, using the change of variable $t = \frac{y}{\rho(x)}$, we have that

$$\begin{aligned}
&\left\langle \frac{\partial}{\partial y} H^{(a,b,c)}_{n,k}, H^{(a,b,c+1)}_{m,j} \right\rangle_{W^{(a,b,c+1)}} \\
&= \iint_\Omega \Big[R^{(a,b,2c+2k+1)}_{n-k}(x)\, \rho(x)^{k-1}\, P^{(c,c)\,\prime}_k\left(\frac{y}{\rho(x)}\right) \\
&\qquad\qquad \cdot\; R^{(a,b,2c+2j+3)}_{m-j}(x)\, \rho(x)^{j}\, P^{(c+1,c+1)}_j\left(\frac{y}{\rho(x)}\right) \Big] \,\mathrm{d}y\,\mathrm{d}x \\
&= \omega_R^{(a,b,2c+2k+1)} \left\langle R^{(a,b,2c+2k+1)}_{n-k}, \rho(x)^{j-k+1}\, R^{(a,b,2c+2j+3)}_{m-j} \right\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\qquad\qquad \cdot\; \omega_P^{(c+1)} \left\langle P^{(c,c)\,\prime}_k,\; P^{(c+1,c+1)}_j \right\rangle_{w_P^{(c+1)}}
\end{aligned}$$

Now, using (3.11), integration-by-parts, and noting that the weight $w_P^{(c)}$ is a polynomial of degree $2c$ and vanishes at the limits of the integral for positive parameter c, we have that

$$\begin{aligned}
\omega_P^{(c+1)} \left\langle P^{(c,c)\,\prime}_k,\; P^{(c+1,c+1)}_j \right\rangle_{w_P^{(c+1)}} &= \int_\gamma^\delta P^{(c,c)\,\prime}_k(y)\, P^{(c+1,c+1)}_j(y)\, w_P^{(c+1)}(y)\,\mathrm{d}y \\
&= -\int_{-1}^{1} P^{(c,c)}_k(y)\, \frac{\mathrm{d}}{\mathrm{d}y}[w_P^{(c+1)}(y)\, P^{(c+1,c+1)}_j(y)]\,\mathrm{d}y \\
&= -\int_{-1}^{1} P^{(c,c)}_k\, [P^{(c+1,c+1)\,\prime}_j\, w_P^{(c+1)} - 2c\, y\, P^{(c+1,c+1)}_j\, w_P^{(c)}]\,\mathrm{d}y \\
&= -\,\omega_P^{(c)} \left\langle P^{(c,c)}_k,\; w_P^{(1)}\, P^{(c+1,c+1)\,\prime}_j - 2c\, y\, P^{(c+1,c+1)}_j \right\rangle_{w_P^{(c)}}
\end{aligned}$$

which is zero for $j < k-1$ by orthogonality. Further, when $j = k-1$, we have that

$$
\begin{aligned}
&\omega_R^{(a,b,2c+2k+1)} \left\langle R_{n-k}^{(a,b,2c+2k+1)}, \rho(x)^{j-k+1}\, R_{m-j}^{(a,b,2c+2j+3)} \right\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&= \omega_R^{(a,b,2c+2k+1)} \left\langle R_{n-k}^{(a,b,2c+2k+1)}, R_{m-j}^{(a,b,2c+2k+1)} \right\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&= \omega_R^{(a,b,2c+2k+1)}\, \delta_{n,m+1},
\end{aligned}
$$

showing that the only possible non-zero coefficient is when $m = n-1, j = k-1$. Finally,

$$
c^y_{n-1,k-1} = \left\langle P_k^{(c,c)\,\prime},\; P_{k-1}^{(c+1,c+1)} \right\rangle_{w_P^{(c+1)}}.
$$

We next consider the case for the operator $D_x^{(a,b,c)}$ for partial differentiation by x. Since $\{H_{m,j}^{(a+1,b+1,c+1)}\}$ for $m = 0,\ldots,n-1$, $j = 0,\ldots,m$ is an orthogonal basis for any degree $n-1$ polynomial, we can expand $\frac{\partial}{\partial x} H_{n,k}^{(a,b,c)} = \sum_{m=0}^{n-1}\sum_{j=0}^{m} c^x_{m,j} H_{m,j}^{(a+1,b+1,c+1)}$. The coefficients of the expansion are then the entries of the relevant operator matrix. As before, we can use an integration-by-parts argument to show that the only non-zero coefficients of this expansion are when $m = n-1, n-2, n-3$, $j = k, k-1, k-2$ and $0 \le j \le m$. First, note that

$$
c^x_{m,j} = \left\langle \frac{\partial}{\partial x} H_{n,k}^{(a,b,c)}, H_{m,j}^{(a+1,b+1,c+1)} \right\rangle_{W^{(a+1,b+1,c+1)}} \left\| H_{m,j}^{(a+1,b+1,c+1)} \right\|^{-2}_{W^{(a+1,b+1,c+1)}}.
$$

Now, again using the change of variable $t = \frac{y}{\rho(x)}$, we have that

$$\begin{aligned}
&\left\langle \frac{\partial}{\partial x} H_{n,k}^{(a,b,c)}, H_{m,j}^{(a+1,b+1,c+1)} \right\rangle_{W^{(a+1,b+1,c+1)}} \\
&= \Big(\int_{\alpha}^{\beta} R_{n-k}^{(a,b,2c+2k+1)\,\prime}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j+1}\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad\qquad \cdot \Big(\int_{\gamma}^{\delta} P_k^{(c,c)}\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\, \mathrm{d}t \Big) \\
&\quad + k \Big(\int_{\alpha}^{\beta} R_{n-k}^{(a,b,2c+2k+1)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j}\, \rho'\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad\qquad \cdot \Big(\int_{\gamma}^{\delta} P_k^{(c,c)}\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\, \mathrm{d}t \Big) \\
&\quad - \Big(\int_{\alpha}^{\beta} R_{n-k}^{(a,b,2c+2k+1)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j}\, \rho'\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad\qquad \cdot \Big(\int_{\gamma}^{\delta} t\, P_k^{(c,c)\,\prime}\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\, \mathrm{d}t \Big).
\end{aligned} \tag{3.13}$$

We will first show that the second factor of each term in (3.13) are zero for $j < k-2$ and also for $j = k-1$. To this end, observe that, for any integer c, $P^{(c,c)}(-t) = (-1)^k\, P^{(c,c)}(t)$ and so $P_k^{(c,c)}$ is an even polynomial for even k, and an odd polynomial for odd k. Thus, $P_k^{(c,c)}\, P_{k-1}^{(c+1,c+1)}$ is an odd polynomial for any k. Hence

$$\int_{\gamma}^{\delta} P_k^{(c,c)}\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\, \mathrm{d}t = \int_{-\delta}^{\delta} P_k^{(c,c)}\, P_j^{(c+1,c+1)}\, w_P^{(1)}\, w_P^{(c)}\, \mathrm{d}t$$

is zero for $j < k-2$ by orthogonality, and is zero for $j = k-1$ due to symmetry over the domain. Moreover, $t\, P_k^{(c,c)\,\prime}(t)\, P_j^{(c+1,c+1)}(t)$ is also an odd polynomial for any k and so

$$\int_{\gamma}^{\delta} t\, P_k^{(c,c)\,\prime}(t)\, P_j^{(c+1,c+1)}(t)\, w_P^{(c+1)}(t)\, \mathrm{d}t$$

is zero for $j = k-1$ due to symmetry over the domain, and

$$\begin{aligned}
&\int_{\gamma}^{\delta} t\, P_k^{(c,c)\,\prime}\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\, \mathrm{d}t \\
&= -\int_{-\delta}^{\delta} P_k^{(c,c)}\, \frac{\mathrm{d}}{\mathrm{d}t}\big[t\, P_j^{(c+1,c+1)}\, w_P^{(c+1)}\big]\, \mathrm{d}t \\
&= -\int_{-\delta}^{\delta} P_k^{(c,c)}\, \big[P_j^{(c+1,c+1)}\, w_P^{(c+1)} + t\, P_j^{(c+1,c+1)\,\prime}\, w_P^{(c+1)} - 2c\, t^2\, P_j^{(c+1,c+1)}\, w_P^{(c)}\big]\, \mathrm{d}t \\
&= -\, \omega_P^{(c)}\, \Big\langle P_k^{(c,c)},\ P_j^{(c+1,c+1)}\, w_P^{(1)} + t\, P_j^{(c+1,c+1)\,\prime}\, w_P^{(1)} - 2c\, t^2\, P_j^{(c+1,c+1)} \Big\rangle_{w_P^{(c)}}
\end{aligned}$$

which is zero for $j < k-2$ by orthogonality. Thus, (3.13) is zero for $j \notin \{k-2, k\}$.

Now, using (3.10), integration-by-parts, and noting that the weight $w_R^{(a,b,2c)}$ is a polynomial degree $a+b+2c$ and vanishes at the limits of the integral for positive parameters a, b, c, we have that

$$
\begin{aligned}
&\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)\,\prime}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j+1}\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \\
&= \int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)\,\prime}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, w_R^{(a+1,b+1,2c+k+j+3)}\, \mathrm{d}x \\
&= -\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)}\, \frac{\mathrm{d}}{\mathrm{d}x}\Big[R_{m-j}^{(a+1,b+1,2c+2j+3)}\, w_R^{(a+1,b+1,2c+k+j+3)}\Big]\, \mathrm{d}x \\
&= -\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)}\, \Big\{R_{m-j}^{(a+1,b+1,2c+2j+3)\,\prime}\, w_R^{(a+1,b+1,2c+k+j+3)} \\
&\qquad\qquad + (2c+k+j+3)\, \rho\, \rho'\, w_R^{(a+1,b+1,2c+k+j+1)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)} \\
&\qquad\qquad + (b+1)\, w_R^{(a+1,b,2c+k+j+3)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)} \\
&\qquad\qquad - (a+1)\, w_R^{(a,b+1,2c+k+j+3)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\Big\}\, \mathrm{d}x \\
&= -\,\omega_R^{(a,b,2c+2k+1)}\, \Big\{ \Big\langle R_{n-k}^{(a,b,2c+2k+1)},\ w_R^{(1,1,j-k+2)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)\,\prime} \Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad + (2c+k+j+3)\, \Big\langle R_{n-k}^{(a,b,2c+2k+1)},\ \rho\, \rho'\, w_R^{(1,1,j-k)} R_{m-j}^{(a+1,b+1,2c+2j+3)} \Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad + (b+1)\, \Big\langle R_{n-k}^{(a,b,2c+2k+1)},\ w_R^{(1,0,j-k+2)} R_{m-j}^{(a+1,b+1,2c+2j+3)} \Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad - (a+1)\, \Big\langle R_{n-k}^{(a,b,2c+2k+1)},\ w_R^{(0,1,j-k+2)} R_{m-j}^{(a+1,b+1,2c+2j+3)} \Big\rangle_{w_R^{(a,b,2c+2k+1)}} \Big\}.
\end{aligned}
\tag{3.14}
$$

By recalling (3.12) and noting that $j-k$ is even by the earlier argument, we can see $\rho\,\rho'\, w_R^{(1,1,j-k)}$, $w_R^{(1,0,j-k+2)}$ and $w_R^{(1,0,j-k+2)}$ are all polynomials, and further that

$$
\deg(\rho\,\rho'\, w_R^{(1,1,j-k)}) = \deg(w_R^{(1,0,j-k+2)}) = \deg(w_R^{(0,1,j-k+2)}) = 3 + j - k.
$$

Hence, by orthogonality, each term in (3.14) is is zero for $m - j + 3 + j - k <$

$n-k \iff m < n-3.$

Finally,

$$\begin{aligned}
&\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j}\, \rho'\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \\
&= \omega_R^{(a,b,2c+2k+1)}\, \left\langle R_{n-k}^{(a,b,2c+2k+1)},\ \rho\, \rho'\, w_R^{(1,1,j-k)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)} \right\rangle_{w_R^{(a,b,2c+2k+1)}}
\end{aligned}$$

which is also zero for $m < n-3$. Thus

$$\left\langle \frac{\partial}{\partial x} H_{n,k}^{(a,b,c)}, H_{m,j}^{(a+1,b+1,c+1)} \right\rangle_{W^{(a+1,b+1,c+1)}} = 0 \quad \text{for} \quad m < n-3,\ j \notin \{k-2, k\},$$

showing that the only possible non-zero coefficients $c_{m,j}^x$ are when $m = n-3, n-2, n-1$ and $j = k-2, k$ $(j \leq m)$.

We can gain the non-zero entries of the weighted differential operators similarly, by noting that for the disk-slice

$$\frac{\partial}{\partial x} W^{(a,b,c)}(x,y) = -aW^{(a-1,b,c)}(x,y) + bW^{(a,b,c)}(x,y) + 2c\rho(x)\, \rho'(x)\, W^{(a,b,c-1)} \tag{3.15}$$

$$\frac{\partial}{\partial y} W^{(a,b,c)}(x,y) = -2c\, y\, W^{(a,b,c-1)}(x,y) \tag{3.16}$$

and also that

$$\left\langle W^{(a,b,c)} H_{n,k}^{(a,b,c)}, W^{(\tilde{a},\tilde{b},\tilde{c})} H_{m,j}^{(\tilde{a},\tilde{b},\tilde{c})} \right\rangle_{W^{(-\tilde{a},-\tilde{b},-\tilde{c})}} = \left\langle H_{n,k}^{(a,b)}, H_{m,j}^{(\tilde{a},\tilde{b})} \right\rangle_{W^{(a,b,c)}}.$$

□

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

Definition 8. *Define the operator matrices*

$$T^{(a,b,c)\to(a+1,b+1,c)}, \quad T^{(a,b,c)\to(a,b,c+1)} \quad \textit{and} \quad T^{(a,b,c)\to(a+1,b+1,c+1)}$$

for conversion between non-weighted spaces, and

$$T_W^{(a,b,c)\to(a-1,b-1,c)}, \quad T_W^{(a,b,c)\to(a,b,c-1)} \quad \textit{and} \quad T_W^{(a,b,c)\to(a-1,b-1,c-1)}$$

for conversion between weighted spaces, according to:

$$\begin{aligned}
\mathbb{H}^{(a,b,c)}(x,y) &= \left(T^{(a,b,c)\to(a+1,b+1,c)}\right)^\top \mathbb{H}^{(a+1,b+1,c)}(x,y) \\
\mathbb{H}^{(a,b,c)}(x,y) &= \left(T^{(a,b,c)\to(a,b,c+1)}\right)^\top \mathbb{H}^{(a,b,c+1)}(x,y) \\
\mathbb{H}^{(a,b,c)}(x,y) &= \left(T^{(a,b,c)\to(a+1,b+1,c+1)}\right)^\top \mathbb{H}^{(a+1,b+1,c+1)}(x,y) \\
\mathbb{W}^{(a,b,c)}(x,y) &= \left(T_W^{(a,b,c)\to(a-1,b-1,c)}\right)^\top \mathbb{W}^{(a-1,b-1,c)}(x,y) \\
\mathbb{W}^{(a,b,c)}(x,y) &= \left(T_W^{(a,b,c)\to(a,b,c-1)}\right)^\top \mathbb{W}^{(a,b,c-1)}(x,y) \\
\mathbb{W}^{(a,b,c)}(x,y) &= \left(T_W^{(a,b,c)\to(a-1,b-1,c-1)}\right)^\top \mathbb{W}^{(a-1,b-1,c-1)}(x,y).
\end{aligned}$$

Lemma 6. *The operator matrices in Definition 16 are sparse, with banded-block-banded structure. More specifically:*

- $T^{(a,b,c)\to(a+1,b+1,c)}$ *has block-bandwidth* $(0,2)$, *with diagonal blocks.*

- $T^{(a,b,c)\to(a,b,c+1)}$ *has block-bandwidth* $(0,2)$ *and sub-block-bandwidth* $(0,2)$.

- $T^{(a,b,c)\to(a+1,b+1,c+1)}$ *has block-bandwidth* $(0,4)$ *and sub-block-bandwidth* $(0,2)$.

- $T_W^{(a,b,c)\to(a-1,b-1,c)}$ *has block-bandwidth* $(2,0)$ *with diagonal blocks.*

- $T_W^{(a,b,c)\to(a,b,c-1)}$ *has block-bandwidth* $(2,0)$ *and sub-block-bandwidth* $(2,0)$.

- $T_W^{(a,b,c)\to(a-1,b-1,c-1)}$ *has block-bandwidth* $(4,0)$ *and sub-block-bandwidth* $(2,0)$.

Proof. We proceed with the case for the non-weighted operators $T^{(a,b)\to(a+\tilde{a},b+\tilde{b},c+\tilde{c})}$, where $\tilde{a},\tilde{b},\tilde{c}\in\{0,1\}$. Since $\{H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}\}$ for $m=0,\ldots,n,\ j=0,\ldots,m$ is an orthogonal basis for any degree n polynomial, we can expand $H_{n,k}^{(a,b,c)}=\sum_{m=0}^{n}\sum_{j=0}^{m}c_{m,j}\ H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}$. The coefficients of the expansion are then the entries of the relevant operator matrix. We will show that the only non-zero coefficients are for $m\geq n-\tilde{a}-\tilde{b}-2\tilde{c}$, $j\geq k-2\tilde{c}$ and $0\leq j\leq m$. First, note that

$$c_{m,j}=\left\langle H_{n,k}^{(a,b,c)},H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}\right\rangle_{W^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}}\left\|H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}\right\|_{W^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}}^{-2}.$$

Then, using the change of variable $t = \frac{y}{\rho(x)}$, we have that

$$\begin{aligned}
&\left\langle H_{n,k}^{(a,b,c)}, H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})} \right\rangle_{W^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}} \\
&\quad = \omega_R^{(a+\tilde{a},b+\tilde{b},2c+2\tilde{c})} \left\langle R_{n-k}^{(a,b,2c+2k+1)}, \rho(x)^{k+j+1}\, R_{m-j}^{(a+\tilde{a},b+\tilde{b},2c+2\tilde{c}+2j+1)} \right\rangle_{w_R^{(a+\tilde{a},b+\tilde{b},2c+2\tilde{c})}} \\
&\qquad \cdot\ \omega_P^{(c+\tilde{c})} \left\langle P_k^{(c,c)},\ P_j^{(c+\tilde{c},c+\tilde{c})} \right\rangle_{w_P^{(c+\tilde{c})}} \\
&\quad = \omega_R^{(a,b,2c+2k+1)} \left\langle R_{n-k}^{(a,b,2c+2k+1)}, w_R^{(\tilde{a},\tilde{b},\, 2\tilde{c}+j-k)}\, R_{m-j}^{(a+\tilde{a},b+\tilde{b},2c+2\tilde{c}+2j+1)} \right\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\qquad \cdot\ \omega_P^{(c)} \left\langle P_k^{(c,c)},\ w_P^{(\tilde{c})}\, P_j^{(c+\tilde{c},c+\tilde{c})} \right\rangle_{w_P^{(c)}}.
\end{aligned}$$

Since $w_P^{(\tilde{c})}$ is a polynomial degree $2\tilde{c}$, we have that the above is then zero for $j < k - 2\tilde{c}$. Further, since $w_R^{(\tilde{a},\tilde{b},\, 2\tilde{c}+j-k)}$ is a polynomial of degree $\tilde{a}+\tilde{b}+2\tilde{c}+j-k$, we have that the above is zero for $m - j + \tilde{a} + \tilde{b} + 2\tilde{c} + j - k < n - k \iff m < n - \tilde{a} - \tilde{b} - 2\tilde{c}$.

The sparsity argument for the weighted parameter transformation operators 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 Laplacian Δ, that will take us from coefficients for expansion in the weighted space

$$\mathbb{W}^{(1,1,1)}(x,y) = W^{(1,1,1)}(x,y)\, \mathbb{H}^{(1,1,1)}(x,y)$$

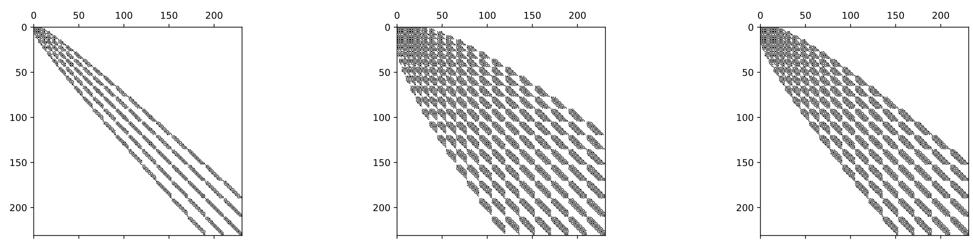


Figure 3.2: "Spy" plots of (differential) operator matrices, showing their sparsity. Left: the Laplace operator $\Delta_W^{(1,1,1)\to(1,1,1)}$. Centre: the weighted variable coefficient Helmholtz operator $\Delta_W^{(1,1,1)\to(1,1,1)} + k^2 T^{(0,0,0)\to(1,1,1)} V(J_x^{(0,0,0)^\top}, J_y^{(0,0,0)^\top}) T_W^{(1,1,1)\to(0,0,0)}$ for $v(x,y) = 1 - (3(x-1)^2 + 5y^2)$ and $k = 200$. Right: the biharmonic operator ${}_2\Delta_W^{(2,2,2)\to(2,2,2)}$.

to coefficients in the non-weighted space $\mathbb{H}^{(1,1,1)}(x,y)$. Note that this construction will ensure the imposition of the Dirichlet zero boundary conditions on Ω. The matrix operator for the Laplacian we denote $\Delta_W^{(1,1,1)\to(1,1,1)}$ acting on the coefficients vector is then given by

$$\Delta_W^{(1,1,1)\to(1,1,1)} := D_x^{(0,0,0)}\, W_x^{(1,1,1)} + T^{(0,0,1)\to(1,1)}\, D_y^{(0,0,0)}\, T_W^{(1,1,0)\to(0,0,0)}\, W_y^{(1,1,1)}.$$

Importantly, this operator will have banded-block-banded structure, and hence will be sparse, as seen in Figure 4.1.

Another important example is the Biharmonic operator Δ^2, where we assume zero Dirichlet and Neumann conditions. To construct this operator, we first note that we can obtain the matrix operator for the Laplacian Δ that will take us from coefficients for expansion in the space $\mathbb{H}^{(0,0,0)}(x,y)$ to coefficients in the space $\mathbb{H}^{(2,2,2)}(x,y)$. We denote this matrix operator that acts on the coefficients vector as $\Delta^{(0,0,0)\to(2,2,2)}$, and is given by

$$\Delta^{(0,0,0)\to(2,2,2)} := D_x^{(1,1,1)}\, D_x^{(0,0,0)} + T^{(1,1,2)\to(2,2,2)}\, D_y^{(1,1,1)}\, T^{(0,0,1)\to(1,1,1)}\, D_y^{(0,0,0)}.$$

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

$$\Delta_W^{(2,2,2)\to(0,0,0)} := W_x^{(1,1,1)}\, W_x^{(2,2,2)} + T_W^{(1,1,0)\to(0,0,0)}\, W_y^{(1,1,1)}\, T_W^{(2,2,1)\to(1,1,1)}\, W_y^{(2,2,2)}.$$

We can then construct a matrix operator for Δ^2 that will take coefficients in the space $\mathbb{W}^{(2,2,2)}$ to coefficients in the space $\mathbb{H}^{(2,2,2)}$. Note that any function expanded in the $\mathbb{W}^{(2,2,2)}$ basis will satisfy both zero Dirichlet and zero Neumann boundary conditions on Ω. The matrix operator for the Biharmonic operator is then given by

$${}_2\Delta_W^{(2,2,2)\to(2,2,2)} = \Delta^{(0,0,0)\to(2,2,2)}\, \Delta_W^{(2,2,2)\to(0,0,0)}.$$

The sparsity and structure of this biharmonic operator are seen in Figure 4.1.

3.3 Computational aspects

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

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

It is possible to obtain the recurrence coefficients for the $\{R_n^{(a,b,c)}\}$ OPs in (3.7), by careful application of the Christoffel–Darboux formula [19, 18.2.12]. We explain the process here for the disk-slice case, however we note that a similar but simpler argument holds for the trapezium case. We thus first need to define a new set of 'interim' 1D OPs.

Definition 9. *Let $w_{\tilde{R}}^{(a,b,c,d)}(x) := (\beta - x)^a \, (x - \alpha)^b \, (1 - x)^c \, (1 + x)^d$ be a weight function on the interval (α, β), and define the associated inner product by:*

$$\langle p,\, q \rangle_{w_{\tilde{R}}^{(a,b,c,d)}} := \frac{1}{\omega_{\tilde{R}}^{(a,b,c,d)}} \int_\alpha^\beta p(x)\, q(x)\, w_{\tilde{R}}^{(a,b,c,d)}(x) \,\mathrm{d}x \tag{3.17}$$

where

$$\omega_{\tilde{R}}^{(a,b,c,d)} := \int_\alpha^\beta w_{\tilde{R}}^{(a,b,c,d)}(x) \,\mathrm{d}x \tag{3.18}$$

Denote the four-parameter family of orthonormal polynomials on $[\alpha, \beta]$ by $\{\tilde{R}_n^{(a,b,c,d)}\}$, orthonormal with respect to the inner product defined in (3.17).

Note that the OPs $\{R_n^{(a,b,2c)}\}$ are then equivalent to the OPs $\{\tilde{R}_n^{(a,b,c,c)}\}$. Let the recurrence coefficients for the OPs $\{\tilde{R}_n^{(a,b,c,d)}\}$ be given by:

$$x\,\tilde{R}_n^{(a,b,c,d)}(x) = \tilde{\beta}_n^{(a,b,c,d)}\,\tilde{R}_{n+1}^{(a,b,c,d)}(x) + \tilde{\alpha}_n^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(x) + \tilde{\beta}_{n-1}^{(a,b,c,d)}\,\tilde{R}_{n-1}^{(a,b,c,d)}(x) \tag{3.19}$$

Proposition 2. *There exist constants $\mathcal{C}_n^{(a,b,c,d)}$, $\mathcal{D}_n^{(a,b,c,d)}$ such that*

$$\tilde{R}_n^{(a,b,c+1,d)}(x) = \mathcal{C}_n^{(a,b,c,d)} \sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(1)\,\tilde{R}_k^{(a,b,c,d)}(x) \tag{3.20}$$

$$\tilde{R}_n^{(a,b,c,d+1)}(x) = \mathcal{D}_n^{(a,b,c,d)} \sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(-1)\,\tilde{R}_k^{(a,b,c,d)}(x) \tag{3.21}$$

Proof. Fix $n, m \in \{0, 1, \dots\}$ and without loss of generality, assume $m \leq n$. First recall that

$$\int_\alpha^\beta \tilde{R}_n^{(a,b,c+1,d)}(x)\,\tilde{R}_m^{(a,b,c+1,d)}(x)\,w_{\tilde{R}}^{(a,b,c+1,d)}(x)\,\mathrm{d}x = \delta_{n,m}\,\omega_{\tilde{R}}^{(a,b,c+1,d)}$$

and define

$$\mathcal{C}_n^{(a,b,c,d)} = \left(\frac{\omega_{\tilde{R}}^{(a,b,c+1,d)}}{\omega_{\tilde{R}}^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(1)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1)\,\tilde{\beta}_n^{(a,b,c,d)}}\right)^{\frac{1}{2}}, \tag{3.22}$$

$$\mathcal{D}_n^{(a,b,c,d)} = (-1)^n \left(\frac{-\omega_{\tilde{R}}^{(a,b,c,d+1)}}{\omega_{\tilde{R}}^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(-1)\,\tilde{R}_{n+1}^{(a,b,c,d)}(-1)\,\tilde{\beta}_n^{(a,b,c,d)}}\right)^{\frac{1}{2}}. \tag{3.23}$$

Now, by the Christoffel–Darboux formula [19, 18.2.12], we have that for any

$x, y \in \mathbb{R}$,

$$\sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(y)\,\tilde{R}_k^{(a,b,c,d)}(x) = \tilde{\beta}_n^{(a,b,c,d)}\,\frac{\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(y) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(y)}{y-x}. \tag{3.24}$$

Then,

$$\begin{aligned}
&\int_\alpha^\beta \Bigl(\bigl[\mathcal{C}_n^{(a,b,c,d)} \sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(1)\,\tilde{R}_k^{(a,b,c,d)}(x)\bigr] \\
&\qquad \cdot \bigl[\mathcal{C}_m^{(a,b,c,d)} \sum_{k=0}^{m} \tilde{R}_k^{(a,b,c,d)}(1)\,\tilde{R}_k^{(a,b,c,d)}(x)\bigr]\, w_{\tilde{R}}^{(a,b,c+1,d)}(x)\Bigr)\,\mathrm{d}x \\
&= \mathcal{C}_n^{(a,b,c,d)}\,\mathcal{C}_m^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c,d)} \\
&\qquad \cdot \sum_{k=0}^{m} \int_\alpha^\beta \Bigl(\tilde{R}_k^{(a,b,c,d)}(1)\,\tilde{R}_k^{(a,b,c,d)}(x) \\
&\qquad\qquad \cdot \bigl[\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(1)\bigr]\, w_{\tilde{R}}^{(a,b,c,d)}(x)\Bigr)\,\mathrm{d}x \\
&= \delta_{m,n}\,\mathcal{C}_n^{(a,b,c,d)^2}\,\tilde{\beta}_n^{(a,b,c,d)}\,\omega_{\tilde{R}}^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(1)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1) \\
&= \delta_{m,n}\,\omega_{\tilde{R}}^{(a,b,c+1,d)}
\end{aligned}$$

using (3.22) and (3.24), showing that the RHS and LHS of (3.20) are equivalent.

Further,

$$
\begin{aligned}
&\int_\alpha^\beta \Big(\big[\mathcal{D}_n^{(a,b,c,d)} \sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(-1)\, \tilde{R}_k^{(a,b,c,d)}(x)\big] \\
&\qquad \cdot \big[\mathcal{D}_m^{(a,b,c,d)} \sum_{k=0}^{m} \tilde{R}_k^{(a,b,c,d)}(-1)\, \tilde{R}_k^{(a,b,c,d)}(x)\big]\, w_{\tilde{R}}^{(a,b,c,d+1)}(x) \Big)\, \mathrm{d}x \\
&= -\mathcal{D}_n^{(a,b,c,d)}\, \mathcal{D}_m^{(a,b,c,d)}\, \tilde{\beta}_n^{(a,b,c,d)} \\
&\qquad \cdot \sum_{k=0}^{m} \int_\alpha^\beta \Big(\tilde{R}_k^{(a,b,c,d)}(-1)\, \tilde{R}_k^{(a,b,c,d)}(x) \\
&\qquad\qquad \cdot \big[\tilde{R}_n^{(a,b,c,d)}(x)\, \tilde{R}_{n+1}^{(a,b,c,d)}(-1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\, \tilde{R}_n^{(a,b,c,d)}(-1)\big]\, w_{\tilde{R}}^{(a,b,c,d)}(x) \Big)\, \mathrm{d}x \\
&= -\delta_{m,n}\, {\mathcal{D}_n^{(a,b,c,d)}}^2\, \tilde{\beta}_n^{(a,b,c,d)}\, \omega_{\tilde{R}}^{(a,b,c,d)}\, \tilde{R}_n^{(a,b,c,d)}(-1)\, \tilde{R}_{n+1}^{(a,b,c,d)}(-1) \\
&= \delta_{m,n}\, \omega_{\tilde{R}}^{(a,b,c,d+1)}
\end{aligned}
$$

using (3.23) and (3.24), showing that the RHS and LHS of (3.21) are also equivalent. □

Proposition 3. *The recurrence coefficients for the OPs* $\{\tilde{R}_n^{(a,b,c+1,d)}\}$ *are given by:*

$$
\tilde{\alpha}_n^{(a,b,c+1,d)} = \frac{\tilde{R}_{n+2}^{(a,b,c,d)}(1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}\, \tilde{\beta}_{n+1}^{(a,b,c,d)} - \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}{\tilde{R}_{n}^{(a,b,c,d)}(1)}\, \tilde{\beta}_{n}^{(a,b,c,d)} + \tilde{\alpha}_{n+1}^{(a,b,c,d)}, \tag{3.25}
$$

$$
\tilde{\beta}_n^{(a,b,c+1,d)} = \frac{\mathcal{C}_n^{(a,b,c,d)}}{\mathcal{C}_{n+1}^{(a,b,c,d)}}\, \frac{\tilde{R}_{n}^{(a,b,c,d)}(1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}\, \tilde{\beta}_{n}^{(a,b,c,d)}. \tag{3.26}
$$

The recurrence coefficients for the OPs $\{\tilde{R}_n^{(a,b,c,d+1)}\}$ *are given by:*

$$\tilde{\alpha}_n^{(a,b,c,d+1)} = \frac{\tilde{R}_{n+2}^{(a,b,c,d)}(-1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_{n+1}^{(a,b,c,d)} - \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}{\tilde{R}_{n}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_{n}^{(a,b,c,d)} + \tilde{\alpha}_{n+1}^{(a,b,c,d)}, \tag{3.27}$$

$$\tilde{\beta}_n^{(a,b,c,d+1)} = \frac{\mathcal{D}_n^{(a,b,c,d)}}{\mathcal{D}_{n+1}^{(a,b,c,d)}}\,\frac{\tilde{R}_{n}^{(a,b,c,d)}(-1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_{n}^{(a,b,c,d)}. \tag{3.28}$$

Proof. First, using (3.20) and (3.24) we have that

$$\begin{aligned}
&(1-x)\,x\,\tilde{R}_n^{(a,b,c+1,d)}(x)\\
&= \mathcal{C}_n^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c,d)}\,x\left[\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(1)\right]\\
&= \mathcal{C}_n^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c,d)}\\
&\qquad\cdot\Bigg[\left(\tilde{\beta}_n^{(a,b,c,d)}\,\tilde{R}_{n+1}^{(a,b,c,d)}(x) + \tilde{\alpha}_n^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(x) + \tilde{\beta}_{n-1}^{(a,b,c,d)}\,\tilde{R}_{n-1}^{(a,b,c,d)}(x)\right)\tilde{R}_{n+1}^{(a,b,c,d)}(1)\\
&\qquad\quad - \left(\tilde{\beta}_{n+1}^{(a,b,c,d)}\,\tilde{R}_{n+2}^{(a,b,c,d)}(x) + \tilde{\alpha}_{n+1}^{(a,b,c,d)}\,\tilde{R}_{n+1}^{(a,b,c,d)}(x) + \tilde{\beta}_n^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(x)\right)\tilde{R}_n^{(a,b,c,d)}(1)\Bigg]
\end{aligned} \tag{3.29}$$

Next, note that the recurrence coefficients for $\tilde{R}_n^{(a,b,c+1,d)}(x)$ satisfy

$$\begin{aligned}
&(1-x)\,x\,\tilde{R}_n^{(a,b,c+1,d)}(x)\\
&= (1-x)\left[\tilde{\beta}_n^{(a,b,c+1,d)}\,\tilde{R}_{n+1}^{(a,b,c+1,d)}(x) + \tilde{\alpha}_n^{(a,b,c+1,d)}\,\tilde{R}_n^{(a,b,c+1,d)}(x) + \tilde{\beta}_{n-1}^{(a,b,c+1,d)}\,\tilde{R}_{n-1}^{(a,b,c+1,d)}(x)\right]\\
&= \mathcal{C}_{n+1}^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c+1,d)}\,\tilde{\beta}_{n+1}^{(a,b,c,d)}\left(\tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_{n+2}^{(a,b,c,d)}(1) - \tilde{R}_{n+2}^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1)\right)\\
&\qquad + \mathcal{C}_n^{(a,b,c,d)}\,\tilde{\alpha}_n^{(a,b,c+1,d)}\,\tilde{\beta}_n^{(a,b,c,d)}\left(\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(1)\right)\\
&\qquad + \mathcal{C}_{n-1}^{(a,b,c,d)}\,\tilde{\beta}_{n-1}^{(a,b,c+1,d)}\,\tilde{\beta}_{n-1}^{(a,b,c,d)}\left(\tilde{R}_{n-1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(1) - \tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n-1}^{(a,b,c,d)}(1)\right)
\end{aligned} \tag{3.30}$$

We can set $\tilde{\beta}_{-1}^{(a,b,c+1,d)} = 0$. By comparing coefficients of $\tilde{R}_{n+2}^{(a,b,c,d)}(x)$ and $\tilde{R}_{n+1}^{(a,b,c,d)}(x)$ in both (3.29) and (3.30) we obtain the desired recurrence coefficients for the OP $\tilde{R}_n^{(a,b,c+1,d)}(x)$. The recurrence coefficients for the OPs $\tilde{R}_n^{(a,b,c,d+1)}(x)$ are found similarly. □

Corollary 2. *The recurrence coefficients for the OPs $\{\tilde{R}_n^{(a,b,c+1,d)}\}$ can be written as:*

$$\tilde{\alpha}_n^{(a,b,c+1,d)} = \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(1)} - \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(1)} + \tilde{\alpha}_n^{(a,b,c,d)}, \tag{3.31}$$

$$\tilde{\beta}_n^{(a,b,c+1,d)} = \left(\frac{1 - \tilde{\alpha}_{n+1}^{(a,b,c,d)} - \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(1)}}{1 - \tilde{\alpha}_n^{(a,b,c,d)} - \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(1)}} \right)^{\frac{1}{2}} \tilde{\beta}_n^{(a,b,c,d)}. \tag{3.32}$$

The recurrence coefficients for the OPs $\{\tilde{R}_n^{(a,b,c,d+1)}\}$ can be written as:

$$\tilde{\alpha}_n^{(a,b,c,d+1)} = \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(-1)} - \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(-1)} + \tilde{\alpha}_n^{(a,b,c,d)}, \tag{3.33}$$

$$\tilde{\beta}_n^{(a,b,c,d+1)} = \left(\frac{-1 + \tilde{\alpha}_{n+1}^{(a,b,c,d)} + \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(-1)}}{-1 + \tilde{\alpha}_n^{(a,b,c,d)} + \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(-1)}} \right)^{\frac{1}{2}} \tilde{\beta}_n^{(a,b,c,d)}. \tag{3.34}$$

where

$$\chi_n^{(a,b,c,d)}(y) := \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(y)}{\tilde{R}_n^{(a,b,c,d)}(y)} \tag{3.35}$$

$$= \frac{1}{\tilde{\beta}_n^{(a,b,c,d)}} \left(y - \tilde{\alpha}_n^{(a,b,c,d)} - \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(y)} \right), \quad y \in \{-1, 1\}. \tag{3.36}$$

These two propositions allow us to recursively obtain the recurrence coefficients for the OPs $\{R_{n-k}^{(a,b,2c+2k+1)}\}$ as k increases to be large.

Remark: The Corollary demonstrates that in order to obtain the recurrence coefficients $\{\alpha_m^{(a,b,2c+2k+1)}\}$, $\{\beta_m^{(a,b,2c+2k+1)}\}$ for some m and k, we require that we obtain the recurrence coefficients $\{\alpha_{m+2}^{(a,b,2c+2(k-1)+1)}\}$, $\{\beta_{m+2}^{(a,b,2c+2(k-1)+1)}\}$. Thus, for large N, this recursive method of obtaining the recurrence coefficients requires a large initialisation (i.e. using the Lanczos algorithm to compute the recurrence coefficients $\{\alpha_n^{(a,b,2c+1)}\}$, $\{\beta_n^{(a,b,2c+1)}\}$ – however, we only need to compute these once, and can store and save this initialisation to disk once computed, for the given values of a, b, c).

3.3.2 Quadrature rule on the disk-slice

In this section we construct a quadrature rule exact for polynomials in the disk-slice Ω that can be used to expand functions in $H_{n,k}^{(a,b,c)}(x, y)$ when Ω is a disk-slice.

Theorem 3. *Denote the Gauss quadrature nodes and weight on $[\alpha, \beta]$ with weight $(\beta - s)^a\ (s - \alpha)^b\ \rho(s)^{2c+1}$ as $(s_k, w_k^{(s)})$, and on $[-1, 1]$ with weight $(1 - t^2)^c$ as*

$(t_k, w_k^{(t)})$. *Define*

$$x_{i+(j-1)N} := s_j, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2} \right\rceil,$$
$$y_{i+(j-1)N} := \rho(s_j)\, t_i, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2} \right\rceil,$$
$$w_{i+(j-1)N} := w_j^{(s)} w_i^{(t)}, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2} \right\rceil.$$

Let $f(x,y)$ *be a polynomial on* Ω. *The quadrature rule is then*

$$\iint_\Omega f(x,y)\, W^{(a,b)}(x,y)\, \mathrm{d}A \approx \frac{1}{2} \sum_{j=1}^{M} w_j \left[f(x_j, y_j) + f(x_j, -y_j) \right],$$

where $M = \left\lceil \frac{1}{2}(N+1) \right\rceil^2$, *and the quadrature rule is exact if* $f(x,y)$ *is a polynomial of degree* $\leq N$.

Proof. We will use the substitution that

$$x = s, \quad y = \rho(s)\, t.$$

First, note that, for $(x,y) \in \Omega$,

$$\begin{aligned} W^{(a,b,c)}(x,y) &= w_R^{(a,b,2c)}(x)\, w_P^{(c)}\left(\frac{y}{\rho(x)}\right) \\ &= w_R^{(a,b,c2)}(s)\, w_P^{(c)}(t) \\ &=: V^{(a,b,c)}(s,t), \quad \text{for } (s,t) \in [\alpha,\beta] \times [-1,1]. \end{aligned}$$

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

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

so that $y \mapsto f_e(x,y)$ for fixed x is an even function, and $y \mapsto f_o(x,y)$ for fixed x is an odd function. Note that if f is a polynomial, then $f_e(s, \rho(s)t)$ is a polynomial in $s \in [\alpha, \beta]$ for fixed t.

Now, we have that

$$\begin{aligned} \iint_\Omega f_e(x,y)\, W^{(a,b,c)}(x,y)\, \mathrm{d}y\, \mathrm{d}x &= \int_\alpha^\beta \int_{-1}^1 f_e\big(s, \rho(s)t\big)\, V^{(a,b,c)}(s,t)\, \rho(s)\, \mathrm{d}t\, \mathrm{d}s \\ &= \int_\alpha^\beta w_R^{(a,b,2c+1)}(s) \, \Big(\int_{-1}^1 f_e\big(s, \rho(s)t\big)\, w_P^{(c)}(t)\, \mathrm{d}t \Big)\, \mathrm{d}s \\ &\approx \int_\alpha^\beta w_R^{(a,b,2c+1)}(s) \sum_{i=1}^{M_2} \Big(w_i^{(t)} f_e\big(s, \rho(s)t_i\big)\Big)\, \mathrm{d}s \quad (\star) \\ &\approx \sum_{j=1}^{M_1} \Bigg(w_j^{(s)} \sum_{i=1}^{M_2} \Big(w_i^{(t)} f_e\big(s_j, \rho(s_j)t_i\big)\Big)\Bigg) \quad (\star\star) \\ &= \sum_{k=1}^{M_1 M_2} w_k\, f_e(x_k, y_k). \end{aligned}$$

Suppose f is a polynomial in x and y of degree N, and hence that f_e is a degree $\leq N$ polynomial. First, note that the degree of the polynomial given by $x \mapsto f_e(x,y)$ for fixed y is $\leq N$ and the degree of the polynomial given by $y \mapsto f_e(x,y)$ for fixed x is $\leq N$. Also note that $s \mapsto f_e\big(s, \rho(s)t\big)$ for fixed t is then a degree N polynomial (since ρ is a degree 1 polynomial). Hence, we achieve equality at $(\star)$

if $2M_2 - 1 \geq N$ and we achieve equality at $(\star\star)$ if also $2M_1 - 1 \geq N$.

Next, note that

$$\begin{aligned}
\iint_\Omega f_o(x,y)\, W^{(a,b,c)}(x,y)\, \mathrm{d}y\, \mathrm{d}x &= \int_\alpha^\beta \int_{-1}^1 f_o\big(s, \rho(s)t\big)\, V^{(a,b,c)}(s,t)\, \rho(s)\, \mathrm{d}t\, \mathrm{d}s \\
&= \int_\alpha^\beta w_R^{(a,b,2c+1)}(s) \left(\int_{-1}^1 f_o\big(s,\rho(s)t\big)\, w_P^{(c)}(t)\, \mathrm{d}t \right) \mathrm{d}s \qquad (\dagger) \\
&= 0
\end{aligned}$$

since the inner integral at $(\dagger)$ over t is zero, due to the symmetry over the domain.

Hence, for a polynomial f in x and y of degree N,

$$\begin{aligned}
\iint_\Omega f(x,y)\, W^{(a,b,c)}(x,y)\, \mathrm{d}y\, \mathrm{d}x &= \iint_\Omega \Big(f_e(x,y) + f_o(x,y)\Big)\, W^{(a,b,c)}(x,y)\, \mathrm{d}y\, \mathrm{d}x \\
&= \iint_\Omega f_e(x,y)\, W^{(a,b,c)}(x,y)\, \mathrm{d}y\, \mathrm{d}x \\
&= \sum_{j=1}^M w_j\, f_e(x_j, y_j),
\end{aligned}$$

where $M = \left\lceil \frac{1}{2}(N+1) \right\rceil^2$. $\square$

3.3.3 Obtaining the coefficients for expansion of a function on the disk-slice

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

$$f(x,y) \approx \sum_{n=0}^{N} \mathbb{H}_n^{(a,b,c)}(x,y)^\top \, \mathbf{f}_n$$

for N sufficiently large, where

$$\mathbb{H}_n^{(a,b,c)}(x,y) := \begin{pmatrix} H_{n,0}^{(a,b,c)}(x,y) \\ \vdots \\ H_{n,n}^{(a,b,c)}(x,y) \end{pmatrix} \in \mathbb{R}^{n+1} \quad \forall n = 0,1,2,\dots,N,$$

and where

$$\mathbf{f}_n := \begin{pmatrix} f_{n,0} \\ \vdots \\ f_{n,n} \end{pmatrix} \in \mathbb{R}^{n+1} \quad \forall n = 0,1,2,\dots,N, \quad f_{n,k} := \frac{\left\langle f,\ H_{n,k}^{(a,b,c)} \right\rangle_{W^{(a,b,c)}}}{\left\| H_{n,k}^{(a,b,c)} \right\|_{W^{(a,b,c)}}}$$

Recall from (3.5) that $\left\| H_{n,k}^{(a,b,c)} \right\|^2_{W^{(a,b,c)}} = \omega_R^{(a,b,2c+2k+1)} \, \omega_P^{(c)}$. Using the quadrature rule detailed in Section 4.2 for the inner product, we can calculate the coefficients $f_{n,k}$ for each $n = 0, \dots, N$, $k = 0, \dots, n$:

$$f_{n,k} = \frac{1}{2\,\omega_R^{(a,b,2c+2k+1)} \, \omega_P^{(c)}} \sum_{j=1}^{M} w_j \left[f(x_j, y_j)\, H_{n,k}^{(a,b,c)}(x_j, y_j) + f(x_j, -y_j)\, H_{n,k}^{(a,b,c)}(x_j, -y_j) \right]$$

where $M = \left\lceil \frac{1}{2}(N+1) \right\rceil^2$.

3.3.4 Calculating non-zero entries of the operator matrices

The proofs of Theorem 4 and Lemma 10 provide a way to calculate the non-zero entries of the operator matrices given in Definition 15 and Definition 16. 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 2D quadrature rule to calculate the 2D inner products, which has a complexity of $\mathcal{O}(N^4)$.

3.4 Examples on the disk-slice 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. We consider Poisson, inhomogeneous variable coefficient Helmholtz equation and the Biharmonic equation, demonstrating the versatility of the approach.

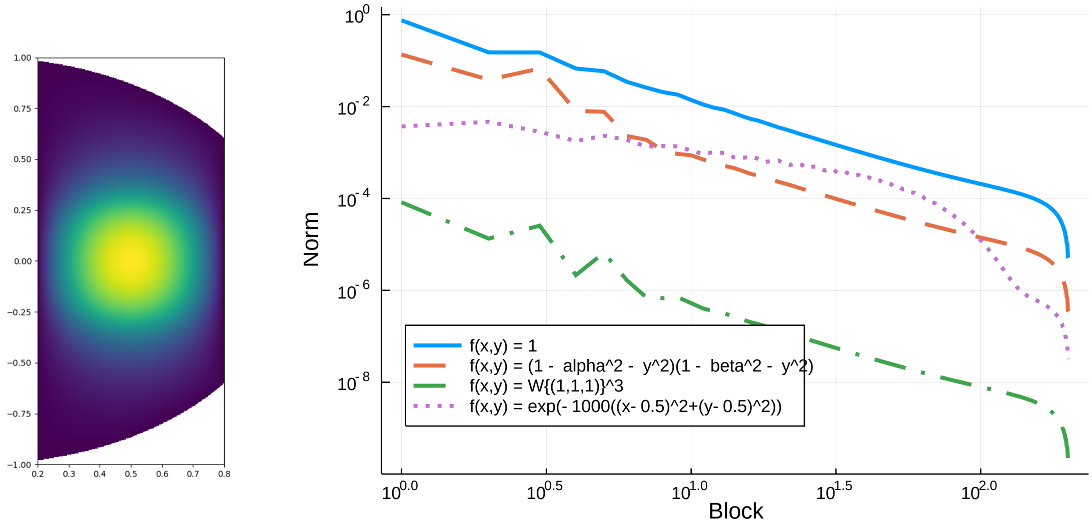


Figure 3.3: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x,y) = 1 + \mathrm{erf}(5(1 - 10((x-0.5)^2 + y^2)))$. Right: The norms of each block of the computed solution of the Poisson equation with the given right hand side functions. This demonstrates algebraic convergence with the rate dictated by the decay at the corners, with spectral convergence observed when the right-hand side vanishes to all orders.

3.4.1 Poisson

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

$$\begin{cases} \Delta u(x,y) = f(x,y) \quad \text{in } \Omega \\ u(x,y) = 0 \quad \text{on } \partial\Omega \end{cases} . \tag{3.37}$$

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 $\mathbb{W}^{(1,1,1)}$ OP basis up to degree N by $\mathbf{u}$, and the coefficient vector for expansion of f in the $\mathbb{H}^{(1,1,1)}$ OP basis up to degree N by $\mathbf{f}$. Since f is known,

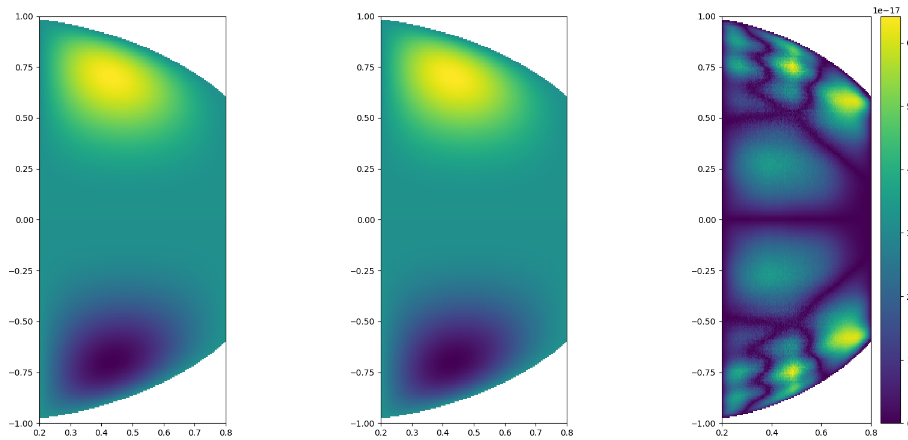


Figure 3.4: The computed solution to $\Delta u = f$ with zero boundary conditions compared with the exact solution $u(x,y) = W^{(1,1,1)}(x,y)y^3 \exp(x)$. Left: Computed. Centre: Exact. Right: Plot of the error (colourbar is shown to demonstrate magnitude of the error is of the order 10^{-17})

we can obtain $\mathbf{f}$ using the quadrature rule above. In matrix-vector notation, our system hence becomes:

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

which can be solved to find $\mathbf{u}$. In Figure 4.2 we see the solution to the Poisson equation with zero boundary conditions given in (4.15) in the disk-slice Ω. In Figure 4.2 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the Poisson equation with $N = 990$, that is, $491,536$ unknowns. 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

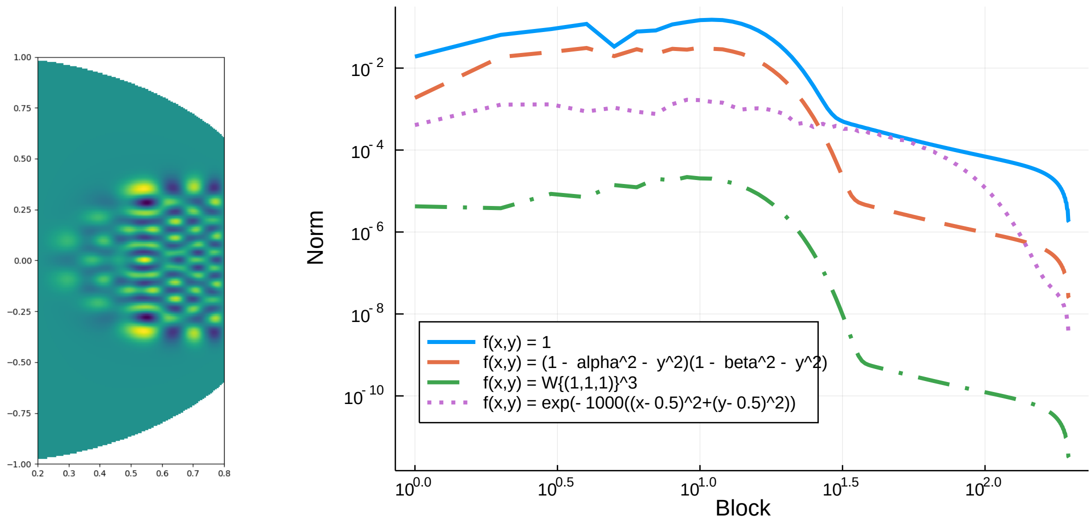


Figure 3.5: Left: The computed solution to $\Delta u + k^2 v u = f$ with zero boundary conditions with $f(x,y) = x(1-x^2-y^2)e^x$, $v(x,y) = 1-(3(x-1)^2+5y^2)$ and $k = 100$. Right: The norms of each block of the computed solution of the Helmholtz equation with the given right hand side functions, with $k = 20$ and $v(x,y) = 1-(3(x-1)^2+5y^2)$.

decay. We see that we achieve algebraic convergence for the first three examples, noting that for right hand-sides that vanish at the corners of our disk-slice ($x \in \{\alpha, \beta\}$, $y = \pm\rho(x)$) we observe faster convergence.

In Figure 3.4 we see an example where the solution calculated to the Poisson equation is shown together with a plot of the exact solution and the error. The example was chosen so that the exact solution was $u(x,y) = W^{(1,1,1)}(x,y)y^3\exp(x)$, and thus the RHS function f would be $f(x,y) = \Delta\left[W^{(1,1,1)}(x,y)y^3\exp(x)\right]$. We see that the computed solution is almost exact.

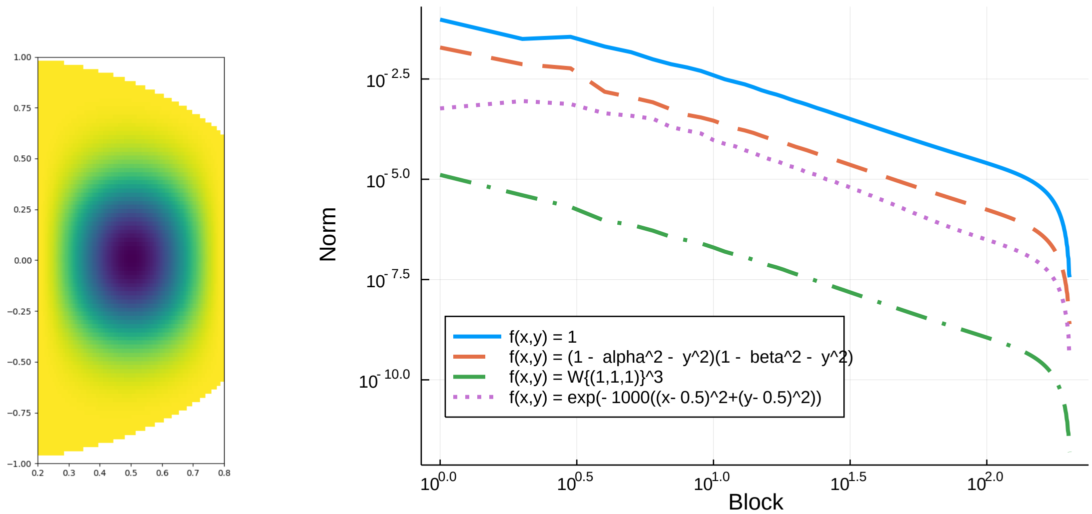


Figure 3.6: Left: The computed solution to $\Delta^2 u = f$ with zero Dirichlet and Neumann boundary conditions with $f(x,y) = 1 + \text{erf}(5(1-10((x-0.5)^2+y^2)))$. Right: The norms of each block of the computed solution of the biharmonic equation with the given right hand side functions.

3.4.2 Inhomogeneous variable-coefficient Helmholtz

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

$$\begin{cases} \Delta u(x,y) + k^2\, v(x,y)\, u(x,y) = f(x,y) & \text{in } \Omega \\ u(x,y) = 0 \quad \text{on } \partial\Omega \end{cases} . \tag{3.38}$$

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 $\mathbb{W}^{(1,1,1)}$ OP basis up to degree N by $\mathbf{u}$, and the coefficient vector for expansion of f in the $\mathbb{H}^{(1,1,1)}$ OP basis up to degree N by $\mathbf{f}$. Since f is known, we can obtain the coefficients $\mathbf{f}$ using the quadrature rule above. We can obtain the matrix operator for the variable-coefficient function $v(x, y)$ by using the Clenshaw algorithm with matrix inputs as the Jacobi matrices $J_x^{(0,0,0)^\top}$, $J_y^{(0,0,0)^\top}$, yielding an operator matrix of the same dimension as the input Jacobi matrices a la the procedure introduced in [22]. We can denote the resulting operator acting on coefficients in the $\mathbb{H}^{(0,0,0)}$ space by $V(J_x^{(0,0,0)^\top}, J_y^{(0,0,0)^\top})$. In matrix-vector notation, our system hence becomes:

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

which can be solved to find $\mathbf{u}$. We can see the sparsity and structure of this matrix system in Figure 4.1 with $v(x, y) = xy^2$ as an example. In Figure 4.3 we see the solution to the inhomogeneous variable-coefficient Helmholtz equation with zero boundary conditions given in (4.16) in the half-disk Ω, with $k = 100$, $v(x, y) = 1-(3(x-1)^2+5y^2)$ and $f(x, y) = x(1-x^2-y^2)e^x$. In Figure 4.3 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 $k = 20$ and $v(x, y) = 1 - (3(x-1)^2 + 5y^2)$ using $N = 500$, that is, $125,751$ unknowns. The rate of decay in the coefficients is a proxy for the rate of convergence of the computed solution. We see that we achieve algebraic convergence for the first three examples, noting that for right hand sides that vanish at the corners of our disk-slice ($x \in \{\alpha, \beta\},\ y = \pm\rho(x)$) we see faster convergence.

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

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

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

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

3.4.3 Biharmonic equation

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

$$\begin{cases} \Delta^2 u(x,y) = f(x,y) \quad \text{in } \Omega \\ u(x,y) = 0, \quad \frac{\partial u}{\partial n}(x,y) = 0 \quad \text{on } \partial\Omega \end{cases} . \tag{3.39}$$

where Δ^2 is the Biharmonic operator, noting the imposition of zero Dirichlet and Neumann boundary conditions on u. In Figure 4.5 we see the solution to the Biharmonic equation (4.17) in the disk-slice Ω. In Figure 4.5 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the biharmonic equation with $N = 500$, that is, $125,751$ unknowns. We see that we achieve algebraic convergence for the first three examples, noting that for right hand sides that vanish at the corners of our disk-slice ($x \in \{\alpha, \beta\}$, $y = \pm\rho(x)$) we see faster convergence.

3.5 Other domains

3.5.1 End-Disk-Slice

The work in this paper on the disk-slice can be easily transferred to the special-case domain of the end-disk-slice, such as half disks, by which we mean

$$\Omega := \{(x, y) \in \mathbb{R}^2 \quad | \quad \alpha < x < \beta,\ \gamma\rho(x) < y < \delta\rho(x)\}$$

with

$$\begin{cases} \alpha & \in (0, 1) \\ \beta & := 1 \\ (\gamma, \delta) & := (-1, 1) \\ \rho(x) & := (1 - x^2)^{\frac{1}{2}}. \end{cases}$$

Our 1D weight functions on the intervals (α, β) and (γ, δ) respectively are then given by:

$$\begin{cases} w_R^{(a,b)}(x) & := (x - \alpha)^a \, \rho(x)^b \\ w_P^{(a)}(x) & := (1 - x^2)^b. \end{cases}$$

Note here how we can remove the need for third parameter, which is why we consider this a special case. This will make some calculations easier, and the operator matrices more sparse. The weight $w_P^{(b)}(x)$ is a still the same ultraspherical weight (and the corresponding OPs are the Jacobi polynomials $\{P_n^{(b,b)}\}$). $w_R^{(a,b)}(x)$ is the (non-classical) weight for the OPs denoted $\{R_n^{(a,b)}\}$. Thus we arrive at the two-parameter family of 2D orthogonal polynomials $\{H_{n,k}^{(a,b)}\}$ on Ω given by, for $0 \le k \le n,\ n = 0, 1, 2, \ldots,$

$$H_{n,k}^{(a,b)}(x,y) := R_{n-k}^{(a,2b+2k+1)}(x)\, \rho(x)^k\, P_k^{(b,b)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega,$$

orthogonal with respect to the weight

$$\begin{aligned} W^{(a,b)}(x,y) &:= w_R^{(a,2b)}(x) w_P^{(b)}\left(\frac{y}{\rho(x)}\right) \\ &= (x-\alpha)^a\, (\rho(x)^2 - y^2)^b \\ &= (x-\alpha)^a\, (1 - x^2 - y^2)^b, \quad (x,y) \in \Omega. \end{aligned}$$

The sparsity of operator matrices for partial differentiation by x, y as well as for parameter transformations generalise to such end-disk-slice domains. For instance, if we inspect the proof of Lemma 4, we see that it can easily generalise to the weights and domain Ω for an end-disk-slice.

In Figure 3.7 we see the solution to the Poisson equation with zero boundary conditions in the half-disk Ω with $(\alpha, \beta) := (0, 1)$.

3.5.2 Trapeziums

We can further extend this work to trapezium shaped domains. Note that for any trapezium there exists an affine map to the canonical trapezium domain that we consider here, given by

$$\Omega := \{(x, y) \in \mathbb{R}^2 \quad | \quad \alpha < x < \beta,\, \gamma\rho(x) < y < \delta\rho(x)\}$$

with

$$\begin{cases} (\alpha, \beta) & := (0, 1) \\ (\gamma, \delta) & := (0, 1) \\ \rho(x) & := 1 - \xi x, \quad \xi \in (0, 1) \\ w_R^{(a,b,c)}(x) & := (\beta - x)^a\,(x - \alpha)^b\,\rho(x)^c = (1 - x)^a\,x^b\,(1 - \xi x)^c \\ w_P^{(a,b)}(x) & := (\delta - x)^a\,(x - \gamma)^b = (1 - x)^a\,x^b. \end{cases}$$

The weight $w_P^{(a,b)}(x)$ is the weight for the shifted Jacobi polynomials on the interval $[0, 1]$, and hence the corresponding OPs are the shifted Jacobi polynomials $\{\tilde{P}_n^{(a,b)}\}$. We note that the shifted Jacobi polynomials relate to the normal Jacobi polynomials by the relationship $\tilde{P}_n^{(a,b)}(x) = P_n^{(a,b)}(2x - 1)$ for any degree $n = 0, 1, 2, \ldots$ and $x \in [0, 1]$. $w_R^{(a,b,c)}(x)$ is the (non-classical) weight for the OPs we dentote $\{R_n^{(a,b,c)}\}$. Thus we arrive at the four-parameter family of 2D orthogonal polynomials $\{H_{n,k}^{(a,b,c,d)}\}$ on Ω given by, for $0 \le k \le n,\ n = 0, 1, 2, \ldots,$

$$H_{n,k}^{(a,b,c,d)}(x,y) := R_{n-k}^{(a,b,c+d+2k+1)}(x)\,\rho(x)^k\,\tilde{P}_k^{(d,c)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega,$$

orthogonal with respect to the weight

$$\begin{aligned} W^{(a,b,c,d)}(x,y) &:= w_R^{(a,b,c+d)}(x)\,w_P^{(d,c)}\left(\frac{y}{\rho(x)}\right) \\ &= (1-x)^a\,x^b\,y^c\,(1-\xi x-y)^d, \quad (x,y) \in \Omega. \end{aligned}$$

In Figure 3.7 we see the solution to the Helmholtz equation with zero boundary conditions in the trapezium Ω with $\xi := \frac{1}{2}$.

3.6 P-finite element methods using sparse operators

It is possible for our framework to be applied to a p-finite element method – that is, one where we can vary the polynomial degree p of the basis functions used in each element (compare this to a normal h-FEM, where we can tune the element size h). For example, one could discretise the disk into disk-slice elements, and apply a p-finite element method to solve PDEs on the disk. As a precursor to this, in this section we limit our discretisation to a single element. Specifically, we follow the method of [3] to construct a sparse p-finite element method in terms of the operators constructed above, with the benefit of ensuring that the

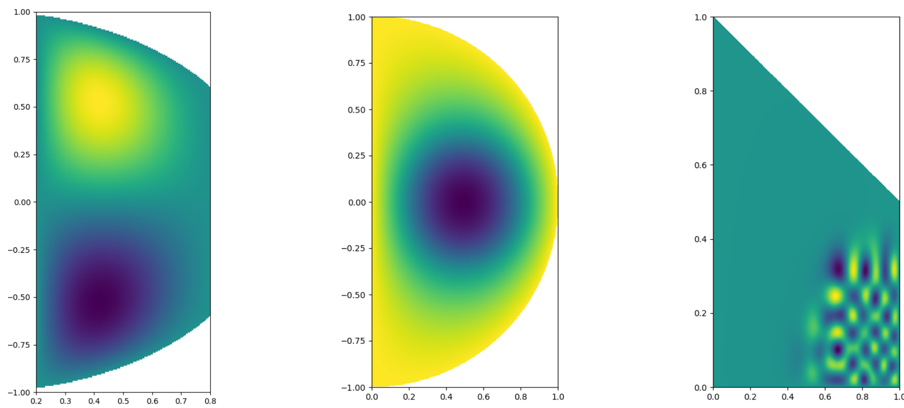


Figure 3.7: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y) = W^{(1,1,1)}(x, y)y \cos(x)$ in the disk-slice using the p-FEM approach with a single element. Centre: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y) = 1 + \text{erf}(5(1 - 10((x - 0.5)^2 + y^2)))$ in the half-disk. Right: The computed solution to $\Delta u + k^2\, v\, u = f$ with zero boundary conditions with $f(x, y) = (1 - x)\, x\, y\, (1 - \frac{1}{2}x - y)\, e^x$, $v(x, y) = 1 - (3(x - 1)^2 + 5y^2)$ and $k = 100.$ in the trapezium.

resulting discretisation is symmetric. Consider the 2D Dirichlet problem on a domain Ω:

$$\begin{cases} -\Delta u(x, y) = f(x, y) \quad \text{in } \Omega \\ u = 0 \quad \text{on } \partial\Omega \end{cases}$$

This has the weak formulation for any test function $v \in V := H_0^1(\Omega) = \{v \in H^1(\Omega) \quad | \quad v|_{\partial\Omega} = 0\}$,

$$L(v) := \int_\Omega f\, v\, d\mathbf{x} = \int_\Omega \nabla u \cdot \nabla v\, d\mathbf{x} =: a(u, v).$$

As eluded to, in general we would let $\mathcal{T}$ be the set of elements τ that make up our finite element discretisation of the domain, where each τ is a trapezium or disk slice for example. However, here we simply consider our domain to be a disk-slice and our discretisation to be a single element – that is we let $\tau = \Omega$ for a disk-slice 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.

$$L(v_p) = a(u_p, v_p) \quad \forall\, v_p \in V_p. \tag{3.40}$$

Recall that the OPs $\mathbb{H}^{(a,b,c)}$ are orthogonal with respect to the weight $W^{(a,b,c)}$ on Ω, and define the matrix $\Lambda^{(a,b,c)} := \left\langle \mathbb{H}^{(a,b,c)},\, \mathbb{H}^{(a,b,c)\top} \right\rangle_{W^{(a,b,c)}}$. Note that due to orthogonality this is a diagonal matrix. We can choose a basis for V_p by using the weighted orthogonal polynomials on τ with parameters $a = b = 1$:

$$\mathbb{W}^{(1,1,1)}(x,y) := \begin{pmatrix} \mathbb{W}^{(1,1,1)}{}_0(x,y) \\ \mathbb{W}^{(1,1,1)}{}_1(x,y) \\ \mathbb{W}^{(1,1,1)}{}_2(x,y) \\ \vdots \\ \mathbb{W}^{(1,1,1)}{}_p(x,y) \end{pmatrix},$$

$$\mathbb{W}^{(1,1,1)}{}_n(x,y) := W^{(1,1,1)}(x,y) \begin{pmatrix} H^{(1,1,1)}_{n,0}(x,y) \\ \vdots \\ H^{(1,1,1)}_{n,n}(x,y) \end{pmatrix} \in \mathbb{R}^{n+1} \quad \forall n = 0, 1, 2, \ldots, p,$$

and rewrite (4.18) in matrix form:

$$\begin{aligned}
a(u_p, v_p) &= \int_\tau \nabla u_p \cdot \nabla v_p \, \mathrm{d}\mathbf{x} \\
&= \int_\tau \begin{pmatrix} \partial_x v_p \\ \partial_y v_p \end{pmatrix}^\top \begin{pmatrix} \partial_x u_p \\ \partial_y u_p \end{pmatrix} \, \mathrm{d}\mathbf{x} \\
&= \int_\tau \begin{pmatrix} \mathbb{H}^{(0,0,0)^\top} W_x^{(1,1,1)} \mathbf{v} \\ \mathbb{H}^{(0,0,0)^\top} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \mathbf{v} \end{pmatrix}^\top \begin{pmatrix} \mathbb{H}^{(0,0,0)^\top} W_x^{(1,1,1)} \mathbf{u} \\ \mathbb{H}^{(0,0,0)^\top} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \mathbf{u} \end{pmatrix} \mathrm{d}\mathbf{x} \\
&= \int_\tau \Big(\mathbf{v}^\top W_x^{(1,1,1)^\top} \mathbb{H}^{(0,0,0)} \mathbb{H}^{(0,0,0)^\top} W_x^{(1,1,1)} \mathbf{u} \\
&\qquad + \mathbf{v}^\top (T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)})^\top \mathbb{H}^{(0,0,0)} \mathbb{H}^{(0,0,0)^\top} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \mathbf{u} \Big) \, \mathrm{d}\mathbf{x} \\
&= \mathbf{v}^\top \Big(W_x^{(1,1,1)^\top} \Lambda^{(0,0,0)} W_x^{(1,1,1)} \\
&\qquad + (T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)})^\top \Lambda^{(0,0,0)} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \Big) \, \mathbf{u}
\end{aligned}$$

where $\mathbf{u}, \mathbf{v}$ are 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), and

$$\begin{aligned}
L(v_p) &= \int_\tau v_p \, f \, \mathrm{d}\mathbf{x} \\
&= \int_\tau \mathbf{v}^\top \, \mathbb{W}^{(1,1,1)} \, \mathbb{H}^{(1,1,1)^\top} \, \mathbf{f} \, \mathrm{d}\mathbf{x} \\
&= \mathbf{v}^\top \, \left\langle \mathbb{H}^{(1,1,1)}, \mathbb{H}^{(1,1,1)^\top} \right\rangle_{W^{(1,1,1)}} \, \mathrm{d}\mathbf{x} \\
&= \mathbf{v}^\top \Lambda^{(1,1,1)} \, \mathbf{f},
\end{aligned}$$

where $\mathbf{f}$ is the coefficient vector for the expansion of the function $f(x, y)$ in the $\mathbb{H}^{(1,1,1)}$ OP basis.

Since (4.18) is equivalent to stating that

$$L(W^{(1,1,1)}H^{(1,1,1)}_{n,k}) = a(u_p, W^{(1,1,1)}H^{(1,1,1)}_{n,k}) \quad \forall\, n = 0,\ldots,p,\ k = 0,\ldots,n,$$

(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

$$A = {W_x^{(1,1,1)}}^\top \Lambda^{(0,0,0)} W_x^{(1,1,1)} + (T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)})^\top \Lambda^{(0,0,0)} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)}$$

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

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

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).

Chapter 4

Spherical Caps

While the work in the previous chapter looked at developing a sparse spectral method inside a two dimensional domain, we move on to investigating the realm of a surface in three dimensional space. Specifically, we look to extend the methodology to a hierarchy of non-classical multivariate orthogonal polynomials on spherical caps, which we will formally define. 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.

4.1 Introduction

Our aim in this chapter is to develop sparse spectral methods for solving linear partial differential equations on certain subsets of the sphere – specifically spherical caps. More precisely, we consider the solution of partial differential equations on the domain Ω given by

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

where $\alpha \in (-1, 1)$ and $\beta := 1$. 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.

Remark: For simplicity we focus on the case of a spherical cap, though there is an extension to a spherical band by taking $\beta \in (\alpha, 1)$. The methods presented here translate to the spherical band case by including the necessary adjustments to the weights and recurrence relations we present in this paper. These adjustments make the mathematics more involved, which is why they are omitted here, but the approach is the same.

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 orthogonal polynomials, whose construction was considered in [23]. 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. Further, we remove the singular nature as α approaches 0 that such a projection would give, since our new approach is applicable for all $\alpha \in (-1, 1)$. 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 $(x, y, z) \in \partial\, \Omega$ when $a > 0$. The corresponding OPs denoted $Q^{(a)}_{n,k,i}(x, y, z)$, where n denotes the polynomial degree, $0 \leq k \leq n$ and $i \in \{0, \min(1, k)\}$. We define these to be orthogonalised lexicographically, that is,

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

where $C_{n,k,i} \neq 0$ and “lower order terms” includes degree n polynomials of the form $x^{j-i}\, y^i\, z^{n-j}$ where $j < k$. The precise normalization arises from their definition in terms of one-dimensional OPs in Definition 11.

We consider partial differential operators involving the spherical Laplacian (the

Laplace–Beltrami operator): in spherical coordinates

$$z = \cos\varphi,$$
$$x = \sin\varphi\cos\theta = \rho(z)\cos\theta,$$
$$y = \sin\varphi\sin\theta = \rho(z)\sin\theta.$$

where $\rho(z) := \sqrt{1-z^2}$, we have

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

i.e. $\Delta_{\mathrm{S}} f(\mathbf{x}) = \Delta f(\frac{\mathbf{x}}{\|\mathbf{x}\|})$ for $\mathbf{x} := (x, y, z) \in \mathbb{R}^3$. 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 4. 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 [20], triangles [22] and disk-slices and trapeziums [26], and the related work on sparse discretisations on disks [31] and spheres [**?** **?**]. As in the disk-slice case in 2D [26], 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 [16, §5]) 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 [26]. 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.

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 axis (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 $O(p^2)$, which is demonstrated in Figure 4.4 with $v(x, y, z) = \cos z$.

4.2 Orthogonal polynomials on spherical caps

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

4.2.1 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 [23], we write here as orthogonal polynomials in x and y:

Definition 10. *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* $k = 0, 1, \dots,\ i = 0, 1$ *on* $(x, y) \in \omega$ *by*

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

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*

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

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

Proposition 4 ([23])**.** *Let* $w : (\alpha, \beta) \to \mathbb{R}$ *be a weight function. For* $n = 0, 1, 2, \dots$, *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

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

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

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

on Ω*, where* $\mathrm{d}A = \sin\varphi\, \mathrm{d}\theta\, \mathrm{d}\varphi$ *is the uniform spherical measure on* Ω*.*

For the spherical cap, we can use Proposition 4 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 11 ([26])**.** *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:

$$\langle p,\ q\rangle_{w_R^{(a,b)}} := \frac{1}{\omega_R^{(a,b)}} \int_\alpha^1 p(x)\, q(x)\, w_R^{(a,b)}(x)\, \mathrm{d}x \tag{4.1}$$

where

$$\omega_R^{(a,b)} := \int_\alpha^1 w_R^{(a,b)}(x)\, \mathrm{d}x \tag{4.2}$$

is a normalising constant. Denote the two-parameter family of orthonormal poly-

nomials on $[\alpha, \beta]$ *by* $\{R_n^{(a,b)}\}$*, orthonormal with respect to the inner product defined in (4.1).*

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

Definition 12. *Define the one-parameter 3D orthogonal polynomials via:*

$$Q_{n,k,i}^{(a)}(x, y, z) := R_{n-k}^{(a,2k)}(z)\, \rho(z)^k\, Y_{k,i}\left(\frac{x}{\rho(z)}, \frac{y}{\rho(z)}\right), \quad (x, y, z) \in \Omega. \tag{4.3}$$

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

$$\begin{aligned}\langle p,\ q\rangle_{Q^{(a)}} &:= \int_\Omega p(\mathbf{x}, z)\, q(\mathbf{x}, z)\, w_R^{(a,0)}(z)\, \mathrm{d}A \\ &= \int_\alpha^1 \int_0^{2\pi} p(\rho(z)\cos\theta, \rho(z)\sin\theta, z)\, q(\rho(z)\cos\theta, \rho(z)\sin\theta, z)\, \mathrm{d}\theta\, w_R^{(a,0)}(z)\, \mathrm{d}z,\end{aligned}$$

with

$$\left\| Q_{n,k,i}^{(a)} \right\|_{Q^{(a)}}^2 := \left\langle Q_{n,k,i}^{(a)},\ Q_{n,k,i}^{(a)} \right\rangle_{Q^{(a)}} = \pi\, \omega_R^{(a,2k)}. \tag{4.4}$$

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 [26], 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 [16, §5]).

4.2.2 Jacobi matrices

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

$$xR_n^{(a,b)}(x) = \beta_n^{(a,b)} R_{n+1}^{(a,b)}(x) + \alpha_n^{(a,b)} R_n^{(a,b)}(x) + \beta_{n-1}^{(a,b)} R_{n-1}^{(a,b)}(x) \tag{4.5}$$

where the coefficients are calculatable (see [26]). We can use (4.5) to determine the 3D recurrences for $Q_{n,k,i}^{(a)}(x, y, z)$. Importantly, we can deduce sparsity in the recurrence relationships. We first require the following lemma.

Lemma 7. *The following identities hold for $k = 2, 3, \ldots,$ $j = 0, 1, \ldots$ and $i, h \in \{0, 1\}$:*

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) $\displaystyle\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \sin\theta\, \mathrm{d}\theta = \frac{1}{2}\, \pi\, \delta_{|i-1|,h}\, ((-1)^{i+1}\, \delta_{k-1,j} + (-1)^i\, \delta_{k+1,j}).$

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

$$2\cos k\theta\cos\theta = \cos(k-1)\theta + \cos(k+1)\theta$$

$$2\sin k\theta\cos\theta = \sin(k-1)\theta + \sin(k+1)\theta$$

$$2\cos k\theta\sin\theta = -\sin(k-1)\theta + \sin(k+1)\theta$$

$$2\sin k\theta\sin\theta = \cos(k-1)\theta - \cos(k+1)\theta.$$

$\square$

Lemma 8. *Define*

$$\eta_k := \begin{cases} 0 & \textit{if } k < 0 \\ Y_0 & \textit{if } k = 0 \\ \frac{1}{2} & \textit{otherwise} \end{cases} \tag{4.6}$$

$Q^{(a)}_{n,k,i}(x,y,z)$ *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*

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

Remark: For z multiplication, note that different Fourier modes do not interact. This is because z is rotationally invariant.

Proof. The 3-term recurrence for multiplication by z follows from (4.5). For the recurrence for multiplication by x, since $\{Q^{(a)}_{m,j,h}\}$ for $m = 0, \ldots, n+1$, $j = 0, \ldots, m$, $h = 0, 1$ 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 (4.4) 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 $(\cos\theta \sin\varphi, \sin\theta \sin\varphi, \cos\varphi) = (x, y, z)$:

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

where $\delta_{k,j}$ is the standard Kronecker delta function, using Lemma 7. 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:

$$
\begin{aligned}
&\left\langle y\, Q^{(a)}_{n,k,i}, Q^{(a)}_{m,j,h} \right\rangle_{Q^{(a)}} \\
&= \int_\Omega Q^{(a)}_{n,k,i}(\mathbf{x}, z)\, Q^{(a)}_{m,j,h}(\mathbf{x}, z)\, y\, w_R^{(a,0)}(z)\, \mathrm{d}A \\
&= \Big(\int_\alpha^1 R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, \rho(z)^{k+j+1}\, w_R^{(a,0)}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \sin\theta\, \mathrm{d}\theta \Big) \\
&= \Big(\int_\alpha^1 R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w_R^{(a,k+j+1)}(z)\, \mathrm{d}z \Big) \cdot \Big(\int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\, \sin\theta\, \mathrm{d}\theta \Big) \\
&= \frac{1}{2}\, \pi\, \delta_{|i-1|,h} \left[(-1)^{i+1}\, \eta_{k-1}\, \delta_{k-1,j} + (-1)^i\, \eta_k\, \delta_{k+1,j} \right] \int_\alpha^1 R^{(a,2k)}_{n-k}(z)\, R^{(a,2j)}_{m-j}(z)\, w_R^{(a,k+j+1)}(z)\, \mathrm{d}z.
\end{aligned}
$$

where again $\delta_{k,j}$ is the standard Kronecker delta function, and we have used Lemma 7.

□

The recurrences in Lemma 8 lead to Jacobi operators that correspond to multiplication by x, y and z. In later sections we will use an ordering of the OPs so that they are grouped by Fourier mode k, which is convenient for the application of differential and other operators to the vector of coefficients of a given function's expansion (some operators will exploit this ordering for operators where Fourier modes do not interact, and thus will be block-diagonal). Before that though, the ordering we will use in the remainder of this section is convenient for establishing Jacobi operators for multiplication by x, y and z, and hence building the OPs and importantly obtaining the associated *recurrence coefficient matrices* necessary for efficient function evaluation using the Clenshaw algorithm. In practice, it is simply a matter of converting coefficients between the two orderings. To this end, we define our OP-building ordering as follows. 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

$$\begin{aligned} \tilde{J}_x^{(a)} \, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= x \, \tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ \tilde{J}_y^{(a)} \, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= y \, \tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ \tilde{J}_z^{(a)} \, \tilde{\mathbb{Q}}^{(a)}(x,y,z) &= z \, \tilde{\mathbb{Q}}^{(a)}(x,y,z). \end{aligned} \tag{4.7}$$

where

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

Note that $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ are *banded-block-banded matrices*:

Definition 13. *A block matrix A with blocks $A_{i,j}$ has block-bandwidths (L, U) if $A_{i,j} = 0$ for $-L \leq j - i \leq U$, 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.*

Each of these Jacobi 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 for $k = 1, \dots, N$, $n = k, \dots, N$

$$
\begin{aligned}
A^{(a)}_{n,k,j} &:= \begin{pmatrix} \alpha^{(a)}_{n,k,j} & 0 \\ 0 & \alpha^{(a)}_{n,k,j} \end{pmatrix} \in \mathbb{R}^{2\times 2}, (k \neq 1 \text{ for } j \text{ odd}) \\
A^{(a)}_{n,0,j} &:= \begin{pmatrix} \alpha^{(a)}_{n,0,j} & 0 \end{pmatrix} \in \mathbb{R}^{1\times 2}, j \text{ even} \\
A^{(a)}_{n,1,j} &:= \begin{pmatrix} \alpha^{(a)}_{n,1,j} \\ 0 \end{pmatrix} \in \mathbb{R}^{2\times 1}, j \text{ odd.}
\end{aligned}
$$

For $\tilde{J}^{(a)}_y$, the sub-blocks have sub-block-bandwidths $(3,3)$:

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

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

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

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

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

$$B^{(a)}_{n,0,j} := \begin{pmatrix} 0 & \beta^{(a)}_{n,0,0,j} \end{pmatrix} \in \mathbb{R}^{1\times 2}, j \text{ even}$$

$$B^{(a)}_{n,1,j} := \begin{pmatrix} 0 \\ \beta^{(a)}_{n,1,1,j} \end{pmatrix} \in \mathbb{R}^{2\times 1}, j \text{ odd.}$$

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

$$\Gamma^{(a)}_{n,k,j} := \begin{pmatrix} \gamma_{n,k,j} & 0 \\ 0 & \gamma_{n,k,j} \end{pmatrix} \in \mathbb{R}^{2\times 2}, \tag{4.8}$$

$$\Gamma^{(a)}_{n,0,j} := \gamma^{(a)}_{n,0,j}. \tag{4.9}$$

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.

4.2.3 Building the OPs

Following the triangle case [22], we can combine each system in (4.7) into a block-tridiagonal system, for any $(x, y, z) \in \Omega$:

$$\begin{pmatrix} 1 & & & \\ B_0 - G_0(x,y,z) & A_0 & & \\ C_1 & B_1 - G_1(x,y,z) & A_1 & \\ & C_2 & B_2 - G_2(x,y,z) & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tilde{\mathbb{Q}}^{(a)}(x,y,z) = \begin{pmatrix} Q_0^{(a)} \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

where we note $Q_0^{(a)} := Q_{0,0,0}^{(a)}(x,y,z) \equiv R_0^{(a,0)}\, Y_0$, and for each $n = 0, 1, 2\ldots$,

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

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

For each $n = 0, 1, 2\ldots$ 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 [9, p78], which can be expanded to obtain the recurrence:

$$\begin{cases} \tilde{\mathbb{Q}}_{-1}^{(a)}(x,y,z) := 0 \\ \tilde{\mathbb{Q}}_0^{(a)}(x,y) := Q_0^{(a)} \\ \tilde{\mathbb{Q}}_{n+1}^{(a)}(x,y) = -D_n^\top(B_n - G_n(x,y,z))\tilde{\mathbb{Q}}_n^{(a)}(x,y,z) - D_n^\top C_n\, \tilde{\mathbb{Q}}_{n-1}^{(a)}(x,y,z), \quad n = 0, 1, 2, \ldots. \end{cases}$$

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

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

for $n = 1, 2, \dots$ where again $\Gamma^{(a)}_{n,k,3}$ are defined in equations (4.8, 4.9) for $k = 0, \dots, n$, and where $\boldsymbol{\eta}_0, \boldsymbol{\eta}_1 \in \mathbb{R}^{3(2n+1)}$ with entries given by

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

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

For $n = 0$, we can simply take

$$D_0^\top := \begin{pmatrix} 0 & 0 & \frac{1}{\gamma^{(a)}_{0,0,3}} \\ \frac{1}{\alpha^{(a)}_{0,0,6}} & 0 & 0 \\ 0 & \frac{1}{\beta^{(a)}_{0,0,6}} & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3}.$$

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.

Definition 14. *The recurrence coefficient matrices associated with the OPs* $\{Q_{n,k,i}^{(a)}\}$ *are given by the matrices* $A_n, B_n, C_n, D_n^\top$ *for* $n = 0, 1, 2, \ldots$ *defined above.*

4.3 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, as alluded to in Section 4.2.2, we introduce new notation for a different ordering of the OP vector, in order to exploit the orthogonality the polynomials $Y_{k,i}$ will bring and thus ensure the operators will be block-diagonal. Let $N \in \mathbb{N}$ and define:

$$\mathbb{Q}^{(a)}_{N,k} := \begin{pmatrix} Q^{(a)}_{k,k,0}(x,y,z) \\ Q^{(a)}_{k,k,1}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,k,0}(x,y,z) \\ Q^{(a)}_{N,k,1}(x,y,z) \end{pmatrix} \in \mathbb{R}^{2(N-k+1)}, \quad k = 1, \ldots, N, \tag{4.10}$$

$$\mathbb{Q}^{(a)}_{N,0} := \begin{pmatrix} Q^{(a)}_{0,0,0}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,0,0}(x,y,z) \end{pmatrix} \in \mathbb{R}^{N+1}, \tag{4.11}$$

$$\mathbb{Q}^{(a)}_{N} := \begin{pmatrix} \mathbb{Q}^{(a)}_{N,0} \\ \vdots \\ \mathbb{Q}^{(a)}_{N,N} \end{pmatrix} \in \mathbb{R}^{(N+1)^2} \tag{4.12}$$

We further denote the weighted set of OPs on Ω by

$$\mathbb{W}^{(a)}_{N}(x,y,z) := w^{(a,0)}_{R}(z)\, \mathbb{Q}^{(a)}_{N}(x,y,z),$$

The operator matrices we derive here act on coefficient vectors, that represent a function $f(x,y,z)$ defined on Ω in spectral space – such a function is approximated by its expansion up to degree N:

$$f(x,y,z) = \mathbb{Q}^{(a)}_{N}(x,y,z)^\top \boldsymbol{f} = \sum_{n=0}^{N} \sum_{k=0}^{n} \sum_{i=0}^{1} f_{n,k,i}\, Q^{(a)}_{n,k,i}(x,y,z),$$

where $\boldsymbol{f} = (f_{n,k,i})$ is the coefficients vector for the function f.

Definition 15. *Let a be a nonnegative parameter, and $\tilde{a} \geq 2$ be a positive integer. Define the operator matrices $D_\varphi^{(a)}$, $W_\varphi^{(a)}$, D_θ, $\mathcal{L}^{(a)\to(a+\tilde{a})}$, $\mathcal{L}_W^{(a)\to(a-\tilde{a})}$, $\Delta_W^{(1)}$ according to:*

$$
\begin{aligned}
\rho \frac{\partial f}{\partial \varphi}(x,y,z) &= \mathbb{Q}_N^{(a+1)}(x,y,z)^\top \, D_\varphi^{(a)} \, \mathbf{f}, \\
\rho \frac{\partial}{\partial \varphi}[w_R^{(a,0)}(z) \, f(x,y,z)] &= \mathbb{W}_N^{(a-1)}(x,y)^\top \, W_\varphi^{(a)} \, \mathbf{f}, \\
\frac{\partial f}{\partial \theta}(x,y,z) &= \mathbb{Q}_N^{(a)}(x,y,z)^\top \, D_\theta \, \mathbf{f}, \\
\Delta_{\mathrm{S}} f(x,y,z) &= \mathbb{Q}_N^{(a+\tilde{a})}(x,y,z)^\top \, \mathcal{L}^{(a)\to(a+\tilde{a})} \, \mathbf{f}, \\
\Delta_{\mathrm{S}}\big(w_R^{(a,0)}(z) \, f(x,y,z)\big) &= \mathbb{W}_N^{(a-\tilde{a})}(x,y,z)^\top \, \mathcal{L}_W^{(a)\to(a-\tilde{a})} \, \mathbf{f}, \qquad \textit{(for } a \geq 2 \textit{ only)} \\
\Delta_{\mathrm{S}}\big(w_R^{(1,0)}(z) \, f(x,y,z)\big) &= \mathbb{Q}_N^{(1)}(x,y,z)^\top \, \Delta_W^{(1)} \, \mathbf{f}, \qquad \textit{(for } a = 1 \textit{ only)}
\end{aligned}
$$

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 [19, (18.9.3)], on the triangle [21], and on the disk-slice [26]. 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 (4.10, 4.11, 4.12) these rotationally invariant operators are block-diagonal, meaning simple and parallelisable practical application.

Theorem 4. *The operator matrices $D_\varphi^{(a)}$, $W_\varphi^{(a)}$, D_θ, $\mathcal{L}^{(a)\to(a+\tilde{a})}$, $\mathcal{L}_W^{(a)\to(a-\tilde{a})}$, $\Delta_W^{(1)}$*

from Definition 15 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* $(1, 1)$
- $\mathcal{L}^{(a)\to(a+\tilde{a})}$ *has block-bandwidths* $(0, 0)$*, and sub-block-bandwidths* $(0, 4)$
- $\mathcal{L}_W^{(a)\to(a-\tilde{a})}$ *has block-bandwidths* $(0, 0)$*, and sub-block-bandwidths* $(4, 0)$
- $\Delta_W^{(1)}$ *has block-bandwidths* $(0, 0)$*, and sub-block-bandwidths* $(2, 2)$

In order to show the last part of Theorem 4, we require the following short lemma.

Lemma 9. *For any general parameter* a *and any* $n = 0, 1, \dots,\ k = 0, \dots, n$ *we have that*

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

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

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

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

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

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

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

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

Proof of Theorem 4. For the operator D_θ for partial differentiation by θ, we simply have that

$$\frac{\partial}{\partial\theta}Q^{(a)}_{n,k,i}(x,y,z) = R^{(a,2k)}_{n-k}(z)\,\rho(z)^k\,\frac{\mathrm{d}}{\mathrm{d}\theta}Y_{k,i}(\theta)$$
$$= \begin{cases} (-1)^{i+1}\,k\,Q^{(a)}_{n,k,|i-1|}(x,y,z) & k>0 \\ 0 & k=0 \end{cases}.$$

We now proceed with the case for the operator $D^{(a)}_{\varphi}$ for partial differentiation by φ. The entries of the operator are given by the coefficients in the expansion

$$\rho\frac{\partial}{\partial\varphi}Q^{(a)}_{n,k,i} = \sum_{m=0}^{n+1}\sum_{j=0}^{m}\sum_{h=0}^{1} c_{m,j,h}\,Q^{(a+1)}_{m,j,h},$$

where the coefficients are

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

Now, note that:

$$\begin{aligned}
w^{(a,b)\,\prime}_{R}(z) &= a\,w^{(a-1,b)}_{R}(z) + c\,\rho(z)\,\rho'(z)\,w^{(a,b-2)}_{R}(z), \\
\rho(z)\,\rho'(z) &= -z \\
\frac{\partial}{\partial\varphi}Q^{(a)}_{n,k,i}(x,y,z) &= -\rho(z)\,\frac{\mathrm{d}}{\mathrm{d}z}\left[\rho(z)^k\,R^{(a,2k)}_{n-k}(z)\right]Y_{k,i}(\theta), \\
\frac{\partial}{\partial\varphi}\left[w^{(a,0)}_{R}(z)\,Q^{(a)}_{n,k,i}(x,y,z)\right] &= -\rho(z)\,\frac{\mathrm{d}}{\mathrm{d}z}\left[w^{(a,k)}_{R}(z)\,R^{(a,2k)}_{n-k}(z)\right]Y_{k,i}(\theta).
\end{aligned}$$

Then,

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

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,

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

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

We move on to the spherical Laplacian operators. Note that the Laplacian acting on the weighted and non-weighted spherical cap OP $Q^{(a)}_{n,k,i}$ yield

$$\begin{aligned}
\Delta_{\mathrm{S}}\, Q^{(a)}_{n,k,i} &= \frac{1}{\rho}\frac{\partial}{\partial\varphi}\Big(\rho\frac{\partial}{\partial\varphi}[R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^k\varphi]\Big)Y_{k,i}(\theta) \\
&\qquad + R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^{k-2}\varphi\frac{\partial^2}{\partial\theta^2}Y_{k,i}(\theta) \\
&= Y_{k,i}(\theta)\rho(z)^k\Big\{-k(k+1)R^{(a,2k)}_{n-k}(z) - 2(k+1)z\, R^{(a,2k)}_{n-k}{}'(z) \\
&\qquad + \rho(z)^2 R^{(a,2k)}_{n-k}{}''(z)\Big\}, \qquad (4.13) \\
\Delta_{\mathrm{S}}\big(w^{(a,0)}_R\, Q^{(a)}_{n,k,i}\big) &= \frac{1}{\rho}\frac{\partial}{\partial\varphi}\Big(\rho\frac{\partial}{\partial\varphi}[w^{(a,0)}_R(\cos\varphi)\, R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^k\varphi]\Big)Y_{k,i}(\theta) \\
&\qquad + w^{(a,0)}_R(\cos\varphi)\, R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^{k-2}\varphi\frac{\partial^2}{\partial\theta^2}Y_{k,i}(\theta) \\
&= Y_{k,i}(\theta)\Big\{R^{(a,2k)}_{n-k}(z)\big[-k(k+1)w^{(a,k)}_R(z) - 2a(k+1)z\, w^{(a-1,k)}_R(z)\big] \\
&\qquad + a(a-1)R^{(a,2k)}_{n-k}(z)\, w^{(a-2,k+1)}_R(z) \\
&\qquad + R^{(a,2k)}_{n-k}{}'(z)\big[-2(k+1)z\, w^{(a,k)}_R(z) + 2a\, w^{(a-1,k+2)}_R(z)\big] \\
&\qquad + R^{(a,2k)}_{n-k}{}''(z)\, w^{(a,k+2)}_R(z)\Big\}. \qquad (4.14)
\end{aligned}$$

For the operator $\mathcal{L}^{(a)\to(a+\tilde{a})}$ for the surface Laplacian on a non-weighted space, the entries of the operator are given by the coefficients in the expansion

$$\Delta_{\mathrm{S}} Q^{(a)}_{n,k,i} = \sum_{m=0}^{n}\sum_{j=0}^{m}\sum_{h=0}^{1} c_{m,j,h}\, Q^{(a+\tilde{a})}_{m,j,h},$$

where the coefficients are

$$c_{m,j,h} = \Big\|Q^{(a+\tilde{a})}_{m,j,h}\Big\|^{-2}_{Q^{(a+\tilde{a})}} \Big\langle \Delta_{\mathrm{S}} Q^{(a)}_{n,k,i},\ Q^{(a+\tilde{a})}_{m,j,h}\Big\rangle_{Q^{(a+\tilde{a})}}.$$

Using equation (4.13), and integrating by parts twice, we then have that

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

where $r_{m-k+\tilde{a}}$ is a degree $m-k+\tilde{a}$ polynomial in z, and so the above is zero for $n-k > m-k+\tilde{a} \iff m < n-\tilde{a}$.

For the operator $\mathcal{L}_W^{(a)\to(a-\tilde{a})}$ for the surface Laplacian on a weighted space, the entries of the operator are given by the coefficients in the expansion

$$
\Delta_{\mathrm{S}}\big(w_R^{(a,0)}\, Q^{(a)}_{n,k,i}\big) = \sum_{m=0}^{n} \sum_{j=0}^{m} \sum_{h=0}^{1} c_{m,j,h}\, w_R^{(a-\tilde{a},0)}\, Q^{(a-\tilde{a})}_{m,j,h},
$$

where the coefficients are

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

Using equation (4.14), and integrating by parts thrice, we then have that

$$
\begin{aligned}
&\Big\langle \Delta_{\mathrm{S}}\big(w_R^{(a,0)}\, Q_{n,k,i}^{(a)}\big),\, Q_{m,j,h}^{(a-\tilde{a})} \Big\rangle_{Q^{(0)}} \\
&\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_{m-j}^{(a-\tilde{a},2j)}\, w_R^{(a-2,k+j)} \Big\{ R_{n-k}^{(a,2k)} [-k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} + a(a-1)\rho^2] \\
&\qquad\qquad + R_{n-k}^{(a,2k)\,\prime} [-2(k+1) z\, w_R^{(2,0)} + 2a w_R^{(1,2)}] \\
&\qquad\qquad + R_{n-k}^{(a,2k)\,\prime\prime}\, w_R^{(2,2)} \Big\}\, \mathrm{d}z \Big) \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \Big\{ R_{m-k}^{(a-\tilde{a},2k)}\, R_{n-k}^{(a,2k)}\, w_R^{(a-2,2k)}\, [-k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} + a(a-1)\rho^2] \\
&\qquad + a\, R_{n-k}^{(a,2k)\,\prime}\, R_{m-k}^{(a-\tilde{a},2k)}\, w_R^{(a-1,2k+2)} \\
&\qquad + R_{m-k}^{(a-\tilde{a},2k)} \frac{\mathrm{d}}{\mathrm{d}z} [R_{n-k}^{(a,2k)\,\prime}\, w_R^{(a,2k+2)}] \Big\}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \Big\{ R_{m-k}^{(a-\tilde{a},2k)}\, R_{n-k}^{(a,2k)}\, w_R^{(a-2,2k)}\, [-k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} + a(a-1)\rho^2] \\
&\qquad + a\, R_{n-k}^{(a,2k)\,\prime}\, R_{m-k}^{(a-\tilde{a},2k)}\, w_R^{(a-1,2k+2)} \\
&\qquad + R_{n-k}^{(a,2k)}\, w_R^{(a-1,2k)} [R_{m-k}^{(a-\tilde{a},2k)\,\prime\prime}\, w_R^{(1,2)} + a R_{m-k}^{(a-\tilde{a},2k)\,\prime}\, \rho^2 - 2(k+1) z\, R_{m-k}^{(a-\tilde{a},2k)}\, w_R^{(1,0)}] \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \Big\{ R_{m-k}^{(a-\tilde{a},2k)}\, R_{n-k}^{(a,2k)}\, w_R^{(a-2,2k)}\, [-k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} + a(a-1)\rho^2] \\
&\qquad + R_{n-k}^{(a,2k)}\, w_R^{(a-1,2k+2)} [R_{m-k}^{(a-\tilde{a},2k)\,\prime\prime}\, \rho^2 - 2(k+1) z\, R_{m-k}^{(a-\tilde{a},2k)\,\prime}] \\
&\qquad + a [R_{n-k}^{(a,2k)}\, R_{m-k}^{(a-\tilde{a},2k)\,\prime} + R_{m-k}^{(a-\tilde{a},2k)}\, R_{n-k}^{(a,2k)\,\prime}]\, w_R^{(a-1,2k+2)} \Big\}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \Big\{ R_{m-k}^{(a-\tilde{a},2k)}\, R_{n-k}^{(a,2k)}\, w_R^{(a-2,2k)}\, [-k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} + a(a-1)\rho^2] \\
&\qquad + R_{n-k}^{(a,2k)}\, w_R^{(a-1,2k+2)} [R_{m-k}^{(a-\tilde{a},2k)\,\prime\prime}\, \rho^2 - 2(k+1) z\, R_{m-k}^{(a-\tilde{a},2k)\,\prime}] \\
&\qquad - a R_{n-k}^{(a,2k)}\, R_{m-k}^{(a-\tilde{a},2k)}\, w_R^{(a-2,2k)}\, [(a-1)\rho^2 - 2(k+1) z\, w_R^{(1,0)}] \Big\}\, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R_{n-k}^{(a,2k)}\, w_R^{(a,2k)}\, r_{m-k}\, \mathrm{d}z
\end{aligned}
$$

where r_{m-k} is a degree $m-k$ polynomial in z, and so the above is zero for $n-k > m-k \iff m < n$.

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 $\Delta_{\mathrm{S}}\big(w_R^{(1,0)}\, Q_{n,k,i}^{(1)}\big) = \sum_{m=0}^{n+2} \sum_{j=0}^{m} \sum_{h=0}^{1} c_{m,j,h}\, Q_{m,j,h}^{(1)}$, where the coefficients are given by

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

Using equation (4.14) with $a = 1$, and Lemma 9, we then have that

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

where the $c_{n-1,k}, c_{n,k}, c_{n+1,k}$ are those derived in Lemma 9. $\square$

By applying these differential operators, we are (in some cases) incrementing or decrementing the parameter value a. It is therefore necessary to also be able to raise or lower the parameter by way of an independent operator. There exist conversion matrix operators that do exactly this, transforming the OPs from one (weighted or non-weighted) parameter space to another.

Definition 16. *Define the operator matrices* $T^{(a)\to(a+\tilde{a})}$, $\quad T_W^{(a)\to(a-\tilde{a})}$ *for conversion between non-weighted spaces and weighted spaces respectively according to*

$$\mathbb{Q}_N^{(a)}(x,y,z) = \left(T^{(a)\to(a+\tilde{a})}\right)^\top \mathbb{Q}_N^{(a+\tilde{a})}(x,y,z)$$
$$\mathbb{W}_N^{(a)}(x,y,z) = \left(T_W^{(a)\to(a-\tilde{a})}\right)^\top \mathbb{W}_N^{(a-\tilde{a})}(x,y,z)$$

Lemma 10. *The operator matrices in Definition 16 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 $\{Q_{m,j,h}^{(a+\tilde{a})}\}$ for $m = 0,\ldots,n$, $j = 0,\ldots,m$, $h = 0,1$ is an orthogonal basis for any degree n polynomial, we can expand $Q_{n,k,i}^{(a)} = \sum_{m=0}^{n} \sum_{j=0}^{m} t_{m,j}\, Q_{m,j,h}^{(a+\tilde{a})}$. The coefficients of the expansion are then 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

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

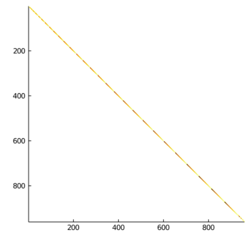
where

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

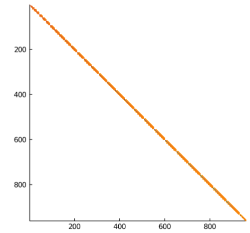
which is zero for $n > m + \tilde{a} \iff m < n - \tilde{a}$. The sparsity argument for the weighted parameter transformation operator follows similarly. □

4.3.1 Further partial differential operators

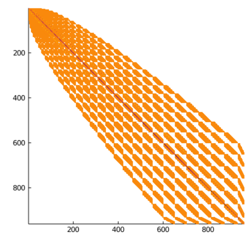
General linear partial differential operators with polynomial variable coefficients can be constructed by composing the sparse representations for partial derivatives, conversion between bases, and Jacobi operators. As a canonical example, we can obtain the matrix operator for the ρ^2-factored spherical Laplacian $\rho(z)^2\, \Delta_{\mathrm{S}}$, that will take us from coefficients for expansion in the weighted space $\mathbb{W}^{(1)}_N(x,y,z) = w_R^{(1,0)}(z)\, \mathbb{Q}^{(1)}_N(x,y,z)$ to coefficients in the non-weighted space $\mathbb{Q}^{(1)}_N(x,y,z)$. 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 $\Delta^{(1)}_W$ in Definition 15. The matrix operator for this ρ^2-



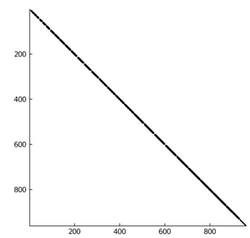
(a) The Laplace-Beltrami operator $\Delta_W^{(1)}$



(b) The ρ^2-factored Laplace-Beltrami operator $D_\varphi^{(0)}\ W_\varphi^{(1)} + T^{(0)\to(1)}\, T_W^{(1)\to(0)}\, (D_\theta)^2$



(c) A variable coefficient Helmholtz operator



(d) The Biharmonic operator $\mathcal{B}_W^{(2)}$

Figure 4.1: "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 $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{1 - x_0^2 - z_0^2}$ and $k = 200$.

factored spherical Laplacian acting on the coefficients vector is then given by

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

Importantly, this operator will have banded-block-banded structure, and hence will be sparse, as seen in Figure 4.1.

Another desirable operator is the Biharmonic operator $\Delta_{\mathbb{S}}^2$, for which we assume zero Dirichlet and Neumann conditions. That is,

$$u(x, y, z) = 0, \quad \frac{\partial u}{\partial n}(x, y, z) = \nabla_S u(x, y, z) \cdot \hat{\boldsymbol{n}}(x, y, z) = 0 \quad \text{for } (x, y, z) \in \partial\Omega$$

where $\partial\Omega$ is the $z = \alpha$ boundary, and $\hat{\boldsymbol{n}}(x, y, z)$ is the outward unit normal vector at the point (x, y, z) on the boundary, i.e. $\hat{\boldsymbol{n}}(x, y, z) = \hat{\boldsymbol{n}}(\boldsymbol{x}) := \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|} = \boldsymbol{x}$. The matrix operator for the Biharmonic operator will take us from coefficients in the space $\mathbb{W}^{(2)}(x, y, z)$ to coefficients in the space $\mathbb{Q}_N^{(2)}(x, y, z)$. To construct this, we can simply multiply together two of the spherical Laplacian operators defined in Definition 15, namely $\mathcal{L}^{(0)\to(2)}$ and $\mathcal{L}_W^{(2)\to(0)}$:

$$\mathcal{B}_W^{(2)} := \mathcal{L}^{(0)\to(2)} \, \mathcal{L}_W^{(2)\to(0)}.$$

Since the operator $\mathcal{L}_W^{(2)\to(0)}$ acts on coefficients in the $\mathbb{W}^{(2)}(x, y, z)$ space, we ensure that we satisfy the zero Dirichlet and Neumann boundary conditions – such a function could be written $u(x, u, z) = w_R^{(2,0)}(z) \, \tilde{u}(x, y, z)$ and thus its spherical gradient would be zero on the boundary $z = \alpha$. This allows us to apply the $\mathcal{L}^{(0)\to(2)}$ operator after, safe in the knowledge that boundary conditions have been accounted for. The sparsity and structure of this biharmonic operator are seen in Figure 4.1.

4.4 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.

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

It is possible to recursively obtain the recurrence coefficients for the $\{R_n^{(a,b)}\}$ OPs in (4.5), see [26], by careful application of the Christoffel–Darboux formula [19, 18.2.12].

4.4.2 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 5. *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* $j = 1, \ldots, M_1,\ l = 1, \ldots, M_2$*:*

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

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

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

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

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 [19, 3.5.23] as $s_j := \cos\Big(\frac{2j-1}{2M_2}\pi\Big)$, $w_j^{(s)} := \frac{\pi}{M_2}$.

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

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

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

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

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

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

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

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

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

4.4.3 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 (4.10, 4.11, 4.12) and where

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

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

Recall from equation (4.4) that $\left\| Q_{n,k,i}^{(a)} \right\|_{Q^{(a)}}^{2} = \omega_R^{(a,2k)} \pi$. Using the quadrature rule detailed in Section 4.4.2 for the inner product, we can calculate the coefficients

$f_{n,k,i}$ for each $n = 0, \dots, N$, $k = 0, \dots, n$, $i = 0, 1$:

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

where the quadrature nodes and weights are those from Theorem 5, 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 $M_1 := \lceil \frac{N+1}{2} \rceil$).

4.4.4 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 4.4.3 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 14, 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 [22] for expansions in the triangle:

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: $f(x,y,z) \approx \boldsymbol{\xi}_0 \, \tilde{\mathbb{Q}}_0^{(a)} = \xi_0 \, Q_0^{(a)}$

4.4.5 Calculating non-zero entries of the operator matrices

The proofs of Theorem 4 and Lemma 10 provide a way to calculate the non-zero entries of the operator matrices given in Definition 15 and Definition 16. We can simply use quadrature to calculate the 1D inner products, which has a complexity of $\mathcal{O}(N^2)$. This proves much cheaper computationally than using the 3D quadrature rule to calculate the surface inner products, which has a complexity of $\mathcal{O}(N^3)$.

4.4.6 Obtaining operator matrices for variable coefficients

The Clenshaw algorithm outlined in Section 4.4.4 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 4.4.4 so that $v(x, y, z) = \tilde{\boldsymbol{v}}^\top\, \tilde{\mathbb{Q}}^{(a)}(x, y, z)$). Denote $X := (J_x^{(a)})^\top$, $Y := (J_y^{(a)})^\top$, $Z := (J_z^{(a)})^\top$. 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 $\boldsymbol{\xi}_n^T = \tilde{\boldsymbol{v}}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T \big(B_n - G_n(X, Y, Z) \big) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$

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.

4.5 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.

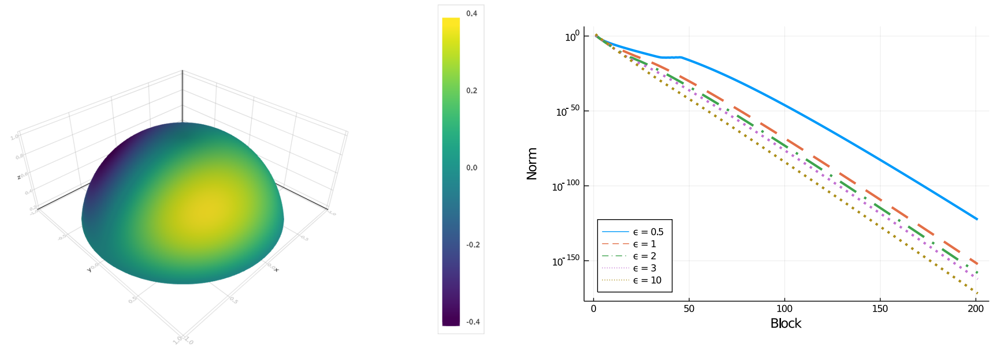


Figure 4.2: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x,y,z) = -2e^x yz(2+x)+w_R^{(1,0)}(z)e^x(y^3+z^2y-4xy-2y)$. Right: The norms of each block of the computed solution of the Poisson equation with right hand side function $f(x,y,z) = \left\|\mathbf{x} - (\epsilon + 1/\sqrt{3})\,(1,1,1)^\top\right\|$ for different ϵ values. This indicates spectral convergence.

4.5.1 Poisson

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

$$\begin{cases} \Delta_{\mathrm{S}} u(x,y,z) = f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = 0 & \text{on } \partial\Omega \end{cases} \tag{4.15}$$

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

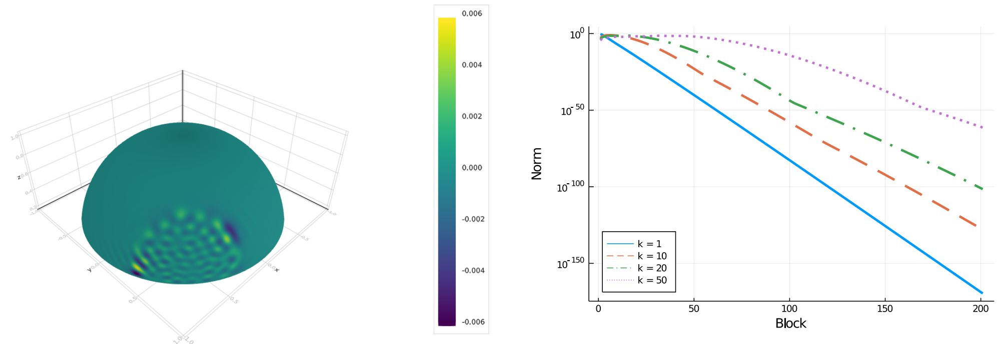


Figure 4.3: Left: The computed solution to $\Delta u + k^2 v u = f$ with zero boundary conditions with $f(x, y, z) = ye^x(z - \alpha)$, $v(x, y, z) = 1 - (3(x - x_0)^2 + 5(y - y_0)^2 + 2(z - z_0)^2)$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{1 - x_0^2 - z_0^2}$ and $k = 100$. Right: The norms of each block of the computed solution of the Helmholtz equation with the right hand side function $f(x, y, z) = 1$ and the same function $v(x, y, z)$, for various k values. This indicates spectral convergence.

rule in Section 4.4.3. In matrix-vector notation, our system hence becomes:

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

which can be solved to find $\mathbf{u}$. In Figure 4.2 we see the solution to the Poisson equation with zero boundary conditions given in (4.15) in the disk-slice Ω. In Figure 4.2 we also show the norms of each block of calculated coefficients of the approximation for four right-hand sides of the Poisson equation with $N = 200$, that is, $(N + 1)^2 = 40,401$ unknowns. The right hand sides we choose here are given by

$$f(x, y, z) = \left\| \left(x - (\epsilon + 1/\sqrt{3}),\ y - (\epsilon + 1/\sqrt{3}),\ z - (\epsilon + 1/\sqrt{3}) \right)^\top \right\|$$

for differing choices of ϵ – this parameter serves to alter the distance from which we would have a singularity. In the plot, a “block” is simply the group of coefficients

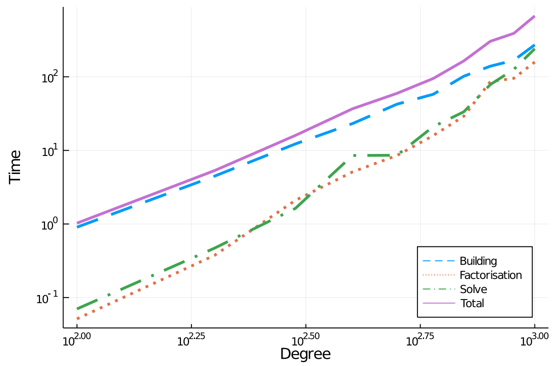


Figure 4.4: Complexity plot showing the length of time taken to construct the operator matrix for $\Delta_{\mathrm{S}} + v(x,y,z)$, with rotationally invariant potential $v(x,y,z) = \cos z$. This shows that the time to build and solve the system $\left[\Delta_{\mathrm{S}} + v(x,y,z)\right] u(x,y,z) = f(x,y,z)$ is roughly of order $\mathcal{O}(N^2)$, where N is the degree to which we approximate the solution. Here, we used $f = -2e^x yz(2+x) + (z-\alpha)e^x(y^3 + z^2 y - 4xy - 2y)$.

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 for these examples.

4.5.2 Inhomogeneous variable-coefficient Helmholtz

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

$$\begin{cases} \Delta_{\mathrm{S}} u(x,y,z) + k^2\, v(x,y,z)\, u(x,y,z) = f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = 0 & \text{on } \partial\Omega \end{cases} \tag{4.16}$$

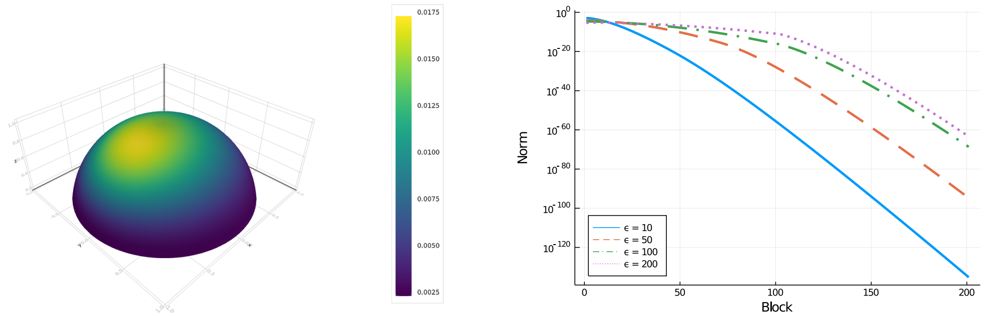


Figure 4.5: Left: The computed solution to $\Delta^2 u = f$ with zero Dirichlet and Neumann boundary conditions with $f(x, y, z) = (1 + \mathrm{erf}(5(1 - 10((x - 0.5)^2 + y^2))))\rho(z)^2$. Right: The norms of each block of the computed solution of the biharmonic equation with the right hand side function $f(x, y, z) = \exp(-\epsilon((x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2))$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{1 - x_0^2 - z_0^2}$, for various ϵ values. This demonstrates algebraic convergence.

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 4.4.3.

Define $X := (J_x^{(0)})^\top$, $Y := (J_y^{(0)})^\top$, $Z := (J_z^{(0)})^\top$. 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 X, Y, Z, yielding an operator matrix of the same dimension as the input Jacobi matrices a la the procedure introduced in [22]. We can denote the resulting operator acting on coefficients in the $\mathbb{Q}_N^{(0)}$ space by $v(X, Y, Z)$. In matrix-vector notation, our system hence becomes:

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

which can be solved to find $\mathbf{u}$. We can see the sparsity and structure of this matrix system in Figure 4.1 with $v(x, y, z) = zxy^2$ as an example. In Figure 4.3 we see the solution to the inhomogeneous variable-coefficient Helmholtz equation with zero boundary conditions given in (4.16) 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 $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{1 - x_0^2 - z_0^2}$ and $k = 100$. In Figure 4.3 we also show the norms of each block of calculated coefficients for the approximation of the solution to the inhomogeneous variable-coefficient Helmholtz equation with various k values. Here, we use $N = 200$, that is, $(N+1)^2 = 40{,}401$ 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.

In Figure 4.4 we plot the time taken[1] to construct the operator for $\Delta_{\mathrm{S}} + v(x, y, z)$, this time with a rotationally invariant $v(x, y, z) = \cos z$, and solve a zero boundary condition Helmholtz problem. The plot demonstrates that as we increase the degree of approximation N, we achieve a complexity of an optimal $\mathcal{O}(N^2)$.

What about other boundary conditions? One simple extension is the case where the value on the boundary takes that of a function depending only on x and y, i.e. $c = c(x, y)$. In this case, the problem

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

[1] measured using the "@belapsed" macro from the BenchmarkTools.jl package [**?**] in Julia.

is equivalent to letting $u(x,y,z) = \tilde{u}(x,y,z) + c(x,y)$ and solving

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

for $\tilde{u}$. This new problem is then a zero boundary condition Helmholtz problem with right hand side

$$g(x,y,z) := f(x,y,z) - k^2\, v(x,y,z)\, c(x,y) - \Delta_{\mathrm{S}}\, c(x,y)$$

for $(x,y,z) \in \Omega$. Notice that the spherical Laplacian applied to $c(x,y)$, expanded in the $\mathbb{Q}_N^{(1)}$ basis with coefficients vector $\boldsymbol{c} = (c_{n,k,i})$, is just

$$\Delta_{\mathrm{S}}\, c(x,y) = \frac{1}{\rho(z)^2} \sum_{n=0}^{N} \sum_{i=0}^{1} c_{n,n,i}\, \frac{\partial^2}{\partial \theta^2} Y_{n,i}(\theta) = -\frac{1}{\rho(z)^2} \sum_{n=0}^{N} \sum_{i=0}^{1} n^2\, c_{n,n,i}\, Y_{n,i}(\theta)$$

since the coefficients $\{c_{n,k,i}\}$ for such a function are zero for $k < n$ due to the dependence on x and y only. Thus, since the function $c(x,y)$ is known, it is simple to evaluate $\frac{\partial^2}{\partial\theta^2} c(x,y)$ and hence one can obtain the coefficients for the expansion of $g(x,y,z)$ in the $\mathbb{Q}_N^{(1)}$ basis in the usual manor.

4.5.3 Biharmonic equation

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

$$\begin{cases} \Delta_{\mathrm{S}}^2 u(x, y, z) = f(x, y, z) & \text{in } \Omega \\ u(x, y, z) = 0, \quad \frac{\partial u}{\partial n}(x, y, z) = \nabla_S \, u(x, y, z) \cdot \hat{\boldsymbol{n}}(x, y, z) = 0 & \text{on } \partial\Omega \end{cases} \tag{4.17}$$

where Δ_{S}^2 is the Biharmonic operator, noting the imposition of zero Dirichlet and Neumann boundary conditions on u. For clarity, we reiterate that the unit normal vector in this sense is simply $\hat{\boldsymbol{n}}(x, y, z) = \hat{\boldsymbol{n}}(\boldsymbol{x}) := \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|} = \boldsymbol{x}$ (see Section 4.3.1). In Figure 4.5 we see the solution to the Biharmonic equation (4.17) in the spherical cap Ω. In Figure 4.5 we also show the norms of each block of calculated coefficients of the approximation for four more complex right-hand sides of the biharmonic equation with $N = 200$, that is, $(N + 1)^2 = 40,401$ 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 algebraic convergence for these more complex functions.

4.6 *p*-finite element methods using sparse operators

As was the case in Section ???, it is possible for our framework in this chapter to be applied to a *p*-finite element method. The ultimate aim here would be to discretise the sphere into spherical cap and spherical band elements, and apply a p-finite element method to solve PDEs on the sphere. As a precursor to this, in this section we limit our discretisation to a single spherical cap element, and follow the method of [3] to construct a sparse p-finite element method in terms of the operators constructed above, once again with the benefit of ensuring that the resulting discretisation is symmetric. Consider the Dirichlet problem on a surface in 3D Ω:

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

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

As mentioned, 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.

$$L(v_p) = a(u_p, v_p) \quad \forall \, v_p \in V_p. \tag{4.18}$$

Define

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

for any a. Note that due to orthogonality this is a diagonal matrix. By choosing suitable bases for our FE spaces, we can rewrite (4.18) 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,

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

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 (4.18) 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).

4.7 Vector-valued functions in the tangent space

We can extend the methodology detailed here to the tangent space of the spherical cap Ω. By creating a basis of orthogonal vector-valued functions (OVFs) for the spherical cap Ω, we can expand vector-valued functions that lie in tangent space we call Ω_T in this basis. Such functions that are useful for the sphere are gradients and perpendicular-gradients of scalar functions. In this section we will define the OVFs, outline the Clenshaw matrices and how to build the OVFs, function evaluation as well as differential operators for gradient, curl and divergence that take us to and from coefficients in either of the OVF or scalar OP expansions.

Any function in the tangent space of Ω can be written as $\nabla f + \hat{\boldsymbol{r}} \times \nabla g$ for some scalar functions f, g on Ω. Let f be a scalar function on Ω that satisfies zero boundary conditions. Then there exist coefficients $\boldsymbol{f}$ such that f can be expanded in the OP basis $\mathbb{W}_N^{(1)}$ for large enough N, i.e. $f = w_R^{(1,0)} \sum_{n,k,i} f_{n,k,i}\, Q_{n,k,i}^{(1)}$. The gradient and perpendicular gradient of f are then

$$\begin{aligned}
\nabla f &= \sum_{n,k,i} f_{n,k,i}\, \nabla\Big(w_R^{(1,0)}\, Q_{n,k,i}^{(1)}\Big) \\
\hat{\boldsymbol{r}} \times \nabla f &= \sum_{n,k,i} f_{n,k,i}\, \hat{\boldsymbol{r}} \times \nabla\Big(w_R^{(1,0)}\, Q_{n,k,i}^{(1)}\Big).
\end{aligned}$$

For the whole sphere, recall from Section ??? that we simply chose the vector spherical harmonics as our tangent space basis, defined simply as the gradient and perpendicular gradients of the scalar spherical harmonics. We could do that because the vector spherical harmonics as defined were naturally orthogonal. Unfortunately, we do not have the same orthogonality here with the set $\{\nabla\left(w_R^{(a,0)}\, Q^{(a)}_{n,k,i}\right), \hat{\boldsymbol{r}} \times \nabla\left(w_R^{(a,0)}\, Q^{(a)}_{n,k,i}\right)\}$ for any parameter a.

The game is to find an orthogonal basis that spans the tangent space of the spherical cap Ω such that we can sparsely expand $\nabla\left(w_R^{(1,0)} Q^{(1)}_{n,k,i}\right)$ and $\hat{\boldsymbol{r}} \times \nabla\left(w_R^{(1,0)} Q^{(1)}_{n,k,i}\right)$ for each n, k, i trio.

Define the OVFs as follows:

$$\boldsymbol{\Phi}_{n,k,i}(x,y,z) := \hat{\boldsymbol{\phi}}\, \frac{1}{\rho(z)}\, Q^{(0)}_{n,k,i}(x,y,z) \tag{4.19}$$

$$\boldsymbol{\Psi}_{n,k,i}(x,y,z) := \hat{\boldsymbol{\theta}}\, \frac{1}{\rho(z)}\, Q^{(0)}_{n,k,i}(x,y,z) \tag{4.20}$$

where

$$\hat{\boldsymbol{\phi}} := \begin{pmatrix} \cos(\theta)\ \cos(\phi) \\ \sin(\theta)\ \cos(\phi) \\ -\sin(\phi) \end{pmatrix} = \begin{pmatrix} xz/\rho(z) \\ yz/\rho(z) \\ -\rho(z) \end{pmatrix} \tag{4.21}$$

$$\hat{\boldsymbol{\theta}} := \begin{pmatrix} -\sin(\theta) \\ \cos(\theta) \\ 0 \end{pmatrix} = \begin{pmatrix} -y/\rho(z) \\ x/\rho(z) \\ 0 \end{pmatrix} \tag{4.22}$$

These are orthogonal with respect to the inner product $\langle \boldsymbol{A}, \boldsymbol{B} \rangle_{\Omega_T} := \int_\Omega \boldsymbol{A}\, \cdot$

$\boldsymbol{B}\,\rho(z)^2\,\mathrm{d}A$:

$$
\begin{aligned}
\langle \mathbf{\Phi}_{n,k,i}, \mathbf{\Phi}_{m,j,h}\rangle_{\Omega_T} &= \int_\Omega \mathbf{\Phi}_{n,k,i}\cdot\mathbf{\Phi}_{m,j,h}\,\rho(z)^2\,\mathrm{d}A \\
&= \int_\Omega Q^{(0)}_{n,k,i}\,Q^{(0)}_{m,j,h}\,\mathrm{d}\Omega \\
&= \pi\,\omega_R^{(0,2k)}\,\delta_{n,m}\,\delta_{k,j}\,\delta_{i,h}, \\
\langle \mathbf{\Psi}_{n,k,i}, \mathbf{\Psi}_{m,j,h}\rangle_{\Omega_T} &= \int_\Omega \mathbf{\Psi}_{n,k,i}\cdot\mathbf{\Psi}_{m,j,h}\,\rho(z)^2\,\mathrm{d}A \\
&= \int_\Omega Q^{(0)}_{n,k,i}\,Q^{(0)}_{m,j,h}\,\mathrm{d}\Omega \\
&= \pi\,\omega_R^{(0,2k)}\,\delta_{n,m}\,\delta_{k,j}\,\delta_{i,h}, \\
\langle \mathbf{\Phi}_{n,k,i}, \mathbf{\Psi}_{m,j,h}\rangle_{\Omega_T} &\equiv 0.
\end{aligned}
$$

To show that these span the tangent space Ω_T, we merely require that we can sparsely expand $\nabla\Big(w_R^{(1,0)}Q^{(1)}_{n,k,i}\Big), \hat{\boldsymbol{r}}\times\nabla\Big(w_R^{(1,0)}Q^{(1)}_{n,k,i}\Big)$ with the vectors $\mathbf{\Phi}_{m,j,h}, \mathbf{\Psi}_{m,j,h}$. First, note that

$$
\begin{aligned}
\nabla\Big(w_R^{(1,0)}\,Q^{(1)}_{n,k,i}\Big) &= \hat{\boldsymbol{\phi}}\,\frac{\partial}{\partial\varphi}\Big(w_R^{(1,0)}\,Q^{(1)}_{n,k,i}\Big) + \hat{\boldsymbol{\theta}}\,\frac{1}{\rho(z)}\,\frac{\partial}{\partial\theta}\Big(w_R^{(1,0)}\,Q^{(1)}_{n,k,i}\Big) \\
&= \hat{\boldsymbol{\phi}}\,\Big[k\,z\,w_R^{(1,0)}(z)\,R^{(1,2k)}_{n-k}(z) - \big(w_R^{(1,0)}(z)\,R^{(1,2k)}_{n-k}(z)\big)'\rho(z)^2\Big]\,\rho(z)^{k-1}\,Y_{k,i}(\theta) \\
&\quad + \hat{\boldsymbol{\theta}}\,(-1)^{i+1}\,k\,w_R^{(1,0)}(z)\,R^{(1,2k)}_{n-k}(z)\,\rho(z)^{k-1}\,Y_{k,|i-1|}(\theta).
\end{aligned}
$$

Then,

$$
\begin{aligned}
&\left\langle \nabla\left(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\right), \boldsymbol{\Phi}_{m,j,h} \right\rangle_{\Omega_T} \\
&\quad = \int_\Omega \nabla\left(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\right) \cdot \boldsymbol{\Phi}_{m,j,h}\, \rho(z)^2 \, \mathrm{d}A \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \left[k\, z\, w_R^{(1,0)}\, R^{(1,2k)}_{n-k} - (w_R^{(1,0)}\, R^{(1,2k)}_{n-k})' \rho^2\right] \rho^{k-1}\, R^{(0,2k)}_{m-k}\, \rho^{k-1}\, \rho^2 \, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \left[k\, z\, w_R^{(1,0)}\, R^{(1,2k)}_{n-k} - (w_R^{(1,0)}\, R^{(1,2k)}_{n-k})' \rho^2\right] R^{(0,2k)}_{m-k}\, \rho^{2k} \, \mathrm{d}z \quad (\star) \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 \Big(kz\, R^{(1,2k)}_{n-k}\, R^{(0,2k)}_{m-k}\, w_R^{(1,2k)} \\
&\qquad\qquad\qquad + w_R^{(1,2k)}\, R^{(1,2k)}_{n-k} \left[R^{(0,2k)\,\prime}_{m-k}\, \rho^2 - (2k+2)\, z\, R^{(0,2k)}_{m-k}\right]\Big) \, \mathrm{d}z \\
&\quad = \pi\, \delta_{k,j}\, \delta_{i,h} \int_\alpha^1 R^{(1,2k)}_{n-k} \left[-\,(k+2)\, z\, R^{(0,2k)}_{m-k} + R^{(0,2k)\,\prime}_{m-k}\, \rho^2\right] w_R^{(1,2k)} \, \mathrm{d}z \quad (\star\star)
\end{aligned}
$$

where by orthogonality of the $\{R_n^{(a,2b)}\}$ OPs we have that the above is zero for $m-k > n-k+2 \iff m > n+2$ at $(\star)$ and also for $n-k > m-k+1 \iff m < n-1$ at $(\star\star)$. Further,

$$
\begin{aligned}
&\left\langle \nabla\left(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\right), \boldsymbol{\Psi}_{m,j,h} \right\rangle_{\Omega_T} \\
&\quad = \int_\Omega \nabla\left(w_R^{(1,0)}\, Q^{(1)}_{n,k,i}\right) \cdot \boldsymbol{\Psi}_{m,j,h}\, \rho(z)^2 \, \mathrm{d}A \\
&\quad = (-1)^{i+1}\, k\, \pi\, \delta_{k,j}\, \delta_{i,|h-1|} \int_\alpha^1 w_R^{(1,0)}\, R^{(1,2k)}_{n-k}\, \rho^{k-1}\, R^{(0,2k)}_{m-k}\, \rho^{k-1}\, \rho^2 \, \mathrm{d}z \\
&\quad = (-1)^{i+1}\, k\, \pi\, \delta_{k,j}\, \delta_{i,|h-1|} \int_\alpha^1 R^{(1,2k)}_{n-k}\, R^{(0,2k)}_{m-k}\, w_R^{(1,2k)} \, \mathrm{d}z
\end{aligned}
$$

which again by orthogonality is zero for $m-k > n-k+1 \iff m > n+1$ and $n-k > m-k \iff m < n$. We of course have similar results for $\hat{\boldsymbol{r}} \times$

$\nabla\left(w_R^{(1,0)}\, Q_{n,k,i}^{(1)}\right)$ since

$$\hat{\boldsymbol{r}} \times \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\theta}}, \quad \hat{\boldsymbol{r}} \times \hat{\boldsymbol{\theta}} = -\hat{\boldsymbol{\phi}}.$$

We now have a set of orthogonal vector valued functions that span the tangent space Ω_T. By construction, we have the same recurrence coefficients for multiplication by x, y, z for each of the OVFs as for the OPs $Q_{n,k,i}^{(0)}$.

Define

$$\tilde{\mathbb{T}}_n := \begin{pmatrix} \boldsymbol{\Phi}_{n,0,0}^\top(x,y,z) \\ \boldsymbol{\Psi}_{n,0,0}^\top(x,y,z) \\ \boldsymbol{\Phi}_{n,1,0}^\top(x,y,z) \\ \boldsymbol{\Psi}_{n,1,0}^\top(x,y,z) \\ \boldsymbol{\Phi}_{n,1,1}^\top(x,y,z) \\ \boldsymbol{\Psi}_{n,1,1}^\top(x,y,z) \\ \vdots \\ \boldsymbol{\Phi}_{n,n,0}^\top(x,y,z) \\ \boldsymbol{\Psi}_{n,n,0}^\top(x,y,z) \\ \boldsymbol{\Phi}_{n,n,1}^\top(x,y,z) \\ \boldsymbol{\Psi}_{n,n,1}^\top(x,y,z) \end{pmatrix} \in \mathbb{R}^{2(2n+1)\times 3}, \qquad \tilde{\mathbb{T}} := \begin{pmatrix} \tilde{\mathbb{T}}_0 \\ \tilde{\mathbb{T}}_1 \\ \tilde{\mathbb{T}}_2 \\ \vdots \end{pmatrix}$$

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

$$\begin{aligned} {}^{T}J_x\, \tilde{\mathbb{T}}(x,y,z) &= x\, \tilde{\mathbb{T}}(x,y,z), \\ {}^{T}J_y\, \tilde{\mathbb{T}}(x,y,z) &= y\, \tilde{\mathbb{T}}(x,y,z), \\ {}^{T}J_z\, \tilde{\mathbb{T}}(x,y,z) &= z\, \tilde{\mathbb{T}}(x,y,z), \end{aligned} \tag{4.23}$$

The matrices ${}^{T}J_x, {}^{T}J_y, {}^{T}J_z$ act on the coefficients vector of a function's expansion in the $\tilde{\mathbb{T}}$ basis. For example, let a function $\boldsymbol{F}(x,y,z) : \Omega \to \Omega_T$ be approximated by its expansion $\boldsymbol{F}(x,y,z)^\top = \tilde{\mathbb{T}}(x,y,z)^\top \boldsymbol{F}_c$, for some coefficients vector $\boldsymbol{F}_c$. Then $x\,\boldsymbol{F}(x,y,z)$ is approximated by $\tilde{\mathbb{T}}(x,y,z)^\top ({}^{T}J_x)^\top \boldsymbol{F}_c$. In other words, $({}^{T}J_x)^\top \boldsymbol{F}_c$ is the coefficients vector for the expansion of the function $(x,y,z) \mapsto x\,\boldsymbol{F}(x,y,z)$ in the $\tilde{\mathbb{T}}$ basis. Further, note that ${}^{T}J_x, {}^{T}J_y, {}^{T}J_z$ are banded-block-banded matrices – they are block-tridiagonal (block-bandwidths $(1,1)$):

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

For ${}^TJ_x$, the sub-blocks have sub-block-bandwidths (?, ?):

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

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

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

where

$$
\begin{aligned}
A_{n,k,j} &:= \alpha_{n,k,j}^{(0)}\, I_4 \in \mathbb{R}^{4\times 4}, \quad k = 1, \ldots, n\, (j \text{ even}), \quad k = 2, \ldots, n\, (j \text{ odd}) \\
A_{n,0,j} &:= \begin{pmatrix} \alpha_{n,0,j}^{(0)} & 0 & 0 & 0 \\ 0 & \alpha_{n,0,j}^{(0)} & 0 & 0 \end{pmatrix} \in \mathbb{R}^{2\times 4}, \quad j \text{ even} \\
A_{n,1,j} &:= \begin{pmatrix} \alpha_{n,1,j}^{(0)} & 0 \\ 0 & \alpha_{n,1,j}^{(0)} \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{4\times 2}, \quad j \text{ odd}
\end{aligned}
$$

For ${}^T J_y$, the sub-blocks have sub-block-bandwidths (?, ?):

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

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

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

where

$$B_{n,k,j} := \begin{pmatrix} 0 & 0 & \beta^{(0)}_{n,k,j} & 0 \\ 0 & 0 & 0 & \beta^{(0)}_{n,k,j} \\ \beta^{(0)}_{n,k,j} & 0 & 0 & 0 \\ 0 & \beta^{(0)}_{n,k,j} & 0 & 0 \end{pmatrix} \in \mathbb{R}^{4\times 4}, \quad k = 1, \ldots, n \, (j \text{ even}), \quad k = 2, \ldots, n \, (j \text{ odd})$$

$$B_{n,0,j} := \begin{pmatrix} 0 & 0 & \beta^{(0)}_{n,0,j} & 0 \\ 0 & 0 & 0 & \beta^{(0)}_{n,0,j} \end{pmatrix} \in \mathbb{R}^{2\times 4}, \quad j \text{ even}$$

$$B_{n,1,j} := \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ \beta^{(0)}_{n,1,j} & 0 \\ 0 & \beta^{(0)}_{n,1,j} \end{pmatrix} \in \mathbb{R}^{4\times 2}, \quad j \text{ odd}$$

For ${}^{T}J_z$, the sub-blocks have sub-block-bandwidths (?, ?):

$$A_{z,n} := \begin{pmatrix} \Gamma_{n,0,3} & 0 & 0 & & \\ 0 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & \Gamma_{n,n,3} & 0 \end{pmatrix} \in \mathbb{R}^{2(2n+1)\times 2(2n+3)}, \quad n = 0, 1, 2, \ldots$$

$$B_{z,n} := \begin{pmatrix} \Gamma_{n,0,2} & 0 & & \\ 0 & \ddots & \ddots & \\ & \ddots & \ddots & 0 \\ & & 0 & \Gamma_{n,n,2} \end{pmatrix} \in \mathbb{R}^{2(2n+1)\times 2(2n+1)} \quad n = 0, 1, 2, \ldots$$

$$C_{z,n} := \begin{pmatrix} \Gamma_{n,0,1} & 0 & & \\ 0 & \ddots & \ddots & \\ & \ddots & \ddots & 0 \\ & & \ddots & \Gamma_{n,n-1,1} \\ & & & 0 \end{pmatrix} \in \mathbb{R}^{2(2n+1)\times 2(2n-1)}, \quad n = 1, 2, \ldots$$

where

$$\Gamma_{n,k,j} := \gamma^{(0)}_{n,k,j}\, I_4 \in \mathbb{R}^{4\times 4}, \quad k = 1, \ldots, n$$
$$\Gamma_{n,0,j} := \begin{pmatrix} \gamma^{(0)}_{n,0,j} & 0 \\ 0 & \gamma^{(0)}_{n,0,j} \end{pmatrix} \in \mathbb{R}^{2\times 2}.$$

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.

4.7.1 Building the OPs

We can combine each system in (4.23) into a block-tridiagonal system, for any $(x, y, z) \in \Omega$:

$$\begin{pmatrix} I_2 & & & \\ B_0 - G_0(x,y,z) & A_0 & & \\ C_1 & B_1 - G_1(x,y,z) & A_1 & \\ & C_2 & B_2 - G_2(x,y,z) & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tilde{\mathbb{T}}(x,y,z) = \begin{pmatrix} \mathbf{\Phi}_0^\top \\ \mathbf{\Psi}_0^\top \\ 0 \\ 0 \\ \vdots \end{pmatrix},$$

where we note $Q_0^{(a)} := Q_{0,0,0}^{(a)}(x,y,z) \equiv R_0^{(a,0)} Y_0$, and for each $n = 0, 1, 2 \ldots,$

$$A_n := \begin{pmatrix} A_{x,n} \\ A_{y,n} \\ A_{z,n} \end{pmatrix} \in \mathbb{R}^{6(2n+1)\times 2(2n+3)}, \quad C_n := \begin{pmatrix} C_{x,n} \\ C_{y,n} \\ C_{z,n} \end{pmatrix} \in \mathbb{R}^{6(2n+1)\times 2(2n-1)} \quad (n \neq 0),$$

$$B_n := \begin{pmatrix} B_{x,n} \\ B_{y,n} \\ B_{z,n} \end{pmatrix} \in \mathbb{R}^{6(2n+1)\times 2(2n+1)}, \quad G_n(x,y,z) := \begin{pmatrix} xI_{2(2n+1)} \\ yI_{2(2n+1)} \\ zI_{2(2n+1)} \end{pmatrix} \in \mathbb{R}^{6(2n+1)\times 2(n+1)}.$$

For each $n = 0, 1, 2\ldots$ let $D_n^\top$ be any matrix that is a left inverse of A_n, i.e. such that $D_n^\top A_n = I_{2(2n+3)}$. 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 [9, p78], which can be expanded to obtain the recurrence:

$$\begin{cases} \tilde{\mathbb{T}}_{-1}(x,y,z) := 0 \\ \tilde{\mathbb{T}}_0(x,y,z) = \begin{pmatrix} \boldsymbol{\Phi}_0^\top \\ \\ \boldsymbol{\Psi}_0^\top \end{pmatrix} := \begin{pmatrix} \boldsymbol{\Phi}_{0,0,0}^\top \\ \\ \boldsymbol{\Phi}_{0,0,0}^\top \end{pmatrix} \\ \tilde{\mathbb{T}}_{n+1}(x,y,z) = -D_n^\top(B_n - G_n(x,y,z))\tilde{\mathbb{T}}_n(x,y,z) - D_n^\top C_n\, \tilde{\mathbb{T}}_{n-1}(x,y,z), \quad n = 0,1,2,\ldots. \end{cases}$$

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

type up DnT for tangent space

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

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

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

$$\left(\boldsymbol{\eta}_1\right)_j = \begin{cases} \left(\boldsymbol{\eta}_0\right)_{j+1} & j = 2n, 3(2n+1)-3 \\ 0 & o/w \end{cases}$$

For $n = 0, 1$, we can simply take

$$D_0^\top := \begin{pmatrix} 0 & 0 & \frac{1}{\gamma^{(a)}_{0,0,3}} \\ \frac{1}{\alpha^{(a)}_{0,0,6}} & 0 & 0 \\ 0 & \frac{1}{\beta^{(a)}_{0,0,6}} & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3},$$

$$D_1^\top := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1/\gamma^{(a)}_{1,0,3} & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\gamma^{(a)}_{1,1,3} & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\gamma^{(a)}_{1,1,3} \\ 0 & 1/\alpha^{(a)}_{1,1,6} & 0 & 0 & 0 & 0 & \eta & 0 & 0 \\ 0 & 0 & 1/\alpha^{(a)}_{1,1,6} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{5\times 9},$$

where $\eta = \frac{-\alpha^{(a)}_{1,1,5}}{\alpha^{(a)}_{1,1,6}\,\gamma^{(a)}_{1,0,3}}$.

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

correct for this case

4.7.2 Operators

Gradient operator on a scalar function is pretty much outlined above. Divergence would either be worked out by knowing what f, g are for a function $\boldsymbol{F} = \nabla f + \hat{\boldsymbol{r}} \times \nabla g$, so that $\nabla \cdot \boldsymbol{F} = \nabla^2 f$. Alternatively, we have expressions for $\rho \frac{\partial}{\partial \varphi} Q^{(a)}_{n,k,i}$ and $\frac{\partial}{\partial \theta} Q^{(a)}_{n,k,i}$ so that we can calculate an operator for $\rho^2 \nabla \cdot$, i.e.

$$\begin{aligned}
\rho^2 \nabla \cdot \boldsymbol{F} &= \rho^2 \, \frac{1}{\rho} \frac{\partial}{\partial \varphi} (\rho F^{\phi}) + \rho^2 \, \frac{1}{\rho} \frac{\partial}{\partial \theta} F^{\theta} \\
&= \sum_{n,k,i} F^{\phi}_{n,k,i} \, \rho \frac{\partial}{\partial \varphi} Q^{(0)}_{n,k,i} + F^{\theta}_{n,k,i} \, \frac{\partial}{\partial \theta} Q^{(0)}_{n,k,i}.
\end{aligned}$$

4.7.3 Linear SWE

$$\begin{aligned}
\boldsymbol{u}_t &= -f \hat{\boldsymbol{r}} \times \boldsymbol{u} + \nabla h \\
h_t &= -\mathcal{H} \nabla \cdot \boldsymbol{u}
\end{aligned}$$

$\implies$

$$\begin{aligned}
\boldsymbol{u}_{n+1} &= \boldsymbol{u}_n - \Delta t \, f \hat{\boldsymbol{r}} \times \boldsymbol{u}_{n+1} + \Delta t \, \nabla h_{n+1} \\
h_{n+1} &= h_n - \Delta t \, \mathcal{H} \nabla \cdot \boldsymbol{u}_{n+1}
\end{aligned}$$

$\Longrightarrow$

$$\begin{aligned}\boldsymbol{u}^c_{n+1} &= \boldsymbol{u}^c_n - \Delta t\, F\boldsymbol{u}^c_{n+1} + \Delta t\, G\boldsymbol{h}^c_{n+1}\\ P\boldsymbol{h}^c_{n+1} &= P\boldsymbol{h}^c_n - \Delta t\, \mathcal{H} D\boldsymbol{u}^c_{n+1}\end{aligned}$$

where $F : \mathbb{T} \to \mathbb{T}$ is the operator for $f\hat{\boldsymbol{r}}\times$, $D : \mathbb{T} \to \mathbb{Q}^{(1)}$ is the operator for $\rho^2\nabla\cdot$, $G : \mathbb{W}^{(1)} \to \mathbb{T}$ is the operator for ∇, and $P : \mathbb{W}^{(1)} \to \mathbb{Q}^{(1)}$ is the operator for multiplication by $\rho(z)^2$.

Chapter 5

Summary and future directions

5.1 Summary

In this thesis, we have developed sparse spectral methods for solving partial differential equations (PDEs) on disk-slices and trapeziums in 2D, and spherical caps as a surface 3D. The work can also be used as a template for developing similar methods on other such similar domains, in particular other subdomains of the sphere.

We began with an introduction to multidimensional sparse spectral methods by looking at the spherical harmonics on the whole sphere, explaining how they can be written as orthogonal polynomials in x, y, z, and how Jacobi and differential operators that apply to coefficient vectors will hence be banded-block-banded.

For the disk-slice in 2D, we defined the OPs that allow similar sparse and banded-block-banded operators required for solving PDEs in the domain, deriving their structure and providing a method to efficiently calculate numerically their entries. The reason they need to be calculated numerically is due to the non-classical univariate OPs that are involved in the 2D OP definitions. Finally, we moved on to use the same arguments for the spherical cap, a 3D surface that is a subdomain of the unit sphere. We once again defined the 3D OPs as orthogonal polynomials in in x, y, z, and showed how the differential operator matrices continue to elicit similar banded-block-banded structure.

5.2 Future directions

We hope that this thesis can serve as somewhat of a blueprint for formalising sparse spectral methods, including how one should define the OPs and derive the accompanying Jacobi and differential operators. The motivation behind this work was to develop sparse spectral methods for subdomains of the unit sphere in 3D space. Thus, the natural direction from this point would be to formalise the framework for spherical bands, which would simply involve slightly more complex arithmetic and the sub-block bands would be slightly larger (this due to the R polynomials we defined now having no zero coefficients in their three-term recurrences, meaning the expressions for multiplication by x, y, z would gain some extra terms).

Ideally, we would like to pair this with a spectral element method for the sphere, where the elements would be the spherical subdomains of spherical bands and spherical caps. The goal here would be to test this method against the full sphere spectral method the is in place in the ECMWF model, with the hypothesis being that by reducing the size of the transforms, we can improve the overall efficiency while still maintaining the accuracy that we achieve from a spectral approach.

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