Imperial College of Science, Technology and Medicine
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Sparse Spectral Methods on Disk-Slices, Trapeziums and Spherical Caps

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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 in 3D. For the latter, the PDEs are surface PDEs involving Laplace-Beltrami operators, spherical gradients and other spherical operators.

We begin with an introduction to sparse spectral methods via viewing spherical harmonics as multidimensional orthogonal polynomials in x, y, and z. We explain how differential operators can be applied as banded-block-banded matrix operators to coefficient vectors for a function's expansion. Further, we demonstrate how vector spherical harmonics in x, y, and z can be used as an orthogonal basis for vector-valued functions, yielding similar banded-block-banded gradient and divergence operators.

We move on to 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.

Piecing together the techniques used thus far, we present a new orthogonal polynomial basis and sparse spectral method for the spherical cap, complete with the same observation of the guaranteed sparsity of operators. The motivation is for one to use spherical caps bands as in a spectral element method for the sphere, with many applications in meteorology and astrophysics – in particular, as a potential replacement of the spherical harmonics approach cur-

rently in use at ECMWF, which is predicted to become too costly due to a parallel scalability bottleneck arising from the global spectral transform.

Foreword

Much of the work in this thesis has already been published, or submitted for publication.

- The contents of Chapter 3 has been published in:

  Ben Snowball and Sheehan Olver. Sparse spectral and p-finite element methods for partial differential equations on disk slices and trapeziums. *Studies in Applied Mathematics*, 145(1):3–35, 2020.

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- The contents of Chapter 4 has been submitted for publication in *Transactions of Mathematics and Its Applications*:

  Ben Snowball and Sheehan Olver. Sparse spectral methods for partial differential equations on spherical caps. arXiv preprint arXiv:2012.11493, 2020.

Declaration

I declare that all the work included in this thesis is, to the best of my knowledge, original unless otherwise attributed.

Ben Snowball, June 2021.

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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. For example, univariate OPs have been used to derive spectral methods to numerically solve one-dimensional differential equations (see e.g. [84, 12, 30, 9, 49, 71, 58]). While there are many famous examples of univariate OPs – such as the Jacobi polynomials, with special cases of the Legendre polynomials and the Chebyshev polynomials but to name a few of the classical families [55, §18.3] – the area of multivariate orthogonal polynomials has a smaller array of research.

One could say this is surprising, given that there is a long history of around 150 years associated with multivariate OPs, beginning with Hermite first presenting the multivariate Hermite polynomials in 1865 [1, 38]. Zernike polynomials [93] were first introduced in 1934, as another example, that are a group of bivariate polynomials orthogonal on a unit circle. Koornwinder in 1975 described a method for constructing two-variable OPs from univariate OPs [41]. However, few books have been published over the years on the topic of multivariate orthogonal polynomials, with the notable exception of the book by Dunkl and Xu [22]. As Dumitriu, Edelman and Shuman said in 2007, "[multivariate orthogonal polynomials] are understudied, underapplied, and important applications may be being missed" [21], while in 2016, Olver opined that "there is still a long way to go before multivariate orthogonal polynomials can reach their full potential in applications". He hypothesised that "[p]art of this neglect may be due to the fact that mutually orthogonal polynomials are not uniquely defined: there is no canonical ordering" and continued "[e]ven when explicit constructions are known, these are often unwieldy" [56].

This branch of mathematics has an encouraging future though, not least as a basis for sparse spectral methods for solving partial differential equations (PDEs) on multidimensional domains. Spectral methods have been developed for solving PDEs as an alternative to finite difference and finite element methods. For example, in recent years spectral methods have been established on the triangle [59] using OPs inspired by the Koornwinder approach for defining them, and on the disk [86] using Zernike polynomials.

There are various interpretations of what a "spectral method" is. It could be described as one that achieves spectral convergence of its solutions [30], or one that uses Laplacian eigenfunctions as basis functions [94], or one that uses OPs as basis functions for the approximation of a solution [59]. It is the latter that we refer to for our purposes as a spectral method in the body of the thesis. By utilising OPs as basis functions, we can develop sparse spectral methods (SSMs), meaning that the naturally sparse relationships between the basis OPs lead to sparse operator matrices that represent the differential operations in the equation to solve. Sparse spectral methods for one dimensional problems have been shown to lead to "almost banded" matrices [58].

In this thesis we expand upon this knowledge by providing frameworks for similar sparse spectral methods for solving PDEs on other multidimensional domains (notably including the disk-slice and trapezium in 2D, and the spherical cap surface in 3D) that also yield matrices that are what is defined as "banded-block-banded". We take inspiration from the work established for the triangle [59] and the unit disk [86], which can be seen as special cases of the disk-slice and trapezium in the framework we present here. The spherical cap work serves to lay a foundation for using spherical caps and spherical bands as elements in a spectral element method for solving PDEs on the whole sphere, as an alternative to the spherical harmonic transform approach that the European Centre for Medium-range Weather Forecasts (ECMWF) use in their weather and climate model [15].

Spherical harmonics (SHs) are of course a long-established and famous group of functions defined on the surface of a sphere with certain useful properties (for example, they are orthogonal to each other on the unit sphere, have sparse recurrences, and are eigenfunctions of the spherical Laplacian) and as a result are widely used in many scientific fields for solving PDEs including computer graphics (e.g. [52, 77]), astrophysics (e.g. [87]), quantum theory (e.g. [85]), biochemistry (e.g.[63, 3]), geosciences (e.g. [26, 34]) and meteorology (e.g. [24, 67, 89, 4, 17, 73, 30]). Spectral methods on the sphere involving spherical harmonics have been used for over 60 years [73]. Notably, spherical harmonics are also used as basis functions for the spectral transform method that makes up part of the model in the Integrated Forecasting System (IFS), which is used by ECMWF for their forecasts [89].

There are other modelling systems using global spectral models too. For example, the AGCM3 model developed by the Canadian Centre for Climate Modelling and Analysis (CCCma) and the Community Earth System Model (CESM) both use a spectral dynamical core[1] [36, 70], while the Geophysical Fluid Dynamics Laboratory (GFDL) has also developed a global spectral atmospheric model [29].

While the whole sphere spectral method using the spherical harmonics has been successful for numerous years [91], 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 IFS [4, 89].

Many implementations of an algorithm to compute the spectral transform (or spherical harmonic transform) exist (see e.g. [75, 81]). For the IFS, the spherical harmonic transform in fact uses two transforms – a Fourier transform (using the well-established Fast Fourier Transform (FFT) [16]) in the longitudinal direction and a Legendre transform in the latitudinal direction – and it is the Legendre transform that has been identified as inhibiting future performance due to its computational cost. While a Fast Legendre Transform (FLT) [89] has been incorporated into the model, along with new grid types [48], to help to extend the lifespan of the spectral method for numerical weather prediction (NWP), it may not be sufficient for certain desired cases and resolutions [88].

The motivation for this project was to help address this problem while still

[1]A *dynamical core* is part of a model that deals with numerically solving the equations of motion on the underlying grid, as opposed to other physical processes.

utilising a spectral approach. More precisely, we aim to develop a sparse spectral method for solving 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. This, however, is future work beyond the scope of this thesis. By spectral element method, we mean a finite element method (FEM) that uses high degree basis polynomials for its elements (this could also be referred to as a p-FEM with large p). In other words, we can use our spectral methods developed for the spherical band and cap elements as part of a finite element framework. By using this approach, one can avoid having to compute the global spectral transform (in particular, the global Legendre transform) and instead simply apply the local element transforms in parallel. Moreover, by still using a spectral approach, one can maintain the high accuracy and excellent error properties that such methods bring. Solving PDEs on a section of the sphere surface is still useful for numerical weather prediction in its own right too, where one could for example perform a more localised simulation near a pole while still using a "global" (in the domain sense) spectral method approach. Moreover, there are also prospective applications in physics, particularly in astrophysics, where solving PDEs on the sphere surface and working in spherical geometries is also desirable (e.g. [87, 66, 7, 85, 76, 67]).

Recently, a method for computing tensor fields in spherical coordinates using Jacobi polynomials has been proposed [87]. In this work the authors present the method for both the surface of the unit sphere and the three-dimensional generalisation of the unit ball. Their method involves using a spectral basis to represent functions too, choosing for the angular part of the basis to be the spin-weighted spherical harmonics (of which the spherical harmonics are a special case, with spin 0) in spherical coordinates. By using these as their basis functions, they are able to derive sparse relations for the Laplacian operator, as well as for multiplication of the basis by $\cos\varphi$ and $\sin\varphi$ (where φ is the polar angle from the z axis in cartesian coordinates), which lead to operators for operations with angular dependencies involving these.

On the other hand, we aim to propose a strictly orthogonal *polynomial* basis, and derive sparse operators for multiplication by the cartesian coordinate axes, which can in turn lead to operators for multiplication by trigonometric functions too. By utilising orthogonal polynomials in cartesian coordinates, we can develop a sparse spectral method on subdomains of the sphere surface (e.g. the spherical cap) using our knowledge of other geometries and methods involving OPs developed for them.

The construction of the spectral methods in this thesis follow a similar pattern that is worth detailing here as a general framework.

1. *Define the domain of interest.*

   It is best to do this via a restriction of one coordinate in terms of the others, using a function ρ that satisfies one of two conditions we will detail later. As an example, for a domain in 2D space, we would define this as $\Omega := \{(x, y) \in \mathbb{R}^2 \quad | \quad \alpha \le x \le \beta,\ \gamma\rho(x) \le y \le \delta\rho(x)\}$ for given constants $\alpha, \beta, \gamma, \delta$.

2. *Express the multivariate and multi-parameter OPs as polynomials in cartesian coordinates.*

The construction of the multivariate OPs takes its inspiration from the Koornwinder approach [41]. The construction will make use of the function ρ. These OPs will be d-parameter, meaning that we can construct operators that raise or lower the parameter values, and thus represent conversion between the OP bases.

3. *Derive expressions for multiplication of the OPs by the coordinates.*

4. *Use these relations to determine the entries to "Jacobi matrices"*

   These "Jacobi matrices" J_x, J_y, etc. represent multiplication by the coordinates when applied to the degree-ordered vector of OPs, $\mathbb{P}$. They will be banded-block-banded in structure – in fact, due to the construction, they will be block-tridiagonal. Continuing with the 2D example:

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

   The degree-ordered vector of OPs, $\mathbb{P}$, can be thought of as being made up of ordered sub-vectors grouped by polynomial degree, $\mathbb{P}_n$ for $n \in \mathbb{N}_0$.

5. *Create a three-term recurrence for the vector of OPs of degree n.*

   This is done by combining the systems $J_x\mathbb{P} = x\mathbb{P}$ and $J_y\mathbb{P} = y\mathbb{P}$ (and $J_z\mathbb{P} = z\mathbb{P}$ if in three-dimensional space). The resulting three-term recurrence will have the form:

$$\mathbb{P}_{n+1}(x,y) = -D_n^\top (B_n - G_n(x,y))\mathbb{P}_n(x,y) - D_n^\top C_n \, \mathbb{P}_{n-1}(x,y).$$

Here, the matrices B_n, C_n and G_n are defined via:

$$C_n := \begin{pmatrix} C_{x,n} \\ C_{y,n} \end{pmatrix} \; (n \neq 0), \quad B_n := \begin{pmatrix} B_{x,n} \\ B_{y,n} \end{pmatrix}, \quad G_n(x,y) := \begin{pmatrix} xI_{n+1} \\ yI_{n+1} \end{pmatrix}.$$

The matrices $D_n^\top$ are left-inverses of the matrices A_n respectively, which are defined similarly:

$$A_n := \begin{pmatrix} A_{x,n} \\ A_{y,n} \end{pmatrix}.$$

6. *Use the multivariate version of the Clenshaw algorithm for evaluation of functions that are expanded in the OP basis.*

7. *Derive (sparse) relationships for various differential operations, and relations for raising and lowering the parameter values of the OPs.*

8. *Construct the sparse operator matrices representing these operations.*

   The differential operators may raise or lower parameter values, which is why the basis conversion operators are required. Further operators can be constructed as combinations of others – for example, a second derivative would be the multiplication of two first derivative operators. Notably, these operator matrices will be banded-block-banded in structure.

9. *Use the "operator Clenshaw algorithm" to construct operator matrices for the action of multiplying by a general function.*

   For instance, this would be useful for constructing an operator matrix that represents a variable coefficient in a Helmholtz example.

By following this framework, one will be able to write down a given PDE in spectral space (i.e. as a matrix-vector equation). The variables are given by their coefficients for their expansion in the OP basis, while the differential and other operations are given by their relevant operator matrices. The resulting system's sparsity is a result of the sparse relations of the OPs.

The structure of the remainder of thesis is as follows.

Chapter 2 of this thesis provides an introduction to sparse spectral methods via the spherical harmonics on the whole sphere surface. Here, we think of the spherical harmonics in a non-traditional way and write them as a group of multidimensional orthogonal polynomials in (x, y, z) as opposed to functions of spherical coordinates. We present an OP 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 a function's expansion. Further, we demonstrate how the vector spherical harmonics (VSHs) can be used as an orthogonal basis for vector valued functions lying in the "tangent bundle" of the sphere, and thus how one can additionally derive gradient and divergence operators.

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. The work in this chapter has been previously published [78].

With a greater knowledge base in our quiver, we can adapt the techniques learnt from the founding of the disk-slice formulation to surfaces in 3D in Chapter 4. Using the same family of (non-classical) 1D OPs, we present a suitable orthogonal polynomial basis for the spherical cap, a subdomain of the surface of a unit sphere, complete with sparse differential operators. A relatively simple adaption permits this framework to be extended to a spherical band. From here, a spectral element method could be devised for the whole sphere using the aforementioned as elements. The work in this chapter has been accepted for publication [79].

Chapter 5 gives a summary of the work we have presented and details avenues for future directions that one could take it.

Finally, as an appendix, we outline how one could approach a vector OP basis for the "tangent bundle" of the spherical cap, analogous to the vector spherical harmonics on the whole sphere. This constitutes Appendix A.

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, and z to evaluate functions and solve PDEs on the whole sphere. More precisely, we desire the solution to partial differential equations on the domain

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

where

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

While it may seem somewhat odd, it should hopefully become apparent why using ρ here is a practical way to define our domain.

It is useful to be able to transform between these cartesian coordinates and the spherical coordinates (φ, θ). Throughout this thesis we will use the convention that the spherical coordinate angles be defined by

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

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

In this chapter, we demonstrate how one can write the spherical harmonics as polynomials in (x, y, z), and how the relationships between them can be used to obtain sparse "Jacobi operators" for multiplication by x, y, and z. We demonstrate how these in turn lead to an algorithm for evaluating the spherical harmonics, an efficient algorithm for evaluating functions when expanded in the SH OP basis, and sparse "banded-block-banded" differential operator matrices. The techniques used here are done so with the aim of applying them to other OP families on other domains (and we do so in later chapters). We will finally demonstrate a proof-of-concept via the examples of the heat equation and the linearised shallow water equations on the unit sphere. These examples consider partial differential operators involving the spherical Laplacian (the Laplace–Beltrami operator): written in spherical coordinates this is

$$\Delta_{\mathrm{S}} = \frac{1}{\sin\varphi}\frac{\partial}{\partial\varphi}\Big(\sin\varphi\frac{\partial}{\partial\varphi}\Big) + \frac{1}{\sin^2\varphi}\frac{\partial^2}{\partial\theta^2} = \frac{1}{\rho}\frac{\partial}{\partial\varphi}\Big(\rho\frac{\partial}{\partial\varphi}\Big) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}, \tag{2.1}$$

i.e. $\Delta_{\mathrm{S}} f(\mathbf{x}) = \Delta f(\frac{\mathbf{x}}{\|\mathbf{x}\|})$ for some function f where $\mathbf{x} := (x, y, z) \in \mathbb{R}^3$.

The code that allows one to produce the numerical examples in this chapter is publicly available as a Julia package[1] that partners with the ApproxFun package [57] – however, this package is purely experimental at this stage.

2.1 Defining the spherical harmonics in three variables

Before we proceed further, let us build up to our definition of the spherical harmonics. We first need to introduce a few classical orthogonal polynomials. Orthogonal polynomials are defined as such by the condition that each polynomial is orthogonal to each other, with respect to a given inner product, and ordered by degree. In particular, they are orthogonal with respect to all lower degree polynomials.

On the unit interval, $[-1, 1]$, we note that there is a hierarchy of OPs in the sense that [55, Table 18.3.1, (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 degree l *Jacobi polynomial* with $a, b > -1$, and $P_l(x) := P_l^{(0,0)}(x)$ is simply the *Legendre polynomial* of degree l. Jacobi polynomials are orthogonal with respect to the weight $w(x) = (1-x)^a(1+x)^b$; that is for

[1] https://github.com/snowball13/SphericalHarmonics.jl

$l, l' \in \mathbb{N}_0$,

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

where $\delta_{l,l'}$ is the regular Kronecker delta function. For the Jacobi polynomials,

$$\omega_{P,l}^{(a,b)} = \frac{2^{a+b+1} \, \Gamma(l+a+1) \, \Gamma(l+b+1)}{(2l+a+b+1) \, \Gamma(l+a+b+1) \, \Gamma(l+1)},$$

where $\Gamma(x)$ is the regular Gamma function [55, (5.2.1)] (with $\Gamma(n) = (n-1)!$ for $n \in \mathbb{N}$). Legendre polynomials are special cases of *Legendre functions* when l is a non-negative integer. Legendre functions are a class of univariate functions that are one set of solutions to the differential equation

$$(1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}y - 2x\frac{\mathrm{d}}{\mathrm{d}x}y + l(l+1)y = 0, \quad x \in [-1,1]$$

which is helpfully known as the *Legendre equation* [55, (14.2.1)]. Further, the *associated Legendre polynomials* are a set of polynomials orthogonal with respect to unit weight on the unit interval, and can be defined as the m^{th} derivative of a Legendre polynomial [5, p.5]:

$$P_l^m(x) := (-1)^m (1-x^2)^{\frac{m}{2}} \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) = (-1)^m \, \frac{(l+m)!}{2^m \, l!} \, (1-x^2)^{\frac{m}{2}} \, P_{l-m}^{(m,m)}(x),$$

for $m = 0, 1, 2, \ldots, l$. It is also standard to include a further definition for the case of m negative – that is we also define:

$$P_l^m(x) := (-1)^m \frac{(l+m)!}{(l-m)!} P_l^{|m|}(x) = \frac{(l+m)!}{2^{|m|}\, l!} (1-x^2)^{\frac{|m|}{2}} P_{l-|m|}^{(|m|,|m|)}(x),$$

for $m = -l, \ldots, -1$.

Once again, associated Legendre polynomials are special cases of *associated Legendre functions* when l is a non-negative integer and $m \in \{0, \ldots, l\}$, which are also a class of univariate functions that are solutions to a modified version of the Legendre equation

$$(1-x^2)\frac{\mathrm{d}^2}{\mathrm{d}x^2}y - 2x\frac{\mathrm{d}}{\mathrm{d}x}y + \left[l(l+1) - \frac{m^2}{1-x^2}\right]y = 0,$$

which is also helpfully known as the *associated Legendre equation* ([5, p.2], [55, (14.2.2)]). We can see that Legendre functions (and polynomials) are just special cases of the associated versions when $m = 0$.

Although often referred to as the associated Legendre "polynomials" as we do here when l is a non-negative integer and $m \in \{0, \ldots, l\}$, P_l^m are not strictly polynomials when m is odd, and as such some authors refer to them as associated Legendre functions regardless instead. Moreover, it should be noted too that the inclusion of the $(-1)^m$ factor in the definition for $m > 0$, known as the *Condon-Shortley phase* in physics, is sometimes omitted.

These relationships for the Jacobi polynomials and associated Legendre polynomials allow us to explicitly see where the normalising constants that we shall be using for our definition of the spherical harmonics come from.

On that note, we can now write down the spherical harmonics. Let $(x, y, z) \in$

Ω. We will use the standard definition – that is, the spherical harmonics, orthonormal on the unit sphere, are [55, (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 $0 \le |m| \le l$, $l \in \mathbb{N}_0$, where

$$c_l^m := \left(\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!}\right)^{\frac{1}{2}} \frac{(l+m)!}{2^{|m|}\,l!} \begin{cases} (-1)^m & \text{if } m \ge 0 \\ 1 & \text{if } m < 0, \end{cases} \tag{2.3}$$

which can be simplified to

$$c_l^m = \left(\frac{(2l+1)\,(l+m)!\,(l-m)!}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^{|m|+1}\,l!} \begin{cases} (-1)^m & \text{if } m \ge 0 \\ 1 & \text{if } m < 0. \end{cases}$$

The spherical harmonics as defined are then orthonormal with respect to the inner product with uniform measure

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

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, and z instead of φ, θ by noting that $\rho(z)^{|m|}e^{im\theta}$ can be expressed in terms of x, y, and z for any $m \in \mathbb{Z}$. Indeed, they are polynomials in x, y, and z, which we denote $Y_l^m(x, y, z)$. They span all polynomials modulo the vanishing ideal associated by the zero set of $x^2 + y^2 + z^2 - 1$ in $\mathbb{R}^3$.

2.2 Jacobi matrices

Jacobi operators are matrices that correspond to multiplication of the orthogonal polynomial basis, in this case the spherical harmonics, by our cartesian coordinates x, y, and z. We can obtain the entries to these operator matrices by determining the coefficients of $x\,Y_l^m(x, y, z)$, $y\,Y_l^m(x, y, z)$, 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. Relations concerning the products of spherical harmonics have already been established, and so the expressions we desire here could just be seen as special cases of these. More specifically, the coefficients of the expansion in the SH basis of the product of two SHs are composed of Clebsch–Gordan coefficients [69, p.231]. Clebsch–Gordan coefficients are important in quantum mechanics and angular momentum, with tables and algorithms existing to calculate them [50]. By simply choosing appropriate combinations, one could gain the desired coefficients for the expansion of each of $x\,Y_l^m(x, y, z)$, $y\,Y_l^m(x, y, z)$, and $z\,Y_l^m(x, y, z)$.

However we reiterate our goal here is to use techniques that can generalise to spectral methods on other domains using multidimensional OPs, and thus we proceed by exploiting the three-term recurrences and other relations of the univariate OPs that make up the spherical harmonics as we have defined them. With that being said, we require a few results concerning the incrementing and decrementing of the parameters for the Jacobi polynomials, and the three-term recurrence for the Jacobi polynomials, that will also prove useful later on in this chapter.

Lemma 1. *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 $n \in \mathbb{N}_0$ the following identities hold:*

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

$$
\begin{aligned}
2) \quad (1-z^2)\, P_n^{(\alpha,\beta)}(z) = \frac{4}{2n+\alpha+\beta+1} \Big\{ &\frac{(n+\alpha)(n+\beta)}{2n+\alpha+\beta} P_n^{(\alpha-1,\beta-1)}(z) \\
&+ (n+1) \Big[\frac{n+\alpha+1}{2n+\alpha+\beta+2} - \frac{n+\beta}{2n+\alpha+\beta} \Big] P_{n+1}^{(\alpha-1,\beta-1)}(z) \\
&- \frac{(n+1)(n+2)}{2n+\alpha+\beta+2} P_{n+2}^{(\alpha-1,\beta-1)}(z) \Big\},
\end{aligned}
$$

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

Proof. The first two results are simply consequences of the relationships established for incrementing and decrementing the parameters of Jacobi polynomials detailed in [55, (18.9.5), (18.9.6)], along with the symmetry relation that $P_n^{(\alpha,\beta)}(-z) \equiv (-1)^n P_n^{(\beta,\alpha)}(z)$. The final one is obtained by rearranging the three-term recurrence in [55, (18.9.1), (18.9.2)]. $\square$

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

Corollary 1. *Let $l, m \in \mathbb{N}_0$ s.t. $0 \le m \le l$ and let $z \in [-1, 1]$. Then:*

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

where

$$\tilde{\alpha}_{l,m,1} := \frac{2l}{2l+1}, \qquad \tilde{\alpha}_{l,m,2} := \begin{cases} -\frac{l}{2(2l+1)} & \text{if } l-m \ge 2 \\ 0 & \text{otherwise}, \end{cases}$$

$$\tilde{\alpha}_{l,m,3} := -\frac{2(l-m+2)(l-m+1)}{(2l+1)(l+1)}, \qquad \tilde{\alpha}_{l,m,4} := \frac{(l+m+2)(l+m+1)}{2(2l+1)(l+1)},$$

$$\tilde{\gamma}_{l,m,1} := \begin{cases} \frac{l}{2l+1} & \text{if } l-m \ge 1 \\ 0 & \text{otherwise}, \end{cases} \qquad \tilde{\gamma}_{l,m,2} := \frac{(l-m+1)(l+m+1)}{(2l+1)(l+1)}.$$

Corollary 1 allows us to easily determine the aforementioned coefficients, that we will formalise in the following Lemma.

Lemma 2. *For $l \in \mathbb{N}_0$, $m \in \mathbb{Z}$ s.t. $0 \le |m| \le l$, the spherical harmonics* *satisfy the relationships:*

$$x\, Y_l^m(x,y,z) = \alpha_{l,m,1} Y_{l-1}^{m-1}(x,y,z) + \alpha_{l,m,2} Y_{l-1}^{m+1}(x,y,z) + \alpha_{l,m,3} Y_{l+1}^{m-1}(x,y,z) + \alpha_{l,m,4} Y_{l+1}^{m+1}(x,y,z), \tag{2.4}$$

$$y\, Y_l^m(x,y,z) = \beta_{l,m,1} Y_{l-1}^{m-1}(x,y,z) + \beta_{l,m,2} Y_{l-1}^{m+1}(x,y,z) + \beta_{l,m,3} Y_{l+1}^{m-1}(x,y,z) + \beta_{l,m,4} Y_{l+1}^{m+1}(x,y,z), \tag{2.5}$$

$$z\, Y_l^m(x,y,z) = \gamma_{l,m,1} Y_{l-1}^{m}(x,y,z) + \gamma_{l,m,2} Y_{l+1}^{m}(x,y,z), \tag{2.6}$$

where

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

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

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

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

where the $c_{l'}^{m'}$ are defined in equation (2.3).

Remark: The results in Lemma 2 can be derived via the relationships established for products of spherical harmonics and Clebsch-Gordan coefficients as mentioned earlier [69, p.231] but we include this proof so as to generalise to other OPs later on in later chapters.

Proof of Lemma 2. The expression for multiplication of the spherical harmonic Y_l^m by z is simply a consequence of the third result in Corollary 1:

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

For multiplication by x and y, note that the complex exponential satisfies

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

Combining this with the results in Corollary 1, the expressions for multiplication of the spherical harmonic Y_l^m by x and y are then:

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

and

$$
\begin{aligned}
y\, Y_l^m(x,y,z) &= c_l^m \sin\theta\, e^{im\theta}\, \rho(z)^{|m|+1} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= -\frac{1}{2} i\, c_l^m (e^{i(m+1)\theta} - e^{i(m-1)\theta})\, \rho(z)^{|m|+1} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= i \Big\{ \alpha_{l,m,1} Y_{l-1}^{m-1}(x,y,z) - \alpha_{l,m,2} Y_{l-1}^{m+1}(x,y,z) \\
&\qquad + \alpha_{l,m,3} Y_{l+1}^{m-1}(x,y,z) - \alpha_{l,m,4} Y_{l+1}^{m+1}(x,y,z) \Big\}.
\end{aligned}
$$

□

These recurrences lead to Jacobi operators that correspond to multiplication by x, y, and z of the OPs. Define for $l \in \mathbb{N}_0$:

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

Note that these OP vectors we have defined are grouped and ordered according to the degree l, and within each degree ordered by the Fourier mode m. Let the Jacobi matrices J_x, J_y, J_z hence be given by

$$
\begin{aligned}
J_x \mathbb{P}(x,y,z) &= x \mathbb{P}(x,y,z), \\
J_y \mathbb{P}(x,y,z) &= y \mathbb{P}(x,y,z), \\
J_z \mathbb{P}(x,y,z) &= z \mathbb{P}(x,y,z),
\end{aligned} \tag{2.7}
$$

for $(x,y,z) \in \Omega$. While J_x, J_y, J_z are not Jacobi matrices in the classical sense, they are block Jacobi matrices. However, it is useful to simply label them as such. These Jacobi matrices can act on the coefficients vector of a function's expansion in the spherical harmonic basis to implement the operation for multiplication by x, y or z. For example, given sufficiently large $n \in \mathbb{N}$ let the function $f(x, y, z) : \Omega \to \mathbb{C}$ be given by its expansion

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

where

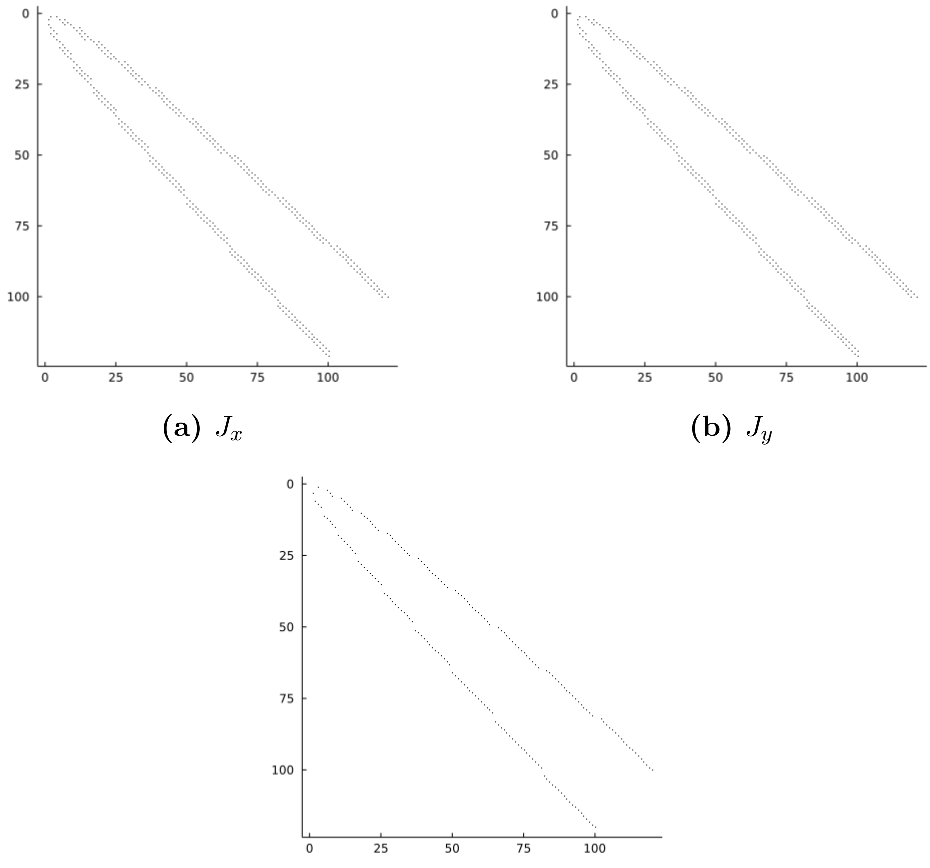
$$\boldsymbol{f}_l := \begin{pmatrix} f_{l,-l} \\ \vdots \\ f_{l,-l} \end{pmatrix} \in \mathbb{C}^{2l+1}, \qquad \boldsymbol{f} := \begin{pmatrix} \boldsymbol{f}_0 \\ \vdots \\ \boldsymbol{f}_N \end{pmatrix}.$$

We say that $\boldsymbol{f}$ is the *coefficients vector* of the function f. Then $xf(x, y, z)$ is approximated by $\mathbb{P}(x, y, z)^\top\, J_x^\top\, \boldsymbol{f}$. In other words, $J_x^\top\, \boldsymbol{f}$ is the coefficient 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 (2.4–2.6), we have that the Jacobi matrices take the following



(a) J_x

(b) J_y

(c) J_z

Figure 2.1: "Spy" plots of the Jacobi operator matrices, showing their sparsity and structure, up to order $N = 10$ (i.e. $(N+1)^2$ unknowns). Dots represent non-zero entries of the operator. Each are block-tridiagonal, with the blocks corresponding to polynomial degree.

block-tridiagonal form (i.e. have block-bandwidths $(1,1)$):

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

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:

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

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

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

The sparsity and structure of the Jacobi matrices as we have defined them can be seen visually in Figure 2.1.

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

Three-term recurrence relations for orthogonal polynomials are well established (see for example [55, §18.9]), including for multidimensional OPs [22, §3.2]. In a similar vein, we can obtain a recurrence relation for the spherical harmonics by combining each system in equation (2.7) in a specific way. It should be emphasised at this point that this is not necessarily the optimal way of computing the spherical harmonics; various efficient methods and algorithms have been proposed (see e.g. [32, 77, 27]). We present this method in order to be able to generalise it to other multidimensional OP families later on in this thesis.

Rewriting equation (2.7), we have that:

$$(J_x - xI)\mathbb{P}(x,y,z) = (J_y - yI)\mathbb{P}(x,y,z) = (J_z - zI)\mathbb{P}(x,y,z) = \mathbf{0}.$$

Combining these relationships into a single system, complete with initial (degree 0) value, results in:

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

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 $l = 0, 1, 2\ldots$,

$$A_l := \begin{pmatrix} A_{x,l} \\ A_{y,l} \\ A_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+3)}, \quad C_l := \begin{pmatrix} C_{x,l} \\ C_{y,l} \\ C_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l-1)} \quad (n \neq 0), \tag{2.8}$$

$$B_l := \begin{pmatrix} B_{x,l} \\ B_{y,l} \\ B_{z,l} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+1)}, \quad G_l(x,y,z) := \begin{pmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{pmatrix} \in \mathbb{C}^{3(2l+1)\times(2l+1)}. \tag{2.9}$$

For each $l = 0, 1, 2\ldots$ 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 [22, §3.2], which can be expanded to obtain the three-term recurrence, for $l = 0, 1, 2, \ldots$:

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

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 order to attempt to maximise sparsity, we define them in the following way[2]. For $l \in \mathbb{N}$, we can set

$$D_l^\top = \begin{pmatrix} & & \boldsymbol{\eta}_0^\top & & & \\ 0 & & 0 & & \frac{1}{\gamma_{l,-l,2}} & \\ & \ddots & & \ddots & & \ddots \\ & 0 & & 0 & & \frac{1}{\gamma_{l,l,2}} \\ & & \boldsymbol{\eta}_1^\top & & & \end{pmatrix} \in \mathbb{R}^{(2l+3)\times 3(2l+1)}, \tag{2.10}$$

where $\boldsymbol{\eta}_0, \boldsymbol{\eta}_1 \in \mathbb{R}^{3(2l+1)}$ are vectors with entries given by

$$\left(\boldsymbol{\eta}_0\right)_j = \begin{cases} \frac{1}{\alpha_{l,-l,3}} & j = 1 \\ \frac{-\alpha_{l,-l,4}}{\alpha_{l,-l,3}\,\gamma_{l,1-l,2}} & j = 2(2l+1)+2 \\ 0 & \text{otherwise}, \end{cases}$$

$$\left(\boldsymbol{\eta}_1\right)_j = \begin{cases} \frac{1}{\alpha_{l,l,4}} & j = 2l+1 \\ \frac{-\alpha_{l,l,3}}{\alpha_{l,l,4}\,\gamma_{l,l-1,2}} & j = 3(2l+1)-1\,\cdot \\ 0 & \text{otherwise}. \end{cases}$$

For $l = 0$ we can simply set

$$D_0^T = \begin{pmatrix} \frac{\beta_{0,0,4}}{\alpha_{0,0,3}\beta_{0,0,4}-\alpha_{0,0,4}\beta_{0,0,3}} & \frac{-\alpha_{0,0,4}}{\alpha_{0,0,3}\beta_{0,0,4}-\alpha_{0,0,4}\beta_{0,0,3}} & 0 \\ 0 & 0 & \frac{1}{\gamma_{0,0,2}} \\ \frac{\beta_{0,0,3}}{\alpha_{0,0,4}\beta_{0,0,3}-\alpha_{0,0,3}\beta_{0,0,4}} & \frac{-\alpha_{0,0,3}}{\alpha_{0,0,4}\beta_{0,0,3}-\alpha_{0,0,3}\beta_{0,0,4}} & 0 \end{pmatrix}. \tag{2.11}$$

It will be convenient for us to give a formal name for these coefficient matrices

[2]There may be a more computationally efficient way of defining these matrices, but in practice we only desire the output of the action of $D_l^\top C_l$ and $D_l^\top(B_l - G_l(x,y,z))$, and so minimising the resulting number of operations is the goal. The choices of the $D_l^\top$ matrices we make in this thesis are designed to do this, but whether there are more computationally efficient ways of defining them is an open question.

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 (2.8–2.11) 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

In coefficient 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

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

using the orthonormality of the spherical harmonics. As discussed in Chapter 1, methods to calculate these coefficients exist known as spectral transforms, and are well established for the spherical harmonics (see e.g. [51, 81]). Additionally, packages are available for public use that implement efficient spherical harmonics transforms, for example the FastTransforms package [75].

2.4.2 Function evaluation

A multivariate analogue of Clenshaw's recursive algorithm for evaluation of a function expanded in an OP basis has been established for methods on other domains in 2D such as the triangle [59], and we proceed similarly here. We can use the Clenshaw algorithm to evaluate this function at a given point (x, y, z) on Ω [64]. The multidimensional *Clenshaw algorithm* is as follows:

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

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

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

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 us explain what we mean by this. 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 $\boldsymbol{\xi}_{N+2} = \mathbf{0}$, $\boldsymbol{\xi}_{N+1} = \mathbf{0}$
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: $V = V(x,y,z) \approx \xi_0 Y_0$

where at each iteration, $\boldsymbol{\xi}_n$ is a vector of matrices[3] (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

We have established that the spherical harmonics can be viewed as a basis of orthonormal polynomials on the sphere. Specifically, given a function $f : \Omega \to$

[3] It may help to think of this symbolically. At each iteration, the entries of $\boldsymbol{\xi}_n$ are polynomials in J_x, J_y and J_z. On the final step, $\boldsymbol{\xi}_0 = \xi_0$ is hence some polynomial expression in J_x, J_y and J_z, which we can then evaluate by inserting the Jacobi matrices.

$\mathbb{C}$, we can write $f = \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m}\ Y_l^m$ where $\{f_{l,m}\}$ are coefficients and $N \in \mathbb{N}$ is sufficiently large. But what about vector-valued functions?

Definition 3. *Let $(x, y, z) \in \Omega$. We refer to the* ***tangent space*** *of the point (x, y, z) as the space of all vectors that are orthogonal to the vector $\hat{\boldsymbol{r}} := [x, y, x]^\top$. We further define the* ***tangent bundle*** *of Ω as the set of all such spaces for every point in Ω.*

For the purposes of this discussion, we will only consider the tangent bundle, and thus wish to write down a basis for vector-valued functions with values in the tangent bundle. Fortunately, there is a simple solution known as the vector spherical harmonics (VSHs) [2]:

$$\begin{aligned}
\boldsymbol{\Psi}_l^m &:= \nabla_{\mathrm{S}} Y_l^m = \frac{\partial}{\partial \phi} Y_l^m \hat{\boldsymbol{\phi}} + \frac{1}{\sin\varphi} \frac{\partial}{\partial \theta} Y_l^m \hat{\boldsymbol{\theta}}, \\
\boldsymbol{\Phi}_l^m &:= \nabla_{\mathrm{S}}^{\perp} Y_l^m \equiv \hat{\boldsymbol{r}} \times \nabla_{\mathrm{S}} Y_l^m = \frac{\partial}{\partial \phi} Y_l^m \hat{\boldsymbol{\theta}} - \frac{1}{\sin\varphi} \frac{\partial}{\partial \theta} Y_l^m \hat{\boldsymbol{\phi}}.
\end{aligned} \tag{2.12}$$

Here, $\hat{\boldsymbol{r}}$ is simply the outward unit normal vector to the surface of the sphere at the point (x, y, z), while $\hat{\boldsymbol{\phi}}, \hat{\boldsymbol{\theta}}$ are the standard spherical coordinate unit vectors, i.e. $\hat{\boldsymbol{\phi}} := [\cos\theta\cos\varphi, \sin\theta\cos\varphi, -\sin\varphi]^\top$, $\hat{\boldsymbol{\theta}} := [-\sin\theta, \cos\theta, 0]^\top$. They are orthogonal with respect to the inner product $\langle \boldsymbol{A}, \boldsymbol{B} \rangle = \iint_\Omega \boldsymbol{A} \cdot \boldsymbol{B}^*\ \sin\varphi\, \mathrm{d}\varphi\, \mathrm{d}\theta$ – in particular, for any $l, l' \in \mathbb{N}$, $m, m' \in \mathbb{Z}$ s.t. $-l \le m \le l$, $-l' \le m' \le l'$,

$$\begin{aligned}
\left\langle \boldsymbol{\Psi}_l^m, \boldsymbol{\Psi}_{l'}^{m'} \right\rangle &= \iint_\Omega \boldsymbol{\Psi}_l^m \cdot \boldsymbol{\Psi}_{l'}^{m'*}\ \sin\varphi\, \mathrm{d}\varphi\, \mathrm{d}\theta = \delta_{l,l'}\delta_{m,m'}\ l(l+1), \\
\left\langle \boldsymbol{\Phi}_l^m, \boldsymbol{\Phi}_{l'}^{m'} \right\rangle &= \iint_\Omega \boldsymbol{\Phi}_l^m \cdot \boldsymbol{\Phi}_{l'}^{m'*}\ \sin\varphi\, \mathrm{d}\varphi\, \mathrm{d}\theta = \delta_{l,l'}\delta_{m,m'}\ l(l+1), \\
\left\langle \boldsymbol{\Psi}_l^m, \boldsymbol{\Phi}_{l'}^{m'} \right\rangle &= \iint_\Omega \boldsymbol{\Phi}_l^m \cdot \boldsymbol{\Phi}_{l'}^{m'*}\ \sin\varphi\, \mathrm{d}\varphi\, \mathrm{d}\theta = 0.
\end{aligned}$$

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. Such a function $\boldsymbol{u}$ we refer to as a *vector-valued function in the tangent bundle* of the sphere. Importantly, the set $\{\boldsymbol{\Psi}_l^m, \boldsymbol{\Phi}_l^m\}$ form a complete and orthogonal basis for such functions [2]. That is, given $\boldsymbol{u}$, there exist coefficients $\{u_{l,m}^{\boldsymbol{\Psi}_l^m}, u_{l,m}^{\boldsymbol{\Phi}_l^m}\}$ such that for large enough N:

$$\boldsymbol{u} = \sum_{l=0}^{N} \sum_{m=-l}^{l} u_{l,m}^{\boldsymbol{\Psi}}\, \boldsymbol{\Psi}_l^m + u_{l,m}^{\boldsymbol{\Phi}}\, \boldsymbol{\Phi}_l^m.$$

Vector spherical harmonics have been widely used in electrostatics (e.g. [2]), electrodynamics (e.g. [13]), and of course fluid dynamics including weather and climate modelling (e.g. [53, 25, 83]). Other definitions for VSHs are used (e.g. [33]), however it is convenient for deriving explicit sparse relations and operators to use the ones described here. In particular, we can note that computing the gradient or divergence of a function is merely a matter of conversion between the SH and the VSH bases.

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. Thus, we we can use the same techniques that we used for the scalar SHs to derive Jacobi matrices, function evaluation and transforms.

2.5.1 Jacobi matrices

We start as before for the scalar case by finding $x\,\mathbf{\Psi}_l^m(x,y,z)$, $y\,\mathbf{\Psi}_l^m(x,y,z)$, $z\,\mathbf{\Psi}_l^m(x,y,z)$, and $x\,\mathbf{\Phi}_l^m(x,y,z)$, $y\,\mathbf{\Phi}_l^m(x,y,z)$, $z\,\mathbf{\Phi}_l^m(x,y,z)$ in terms of $\mathbf{\Psi}_{l'}^{m'}(x,y,z)$, $\mathbf{\Phi}_{l'}^{m'}(x,y,z)$. 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:

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

$$\int_0^{2\pi} e^{im\theta}\, e^{-im'\theta}\, \sin(\theta)\mathrm{d}\theta = i\,\pi(\delta_{m',m-1} - \delta_{m',m+1}), \tag{2.14}$$

and, for $l \in \mathbb{N}_0, m \in \mathbb{Z}$ s.t. $-l \le m \le l$,

$$\int_{-1}^{1} P_{l-|m|}^{(|m|,|m|)}(z)\, P_{l'-|m|}^{(|m|,|m|)}(z)\, \rho(z)^{2|m|}\, \mathrm{d}z = \delta_{l',l}\, \frac{1}{2\pi(c_l^m)^2}, \tag{2.15}$$

$$P_{l-|m|}^{(|m|,|m|)}{}'(z) = d_{l,m}\, P_{l-(|m|+1)}^{(|m|+1,|m|+1)}, \quad \text{where } d_{l,m} := \begin{cases} \frac{1}{2}(l+|m|+1) & l > |m| \\ 0 & l = |m|\,. \end{cases} \tag{2.16}$$

Equation (2.15) and equation (2.16) are simply consequences of the definition of the Jacobi polynomials – see [55, Table 18.3.1] and [55, (18.9.15)].

The expressions for the VSHs as given in equation (2.12) together with the above allow us to be able to find the coefficients for our desired expressions for

$x\mathbf{\Psi}_l^m$, $y\mathbf{\Psi}_l^m$, $z\mathbf{\Psi}_l^m$, $x\mathbf{\Phi}_l^m$, $y\mathbf{\Phi}_l^m$ and $z\mathbf{\Phi}_l^m$.

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

$$\begin{aligned}
x\mathbf{\Psi}_l^m &= A_{l,m,1}\mathbf{\Psi}_{l-1}^{m-1} + A_{l,m,2}\mathbf{\Psi}_{l-1}^{m+1} + A_{l,m,3}\mathbf{\Psi}_{l+1}^{m-1} + A_{l,m,4}\mathbf{\Psi}_{l+1}^{m+1} \\
&\quad + A_{l,m,5}\mathbf{\Phi}_l^{m-1} + A_{l,m,6}\mathbf{\Phi}_l^{m+1}, \\
x\mathbf{\Phi}_l^m &= A_{l,m,1}\mathbf{\Phi}_{l-1}^{m-1} + A_{l,m,2}\mathbf{\Phi}_{l-1}^{m+1} + A_{l,m,3}\mathbf{\Phi}_{l+1}^{m-1} + A_{l,m,4}\mathbf{\Phi}_{l+1}^{m+1} \\
&\quad - A_{l,m,5}\mathbf{\Psi}_l^{m-1} - A_{l,m,6}\mathbf{\Psi}_l^{m+1}, \\
y\mathbf{\Psi}_l^m &= B_{l,m,1}\mathbf{\Psi}_{l-1}^{m-1} + B_{l,m,2}\mathbf{\Psi}_{l-1}^{m+1} + B_{l,m,3}\mathbf{\Psi}_{l+1}^{m-1} + B_{l,m,4}\mathbf{\Psi}_{l+1}^{m+1} \\
&\quad + B_{l,m,5}\mathbf{\Phi}_l^{m-1} + B_{l,m,6}\mathbf{\Phi}_l^{m+1}, \\
y\mathbf{\Phi}_l^m &= B_{l,m,1}\mathbf{\Phi}_{l-1}^{m-1} + B_{l,m,2}\mathbf{\Phi}_{l-1}^{m+1} + B_{l,m,3}\mathbf{\Phi}_{l+1}^{m-1} + B_{l,m,4}\mathbf{\Phi}_{l+1}^{m+1} \\
&\quad - B_{l,m,5}\mathbf{\Psi}_l^{m-1} - B_{l,m,6}\mathbf{\Psi}_l^{m+1}, \\
z\mathbf{\Psi}_l^m &= \Gamma_{l,m,1}\mathbf{\Psi}_{l-1}^{m} + \Gamma_{l,m,2}\mathbf{\Psi}_{l+1}^{m} + \Gamma_{l,m,3}\mathbf{\Phi}_l^{m}, \\
z\mathbf{\Phi}_l^m &= \Gamma_{l,m,1}\mathbf{\Phi}_{l-1}^{m} + \Gamma_{l,m,2}\mathbf{\Phi}_{l+1}^{m} - \Gamma_{l,m,3}\mathbf{\Psi}_l^{m},
\end{aligned}$$

where,

$$A_{l,m,1} := \frac{c_l^m c_{l-1}^{m-1}}{2l(l-1)} \begin{cases} \tilde{A}_{l,m,1} & \text{if } m > 0 \\ \tilde{A}_{l,|m|,2} & \text{if } m \leq 0, \end{cases}$$

$$A_{l,m,2} := \frac{c_l^m c_{l-1}^{m+1}}{2l(l-1)} \begin{cases} \tilde{A}_{l,m,2} & \text{if } m \geq 0 \\ \tilde{A}_{l,|m|,1} & \text{if } m < 0, \end{cases}$$

$$A_{l,m,3} := \frac{c_l^m c_{l+1}^{m-1}}{2(l+1)(l+2)} \begin{cases} \tilde{A}_{l,m,3} & \text{if } m > 0 \\ \tilde{A}_{l,|m|,4} & \text{if } m \leq 0, \end{cases}$$

$$A_{l,m,4} := \frac{c_l^m c_{l+1}^{m+1}}{2(l+1)(l+2)} \begin{cases} \tilde{A}_{l,m,4} & \text{if } m \geq 0 \\ \tilde{A}_{l,|m|,3} & \text{if } m < 0, \end{cases}$$

$$A_{l,m,5} := \frac{i}{2l(l+1)} \begin{cases} -i\, d_{l,m-1} \frac{c_l^{m-1}}{2c_l^m} & \text{if } m > 0 \\ i\, d_{l,|m|} \frac{c_l^m}{2c_l^{m-1}} & \text{if } m \leq 0, \end{cases}$$

$$A_{l,m,6} := \frac{i}{2l(l+1)} \begin{cases} -d_{l,m} \frac{c_l^m}{c_l^{m+1}} & \text{if } m \geq 0 \\ d_{l,|m|-1} \frac{c_l^{m+1}}{c_l^m} & \text{if } m < 0, \end{cases}$$

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

$$\Gamma_{l,m,1} := \frac{c_l^m c_{l-1}^m}{l(l-1)} \left[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,1}}{(c_{l-1}^{|m|})^2} + d_{l,|m|} d_{l-1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,1}}{(c_{l-1}^{|m|+1})^2} \right],$$

$$\Gamma_{l,m,2} := \frac{c_l^m c_{l+1}^m}{(l+1)(l+2)} \left[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,2}}{(c_{l+1}^{|m|})^2} + d_{l,|m|} d_{l+1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,2}}{(c_{l+1}^{|m|+1})^2} \right],$$

$$\Gamma_{l,m,3} := \frac{i\, m}{l(l+1)},$$

where the $c_{l'}^{m'}$, $d_{l',m'}$, $\tilde{\gamma}_{l',m',j}$ *are defined in equation (2.3), equation (2.16) and*

Corollary 1 respectively, and

$$\begin{aligned}
\tilde{A}_{l,m,1} &:= \Big((m^2-1)\tilde{\alpha}_{l-1,m-1,4} - d_{l-1,m-1}\tilde{\gamma}_{l-1,m,2}\Big)\frac{1}{(c_l^m)^2} + d_{l,m}d_{l-1,m-1}\frac{\tilde{\alpha}_{l,m+1,1}}{(c_{l-1}^m)^2},\\
\tilde{A}_{l,m,2} &:= \Big(m(m+2)\tilde{\alpha}_{l,m,2} - d_{l,m}\tilde{\gamma}_{l,m+1,1}\Big)\frac{1}{(c_{l-1}^{m+1})^2} + d_{l,m}d_{l-1,m+1}\frac{\tilde{\alpha}_{l-1,m+2,3}}{(c_l^{m+1})^2},\\
\tilde{A}_{l,m,3} &:= \Big((m^2-1)\tilde{\alpha}_{l+1,m-1,2} - d_{l+1,m-1}\tilde{\gamma}_{l+1,m,1}\Big)\frac{1}{(c_l^m)^2} + d_{l,m}d_{l+1,m-1}\frac{\tilde{\alpha}_{l,m+1,3}}{(c_{l+1}^m)^2},\\
\tilde{A}_{l,m,4} &:= \Big(m(m+2)\tilde{\alpha}_{l,m,4} - d_{l,m}\tilde{\gamma}_{l,m+1,2}\Big)\frac{1}{(c_{l+1}^{m+1})^2} + d_{l,m}d_{l+1,m+1}\frac{\tilde{\alpha}_{l+1,m+2,1}}{(c_l^{m+1})^2},
\end{aligned}$$

where again the $\tilde{\alpha}_{l',m',j}$ are defined in Corollary 1 too.

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 $l \in \mathbb{N}$ and $m \in \mathbb{Z}$ s.t. $-l \le m \le l$. The proof we will use is to directly calculate the nonzero coefficients in each expansion using inner products. To this end, note that

$$x\mathbf{\Psi}_l^m = \sum_{l'=1}^{l+1}\sum_{m'=-l'}^{l'} \mathcal{A}_{l',m'}\mathbf{\Psi}_{l'}^{m'} + \mathcal{A}_{l',m'}^{\perp}\mathbf{\Phi}_{l'}^{m'},$$

where the coefficients are given by

$$\begin{aligned}
\mathcal{A}_{l',m'} &= \frac{\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'}\right\rangle}{\left\|\mathbf{\Psi}_{l'}^{m'}\right\|^2} = \frac{1}{l'(l'+1)}\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'}\right\rangle,\\
\mathcal{A}_{l',m'}^{\perp} &= \frac{\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Phi}_{l'}^{m'}\right\rangle}{\left\|\mathbf{\Phi}_{l'}^{m'}\right\|^2} = \frac{1}{l'(l'+1)}\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Phi}_{l'}^{m'}\right\rangle.
\end{aligned}$$

The aim will be to show that the only nonzero coefficients $\mathcal{A}_{l',m'}$, $\mathcal{A}_{l',m'}^{\perp}$ match the $A_{l,m,j}$ for $j = 1, \ldots, 6$ in the Lemma. Now, using a change of variable, we have that

$$
\begin{aligned}
&\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'}\right\rangle \\
&= \iint_\Omega \cos\theta \sin\varphi \, \mathbf{\Psi}_l^m \cdot \mathbf{\Psi}_{l'}^{m'*} \sin\varphi \, \mathrm{d}\phi \, \mathrm{d}\theta \\
&= c_l^m c_{l'}^{m'} \Big(\int_0^{2\pi} e^{im\theta} e^{im'\theta} \cos\theta \, \mathrm{d}\theta \Big) \\
&\qquad \cdot \Big(\int_{-1}^1 \Big\{ \big[\, |m|\, z P_{l-|m|}^{(|m|,|m|)}(z) - \rho(z)^2 P_{l-|m|}^{(|m|,|m|)}{}'(z) \big] \\
&\qquad\qquad\qquad \cdot \big[\, |m'|\, z P_{l'-|m'|}^{(|m'|,|m'|)}(z) - \rho(z)^2 P_{l'-|m'|}^{(|m'|,|m'|)}(z) \big] \\
&\qquad\qquad + mm' P_{l-|m|}^{(|m|,|m|)}(z) P_{l'-|m'|}^{(|m'|,|m'|)}(z) \Big\} \, \rho(z)^{|m|+|m'|-1} \, \mathrm{d}z \Big) \\
&= c_l^m c_{l'}^{m'} \pi (\delta_{m',m-1} + \delta_{m',m+1}) \\
&\qquad \cdot \Big(\int_{-1}^1 \Big\{ P_{l-|m|}^{(|m|,|m|)} P_{l'-|m'|}^{(|m'|,|m'|)} \rho^{|m|+|m'|-1} \big(mm' + |m|\,|m'|\, z^2 \big) \\
&\qquad\qquad - |m|\, z P_{l-|m|}^{(|m|,|m|)} P_{l'-|m'|}^{(|m'|,|m'|)}{}' \rho^{|m|+|m'|+1} \\
&\qquad\qquad - |m'|\, z P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m'|}^{(|m'|,|m'|)} \rho^{|m|+|m'|+1} \\
&\qquad\qquad + P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m'|}^{(|m'|,|m'|)}{}' \rho^{|m|+|m'|+3} \Big\} \, \mathrm{d}z \Big).
\end{aligned} \tag{2.17}
$$

We can conclude that the only possible nonzero coefficients are when $m' = m \pm 1$, and so it is left to evaluate the integral that is left at equation (2.17) when m' takes either value. Since we need to take account of the fact that m can be negative, to simplify our argument we make use of the fact that $m' = m - 1$ for $m < 0$ is analogous to the case $m' = m + 1$ for $m > 0$, and vice versa.

On that note, we will first consider the case that $m > 0$ and $m' = m - 1$, and calculate the integral in equation (2.17):

$$\begin{aligned}
&\int_{-1}^{1} \Big\{ m(m-1) P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m-2}(1+z^2) - mz P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \\
&\qquad - (m-1) z P_{l-m}^{(m,m)\,\prime} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m} + P_{l-m}^{(m,m)\,\prime} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m+2} \Big\}\,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m(m-1) P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m-2}(1+z^2) - mz P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \\
&\quad + (m-1) P_{l-m}^{(m,m)} \rho^{2m-2} \big(P_{l'-(m-1)}^{(m-1,m-1)} \rho^2 - z P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^2 - 2mz^2 P_{l'-(m-1)}^{(m-1,m-1)} \big) \\
&\quad + P_{l-m}^{(m,m)\,\prime} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m+2} \Big\}\,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ (m-1)(m+1) P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m} - z P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \\
&\qquad + P_{l-m}^{(m,m)\,\prime} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m+2} \Big\}\,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ (m-1)(m+1) P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m} - d_{l',m-1} z P_{l-m}^{(m,m)} P_{l'-m}^{(m,m)} \rho^{2m} \\
&\qquad + d_{l,m} d_{l',m-1} P_{l-(m+1)}^{(m+1,m+1)} P_{l'-m}^{(m,m)} \rho^{2m+2} \Big\}\,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ (m^2-1) P_{l-m}^{(m,m)} \big(\tilde{\alpha}_{l',m-1,2} P_{l'-1-m}^{(m,m)} + \tilde{\alpha}_{l',m-1,4} P_{l'+1-m}^{(m,m)} \big) \rho^{2m} \\
&\qquad - d_{l',m-1} P_{l-m}^{(m,m)} \big(\tilde{\gamma}_{l',m,1} P_{l'-1-m}^{(m,m)} + \tilde{\gamma}_{l',m,2} P_{l'+1-m}^{(m,m)} \big) \rho^{2m} \\
&\qquad + d_{l,m} d_{l',m-1} P_{l'-m}^{(m,m)} \big(\tilde{\alpha}_{l,m+1,1} P_{l-1-m}^{(m,m)} + \tilde{\alpha}_{l,m+1,3} P_{l+1-m}^{(m,m)} \big) \rho^{2m} \Big\}\,\mathrm{d}z \\
&= \frac{\delta_{l',l-1}}{2\pi} \Big\{ \big[(m^2-1) \tilde{\alpha}_{l-1,m-1,4} - d_{l-1,m-1} \tilde{\gamma}_{l-1,m,2} \big] \frac{1}{(c_l^m)^2} + d_{l,m} d_{l-1,m-1} \frac{\tilde{\alpha}_{l-1,m-1,1}}{(c_{l-1}^m)^2} \Big\} \\
&\quad + \frac{\delta_{l',l+1}}{2\pi} \Big\{ \big[(m^2-1) \tilde{\alpha}_{l+1,m-1,2} - d_{l+1,m-1} \tilde{\gamma}_{l+1,m,1} \big] \frac{1}{(c_l^m)^2} \\
&\qquad\qquad + d_{l,m} d_{l+1,m-1} \frac{\tilde{\alpha}_{l-1,m-1,3}}{(c_{l+1}^m)^2} \Big\}.
\end{aligned} \tag{2.18}$$

As we can see, the coefficients zero for $l' \neq l \pm 1$. Combining the above with the equation (2.17), we have that our two coefficients for $\mathcal{A}_{l-1,m-1}, \mathcal{A}_{l+1,m-1}$ are those stated in the Lemma as $A_{l,m,1}$ and $A_{l,m,3}$, for $m > 0$.

Next, assume $m \geq 0$ and consider the case $m' = m + 1$. The integral in equation (2.17) is then:

$$
\begin{aligned}
&\int_{-1}^{1} \Big\{ m(m+1) P_{l-m}^{(m,m)} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m}(1+z^2) - mz P_{l-m}^{(m,m)} P_{l'-(m+1)}^{(m+1,m+1)\,\prime} \rho^{2m+2} \\
&\qquad - (m+1) z P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} + P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)\,\prime} \rho^{2m+4} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m(m+1) P_{l-m}^{(m,m)} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m}(1+z^2) \\
&\qquad - (m+1) z P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} \\
&\qquad + m P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m} \big(-2(m+1) z^2 P_{l-m}^{(m,m)} + P_{l-m}^{(m,m)} \rho^2 - z P_{l-m}^{(m,m)\,\prime} \rho^2 \big) \\
&\qquad + P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)\,\prime} \rho^{2m+2} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m(m+2) P_{l-m}^{(m,m)} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} - z P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} \\
&\qquad + P_{l-m}^{(m,m)\,\prime} P_{l'-(m+1)}^{(m+1,m+1)\,\prime} \rho^{2m+4} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m(m+2) P_{l-m}^{(m,m)} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} - d_{l,m} z P_{l-(m+1)}^{(m+1,m+1)} P_{l'-(m+1)}^{(m+1,m+1)} \rho^{2m+2} \\
&\qquad + d_{l,m} d_{l',m+1} P_{l-(m+1)}^{(m+1,m+1)} P_{l'-(m+2)}^{(m+2,m+2)} \rho^{2m+4} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m(m+2) P_{l'-(m+1)}^{(m+1,m+1)} \big(\tilde{\alpha}_{l,m,2} P_{l-1-(m+1)}^{(m+1,m+1)} + \tilde{\alpha}_{l,m,4} P_{l+1-(m+1)}^{(m+1,m+1)} \big) \rho^{2m+2} \\
&\quad - d_{l,m} P_{l'-(m+1)}^{(m+1,m+1)} \big(\tilde{\gamma}_{l,m+1,1} P_{l-1-(m+1)}^{(m+1,m+1)} + \tilde{\gamma}_{l,m+1,2} P_{l+1-(m+1)}^{(m+1,m+1)} \big) \rho^{2m+2} \\
&\quad + d_{l,m} d_{l',m+1} P_{l-(m+1)}^{(m+1,m+1)} \big(\tilde{\alpha}_{l',m+2,1} P_{l'-1-(m+1)}^{(m+1,m+1)} + \tilde{\alpha}_{l',m+2,3} P_{l'+1-(m+1)}^{(m+1,m+1)} \big) \rho^{2m+2} \Big\}\, \mathrm{d}z \\
&= \frac{\delta_{l',l-1}}{2\pi} \Big\{ \big[m(m+2)\tilde{\alpha}_{l,m,2} - d_{l,m}\tilde{\gamma}_{l,m+1,1} \big] \frac{1}{(c_{l-1}^{m+1})^2} + d_{l,m} d_{l-1,m+1} \frac{\tilde{\alpha}_{l-1,m+2,3}}{(c_l^{m+1})^2} \Big\} \\
&\quad + \frac{\delta_{l',l+1}}{2\pi} \Big\{ \big[m(m+2)\tilde{\alpha}_{l,m,4} - d_{l,m}\tilde{\gamma}_{l,m+1,2} \big] \frac{1}{(c_{l-1}^{m+1})^2} + d_{l,m} d_{l+1,m+1} \frac{\tilde{\alpha}_{l+1,m+2,1}}{(c_l^{m+1})^2} \Big\}.
\end{aligned}
\tag{2.19}
$$

Again, we can see that the coefficients hence zero for $l' \neq l \pm 1$. Combining the above with the equation (2.17), we have that our two coefficients for $\mathcal{A}_{l-1,m-1}, \mathcal{A}_{l+1,m-1}$ are those stated in the Lemma as $A_{l,m,2}$ and $A_{l,m,4}$, for

$m \geq 0$.

We still have to account for the remaining $m = 0$ cases and m negative cases. Thankfully, as noted earlier, the case of $m \leq 0$, $m' = m - 1$ is the same as replacing m with $|m|$ in equation (2.19). Thus, our two coefficients for $\mathcal{A}_{l-1,m-1}, \mathcal{A}_{l+1,m-1}$ are those stated in the Lemma as $A_{l,m,1}$ and $A_{l,m,3}$, for $m \leq 0$. Similarly the case of $m < 0$, $m' = m + 1$ is the same as replacing m with $|m|$ in equation (2.18), and thus our two coefficients for $\mathcal{A}_{l-1,m+1}, \mathcal{A}_{l+1,m+1}$ are those stated in the Lemma as $A_{l,m,2}$ and $A_{l,m,4}$ for $m < 0$.

The remaining coefficients we need to determine are $\mathcal{A}^{\perp}_{l',m'}$. To this end, we have that

$$\begin{aligned}
&\left\langle x\mathbf{\Psi}_l^m, \mathbf{\Phi}_{l'}^{m'} \right\rangle \\
&= \iint_\Omega \cos\theta \sin\varphi \, \mathbf{\Psi}_l^m \cdot \mathbf{\Phi}_{l'}^{m'^*} \sin\varphi \, \mathrm{d}\phi \, \mathrm{d}\theta \\
&= c_l^m c_{l'}^{m'} \Big(\int_0^{2\pi} e^{im\theta} e^{im'\theta} \cos\theta \, \mathrm{d}\theta \Big) \\
&\quad \cdot \Big(\int_{-1}^1 \rho(z)^{|m|+|m'|-1} \Big\{ im' P_{l'-|m'|}^{(|m'|,|m'|)}(z) \big[\, |m| \, z P_{l-|m|}^{(|m|,|m|)}(z) - \rho(z)^2 P_{l-|m|}^{(|m|,|m|)\,\prime}(z) \big] \\
&\qquad\quad + im P_{l-|m|}^{(|m|,|m|)}(z) \big[\, |m'| \, z P_{l'-|m'|}^{(|m'|,|m'|)}(z) - \rho(z)^2 P_{l'-|m'|}^{(|m'|,|m'|)}(z) \big] \Big\} \, \mathrm{d}z \Big) \\
&= c_l^m c_{l'}^{m'} \pi (\delta_{m',m-1} + \delta_{m',m+1}) \\
&\qquad \cdot \Big(\int_{-1}^1 \Big\{ \mathrm{sgn}(m) \, 2i \, m \, m' \, z P_{l-|m|}^{(|m|,|m|)} P_{l'-|m'|}^{(|m'|,|m'|)} \rho^{|m|+|m'|-1} \\
&\qquad\qquad - im P_{l-|m|}^{(|m|,|m|)\,\prime} P_{l'-|m'|}^{(|m'|,|m'|)} \rho^{|m|+|m'|+1} \\
&\qquad\qquad - im' P_{l-|m|}^{(|m|,|m|)} P_{l'-|m'|}^{(|m'|,|m'|)\,\prime} \rho^{|m|+|m'|+1} \Big\} \, \mathrm{d}z \Big),
\end{aligned} \tag{2.20}$$

since when the above is nonzero, m, m' will have the same sign (or one is zero) and so $|m| \, m' + |m'| \, m = \mathrm{sgn}(m) m m'$. Once again, we can conclude that $\mathcal{A}^{\perp}_{l',m'}$

are zero for $m' \notin \{m-1, m+1\}$. It is left to evaluate the integral that is left at equation (2.20) when m' takes either $m \pm 1$ value. First, consider the case that $m > 0$ and $m' = m - 1$. The integral is then, using integration by parts:

$$\begin{aligned}
&= \int_{-1}^{1} \Big\{ 2i\, m(m-1)\, z P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m-2} - im P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \\
&\qquad - i(m-1) P_{l-m}^{(m,m)\,\prime} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m} \Big\} \,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ 2i\, m(m-1)\, z P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)} \rho^{2m-2} - im P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \\
&\qquad + i(m-1) P_{l-m}^{(m,m)} \rho^{2m-2} \big[P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^2 - 2mz P_{l'-(m-1)}^{(m-1,m-1)} \big] \Big\} \,\mathrm{d}z \\
&= -\int_{-1}^{1} i P_{l-m}^{(m,m)} P_{l'-(m-1)}^{(m-1,m-1)\,\prime} \rho^{2m} \,\mathrm{d}z \\
&= -\int_{-1}^{1} i\; d_{l',m-1}\; P_{l-m}^{(m,m)} P_{l'-m}^{(m,m)} \rho^{2m} \,\mathrm{d}z \\
&= -i\, \frac{d_{l,m-1}}{2\pi (c_l^m)^2}\, \delta_{l',l}.
\end{aligned} \tag{2.21}$$

Combining equation (2.21) with equation (2.20) means we retrieve the correct values for our coefficients $\mathcal{A}^{\perp}_{l,m-1}$ when $m > 0$, i.e. they are $A_{l,m,5}$ as stated in the Lemma for $m > 0$. The case of $m < 0$ and $m' = m + 1$ is very similar with the integral becoming:

$$
\begin{aligned}
&= \int_{-1}^{1} \Big\{ -2i\, m(m+1)\, z P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)} \rho^{2|m|-2} \\
&\qquad - im P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)\,\prime} \rho^{2|m|} \\
&\qquad - i(m+1) P_{l-|m|}^{(|m|,|m|)\,\prime} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)} \rho^{2|m|} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ -2i\, m(m+1)\, z P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)} \rho^{2|m|-2} \\
&\qquad - im P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)\,\prime} \rho^{2|m|} \\
&\qquad + i(m+1) P_{l-|m|}^{(|m|,|m|)} \rho^{2|m|-2} \big[P_{l'-(|m|-1)}^{(|m|-1,|m|-1)\,\prime} \rho^2 - 2\,|m|\, z P_{l'-(|m|-1)}^{(|m|-1,|m|-1)} \big] \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} i P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|-1)}^{(|m|-1,|m|-1)\,\prime} \rho^{2|m|}\, \mathrm{d}z \\
&= \int_{-1}^{1} i\, d_{l',|m|-1}\, P_{l-|m|}^{(|m|,|m|)} P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|}\, \mathrm{d}z \\
&= i\, \frac{d_{l,|m|-1}}{2\pi (c_l^{|m|})^2}\, \delta_{l',l}.
\end{aligned} \tag{2.22}
$$

Combining equation (2.22) with equation (2.20) means we retrieve the correct values for our coefficients $\mathcal{A}_{l,m+1}^{\perp}$ when $m < 0$, i.e. they are $A_{l,m,6}$ as stated in the Lemma for $m < 0$.

Next, assume $m \geq 0$ and $m' = m + 1$. Then the integral in equation (2.20) becomes:

$$
\begin{aligned}
&= \int_{-1}^{1} \Big\{ 2i\, m(m+1)\, z P^{(m,m)}_{l-m} P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m} - im P^{(m,m)}_{l-m} P^{(m+1,m+1)}_{l'-(m+1)}{}' \rho^{2m+2} \\
&\qquad - i(m+1) P^{(m,m)}_{l-m}{}' P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m+2} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ 2i\, m(m+1)\, z P^{(m,m)}_{l-m} P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m} - i(m+1) P^{(m,m)}_{l-m}{}' P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m+2} \\
&\qquad + im P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m} \big[P^{(m,m)}_{l-m}{}' \rho^2 - 2(m+1) z P^{(m,m)}_{l-m} \big] \Big\}\, \mathrm{d}z \\
&= -\int_{-1}^{1} i P^{(m,m)}_{l-m}{}' P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m+2}\, \mathrm{d}z \\
&= -\int_{-1}^{1} i\, d_{l,m}\, P^{(m+1,m+1)}_{l-(m+1)} P^{(m+1,m+1)}_{l'-(m+1)} \rho^{2m+2}\, \mathrm{d}z \\
&= -i\, \frac{d_{l,m}}{2\pi (c_l^{m+1})^2}\, \delta_{l',l}.
\end{aligned} \tag{2.23}
$$

Again, combining equation (2.23) with equation (2.20) means we retrieve the correct values for our coefficients $\mathcal{A}^{\perp}_{l,m+1}$ when $m \geq 0$, i.e. they are $A_{l,m,6}$ as stated in the Lemma for $m \geq 0$. In a similar vein, the integral for the case

$m \leq 0$ and $m' = m - 1$ is:

$$\begin{aligned}
&= \int_{-1}^{1} \Big\{ -2i\, m(m-1)\, z P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|} \\
&\qquad - im P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)\,\prime} \rho^{2|m|+2} \\
&\qquad - i(m-1) P_{l-|m|}^{(|m|,|m|)\,\prime} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \Big\} \,\mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ -2i\, m(m-1)\, z P_{l-|m|}^{(|m|,|m|)} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|} \\
&\qquad - i(m-1) P_{l-|m|}^{(|m|,|m|)\,\prime} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \\
&\qquad + im P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|} \big[P_{l-|m|}^{(|m|,|m|)\,\prime} \rho^2 - 2(|m|+1) z P_{l-|m|}^{(|m|,|m|)} \big] \Big\} \,\mathrm{d}z \\
&= \int_{-1}^{1} i P_{l-|m|}^{(|m|,|m|)\,\prime} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \,\mathrm{d}z \\
&= \int_{-1}^{1} i\; d_{l,|m|}\; P_{l-(|m|+1)}^{(|m|+1,|m|+1)} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \,\mathrm{d}z \\
&= i\, \frac{d_{l,|m|}}{2\pi (c_l^{|m|+1})^2}\, \delta_{l',l},
\end{aligned} \tag{2.24}$$

and so combining equation (2.24) with equation (2.20), we have that our coefficients for $\mathcal{A}_{l,m-1}^{\perp}$ are those stated in the Lemma as $A_{l,m,5}$ for $m \leq 0$, concluding the argument for the expansion of $x\mathbf{\Psi}_l^m$.

An almost identical argument holds for multiplication by y, since

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

replaces the integrals over θ in equation (2.17) and equation (2.20).

For multiplication by z, we will use the same method to directly calculate the nonzero coefficients in each expansion using inner products. To this end, note that

$$z\mathbf{\Psi}_l^m = \sum_{l'=1}^{l+1} \sum_{m'=-l'}^{l'} \mathcal{C}_{l',m'} \mathbf{\Psi}_{l'}^{m'} + \mathcal{C}_{l',m'}^{\perp} \mathbf{\Phi}_{l'}^{m'},$$

where the coefficients are given by

$$\begin{aligned}\mathcal{C}_{l',m'} &= \frac{\left\langle z\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'} \right\rangle}{\left\| \mathbf{\Psi}_{l'}^{m'} \right\|^2} = \frac{1}{l'(l'+1)} \left\langle z\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'} \right\rangle, \\ \mathcal{C}_{l',m'}^{\perp} &= \frac{\left\langle z\mathbf{\Psi}_l^m, \mathbf{\Phi}_{l'}^{m'} \right\rangle}{\left\| \mathbf{\Phi}_{l'}^{m'} \right\|^2} = \frac{1}{l'(l'+1)} \left\langle z\mathbf{\Psi}_l^m, \mathbf{\Phi}_{l'}^{m'} \right\rangle.\end{aligned}$$

The aim once again will be to show that the only nonzero coefficients $\mathcal{C}_{l',m'}$, $\mathcal{C}_{l',m'}^{\perp}$ match the $\Gamma_{l,m,j}$ for $j = 1, 2, 3$ in the Lemma. Now, using a change of variable and integration by parts, we have that

$$\begin{aligned}&\left\langle z\mathbf{\Psi}_l^m, \mathbf{\Psi}_{l'}^{m'} \right\rangle \\ &= \iint_{\Omega} \cos\varphi \; \mathbf{\Psi}_l^m \cdot \mathbf{\Psi}_{l'}^{m'*} \sin\varphi \, \mathrm{d}\varphi \, \mathrm{d}\theta \\ &= c_l^m c_{l'}^{m'} \Big(\int_0^{2\pi} e^{im\theta} e^{im'\theta} \, \mathrm{d}\theta \Big) \\ &\quad \cdot \Big(\int_{-1}^{1} \Big\{ \big[|m| \, z P_{l-|m|}^{(|m|,|m|)}(z) - \rho(z)^2 P_{l-|m|}^{(|m|,|m|)\,\prime}(z) \big] \\ &\qquad\qquad \cdot \big[|m'| \, z P_{l'-|m'|}^{(|m'|,|m'|)}(z) - \rho(z)^2 P_{l'-|m'|}^{(|m'|,|m'|)}(z) \big] \\ &\qquad\qquad + mm' P_{l-|m|}^{(|m|,|m|)}(z) P_{l'-|m'|}^{(|m'|,|m'|)}(z) \Big\} \; z \; \rho(z)^{|m|+|m'|-2} \, \mathrm{d}z \Big). \qquad (2.25)\end{aligned}$$

The integral over θ in equation (2.25) is simply $2\pi\delta_{m',m}$ showing the above is zero when $m' \neq m$, and thus so will the coefficients $\mathcal{C}_{l',m'}$ be when this is the case. Focusing on the second integral (over z) when $m' = m$, this becomes:

$$
\begin{aligned}
&\int_{-1}^{1} \Big\{ m^2 z P_{l-|m|}^{(|m|,|m|)} P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|-2}(1+z^2) \\
&\qquad - |m|\, z^2 P_{l-|m|}^{(|m|,|m|)} P_{l'-|m|}^{(|m|,|m|)}{}' \rho^{2|m|} \\
&\qquad - |m|\, z^2 P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|} \\
&\qquad + z P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m|}^{(|m|,|m|)}{}' \rho^{2|m|+2} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ m^2 z P_{l-|m|}^{(|m|,|m|)} P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|-2}(1+z^2) \\
&\qquad + |m|\, P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|-2} \big[z^2 P_{l-|m|}^{(|m|,|m|)}{}' \rho^2 + 2z P_{l'-|m|}^{(|m|,|m|)} - 2\,|m|\, z^3 P_{l'-|m|}^{(|m|,|m|)} \rho^2 \big] \\
&\qquad - |m|\, z^2 P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|} \\
&\qquad + z P_{l-|m|}^{(|m|,|m|)}{}' P_{l'-|m|}^{(|m|,|m|)}{}' \rho^{2|m|+2} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ |m|\,(|m|+2) z P_{l-|m|}^{(|m|,|m|)} P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|} \\
&\qquad + z d_{l,|m|} d_{l',|m|} P_{l-(|m|+1)}^{(|m|+1,|m|+1)} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \Big\}\, \mathrm{d}z \\
&= \int_{-1}^{1} \Big\{ |m|\,(|m|+2) P_{l'-|m|}^{(|m|,|m|)} \rho^{2|m|} \big[\tilde{\gamma}_{l,|m|,1} P_{l-1-|m|}^{(|m|,|m|)} + \tilde{\gamma}_{l,|m|,2} P_{l+1-|m|}^{(|m|,|m|)} \big] \\
&\qquad + d_{l,|m|} d_{l',|m|} P_{l'-(|m|+1)}^{(|m|+1,|m|+1)} \rho^{2|m|+2} \\
&\qquad\quad \cdot \big[\tilde{\gamma}_{l,|m|+1,1} P_{l-1-(|m|+1)}^{(|m|+1,|m|+1)} + \tilde{\gamma}_{l,|m|+1,2} P_{l+1-(|m|+1)}^{(|m|+1,|m|+1)} \big] \Big\}\, \mathrm{d}z \\
&= c_{l-1}^{m} \delta_{l',l-1} \Big[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,1}}{2\pi (c_{l-1}^{|m|})^2} + d_{l,|m|} d_{l-1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,1}}{2\pi (c_{l-1}^{|m|+1})^2} \Big] \\
&\quad + c_{l+1}^{m} \delta_{l',l+1} \Big[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,2}}{2\pi (c_{l+1}^{|m|})^2} + d_{l,|m|} d_{l+1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,2}}{2\pi (c_{l+1}^{|m|+1})^2} \Big] \\
&= c_{l-1}^{m} \delta_{l',l-1} \Big[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,1}}{(c_{l-1}^{|m|})^2} + d_{l,|m|} d_{l-1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,1}}{(c_{l-1}^{|m|+1})^2} \Big] \\
&\quad + c_{l+1}^{m} \delta_{l',l+1} \Big[|m|\,(|m|+2) \frac{\tilde{\gamma}_{l,|m|,2}}{(c_{l+1}^{|m|})^2} + d_{l,|m|} d_{l+1,|m|} \frac{\tilde{\gamma}_{l,|m|+1,2}}{(c_{l+1}^{|m|+1})^2} \Big].
\end{aligned}
\tag{2.26}
$$

Combining equation (2.26) with equation (2.25), we obtain that

$$\begin{aligned}\left\langle z\boldsymbol{\Psi}_l^m, \boldsymbol{\Psi}_{l'}^{m'}\right\rangle = c_l^m \delta_{m',m}\Big\{ & c_{l-1}^m \delta_{l',l-1}\big[\,|m|\,(|m|+2)\frac{\tilde{\gamma}_{l,|m|,1}}{(c_{l-1}^{|m|})^2} + d_{l,|m|}d_{l-1,|m|}\frac{\tilde{\gamma}_{l,|m|+1,1}}{(c_{l-1}^{|m|+1})^2}\big] \\ & + c_{l+1}^m \delta_{l',l+1}\big[\,|m|\,(|m|+2)\frac{\tilde{\gamma}_{l,|m|,2}}{(c_{l+1}^{|m|})^2} + d_{l,|m|}d_{l+1,|m|}\frac{\tilde{\gamma}_{l,|m|+1,2}}{(c_{l+1}^{|m|+1})^2}\big]\Big\}.\end{aligned} \tag{2.27}$$

We can see here in equation (2.27) that the nonzero coefficients $\mathcal{C}_{l',m'}$ are those described in the Lemma as $\Gamma_{l,m,1}$ and $\Gamma_{l,m,2}$.

Next, we also have that

$$\begin{aligned}&\left\langle z\boldsymbol{\Psi}_l^m, \boldsymbol{\Phi}_{l'}^{m'}\right\rangle \\ &= \iint_\Omega \cos\varphi\, \boldsymbol{\Psi}_l^m \cdot \boldsymbol{\Phi}_{l'}^{m'\,*} \sin\varphi \,\mathrm{d}\varphi\,\mathrm{d}\theta \\ &= c_l^m c_{l'}^{m'}\Big(\int_0^{2\pi} e^{im\theta}e^{im'\theta}\,\mathrm{d}\theta\Big) \\ &\quad\cdot\Big(\int_{-1}^1 \rho^{|m|+|m'|-2}\Big\{im'zP_{l'-|m'|}^{(|m'|,|m'|)}\big[\,|m|\,zP_{l-|m|}^{(|m|,|m|)} - \rho^2 P_{l-|m|}^{(|m|,|m|)\,\prime}\big] \\ &\qquad\qquad + imzP_{l-|m|}^{(|m|,|m|)}\big[\,|m'|\,zP_{l'-|m'|}^{(|m'|,|m'|)} - \rho^2 P_{l'-|m'|}^{(|m'|,|m'|)}\big]\Big\}\,\mathrm{d}z\Big) \\ &= c_l^m c_{l'}^m 2\pi\delta_{m',m}\int_{-1}^1 \Big\{2im\,|m|\,z^2 P_{l-|m|}^{(|m|,|m|)}P_{l'-|m|}^{(|m|,|m|)}\rho^{2|m|-2} \\ &\qquad\qquad - imzP_{l-|m|}^{(|m|,|m|)}P_{l'-|m|}^{(|m|,|m|)\,\prime}\rho^{2|m|} \\ &\qquad\qquad - imzP_{l-|m|}^{(|m|,|m|)\,\prime}P_{l'-|m|}^{(|m|,|m|)}\rho^{2|m|}\Big\}\,\mathrm{d}z \\ &= c_l^m c_{l'}^m\, 2\pi\,\delta_{m',m}\int_{-1}^1 imP_{l-|m|}^{(|m|,|m|)}(z)P_{l'-|m|}^{(|m|,|m|)}(z)\rho(z)^{2|m|}\,\mathrm{d}z \\ &= \delta_{l',l}\,\delta_{m',m}\,i\,m.\end{aligned} \tag{2.28}$$

Again, we can see here in equation (2.28) that the coefficients $\mathcal{C}_{l',m'}^{\perp}$ are zero when $l' \neq l$ or $m' \neq m$, and that the nonzero coefficients are those described in the Lemma as $\Gamma_{l,m,3}$.

Finally, to complete our proof, for multiplication by x, y, and z of the other VSHs $\boldsymbol{\Phi}_l^m$, simply take the cross product by $\hat{\boldsymbol{r}}$ of $x\boldsymbol{\Psi}_l^m$, etc. noting that $\hat{\boldsymbol{r}} \times \boldsymbol{\Psi}_l^m = \boldsymbol{\Phi}_l^m$ and $\hat{\boldsymbol{r}} \times \boldsymbol{\Phi}_l^m = -\left\|\hat{\boldsymbol{r}}\right\| \boldsymbol{\Psi}_l^m = -\boldsymbol{\Psi}_l^m$ by the triple vector product and orthogonality. $\square$

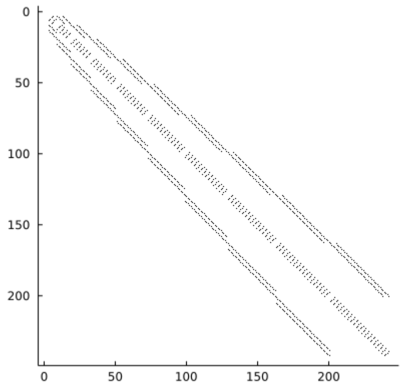
As for the scalar case, these coefficients detailed above are then the nonzero entries of the Jacobi matrices for the VSHs. Define $\tilde{\mathbb{T}}$ by

$$\tilde{\mathbb{T}} = \begin{pmatrix} \tilde{\mathbb{T}}_0 \\ \tilde{\mathbb{T}}_1 \\ \vdots \end{pmatrix}, \quad \text{where} \quad \tilde{\mathbb{T}}_l = \begin{pmatrix} (\boldsymbol{\Psi}_l^{-l})^\top \\ (\boldsymbol{\Phi}_l^{-l})^\top \\ \vdots \\ (\boldsymbol{\Psi}_l^{l})^\top \\ (\boldsymbol{\Phi}_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{2(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0. \tag{2.29}$$

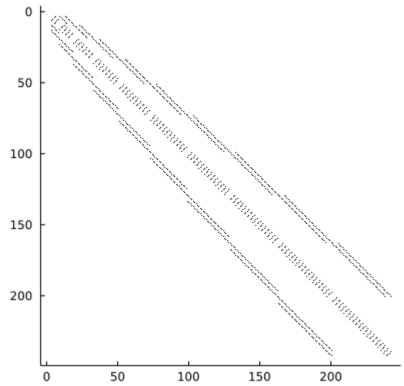
The Jacobi matrices are then defined according to the matrices ${}^T J_x, {}^T J_y, {}^T J_z$ satisfying

$$\begin{aligned} {}^T J_x \tilde{\mathbb{T}}(x,y,z) &= x\tilde{\mathbb{T}}(x,y,z), \\ {}^T J_y \tilde{\mathbb{T}}(x,y,z) &= y\tilde{\mathbb{T}}(x,y,z), \\ {}^T J_z \tilde{\mathbb{T}}(x,y,z) &= z\tilde{\mathbb{T}}(x,y,z), \end{aligned} \tag{2.30}$$

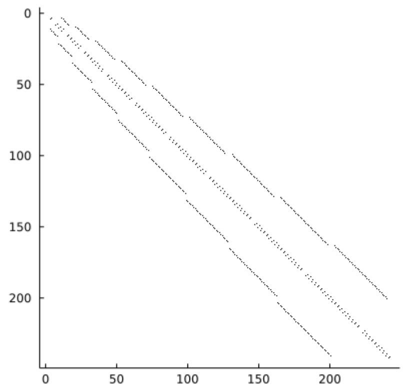
for each $(x,y,z) \in \Omega$. The VSH Jacobi matrices are banded-block-banded due to the sparse relationships we obtain from Lemma 3. Specifically, they each



(a) $^{T}J_x$



(b) $^{T}J_y$



(c) $^{T}J_z$

Figure 2.2: "Spy" plots of the Jacobi operator matrices for the vector spherical harmonic OP basis, showing their sparsity and structure, up to order $N = 10$. These are block-tridiagonal, with sub-block bandwidths: (a) (4,4), (b) (4,4), (c) (2,2).

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 zero matrix. ${}^T J_x$ has subblock-bandwidths $(4, 4)$ since for $l \in \mathbb{N}_0$:

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

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

and

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

where

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

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

$$A_{y,l} := \begin{pmatrix} \mathcal{B}_{l,-l,3} & 0_2 & \mathcal{B}_{l,-l,4} & & \\ & \ddots & \ddots & \ddots & \\ & & \mathcal{B}_{l,l,3} & 0_2 & \mathcal{B}_{l,l,4} \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)},$$
$$B_{y,l} := \begin{pmatrix} 0_2 & \mathcal{B}_{l,-l,6} & & \\ \mathcal{B}_{l,-l+1,5} & \ddots & \ddots & \\ & \ddots & \ddots & \mathcal{B}_{l,l-1,6} \\ & & \mathcal{B}_{l,l,5} & 0_2 \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)},$$

and

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

where

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

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

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

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

and

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

The sparsity and structure of the Jacobi matrices for the VSHs as we have defined them can be seen visually in Figure 2.2.

2.5.2 Three-term recurrence relation for $\tilde{\mathbb{T}}$

We can combine each system in equation (2.30) into a block-tridiagonal system for any $(x, y, z) \in \Omega$:

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

where

$$\tilde{\mathbb{T}}_1(x,y,z) := \begin{pmatrix} \mathbf{\Psi}_1^{-1}(x,y,z)^\top \\ \mathbf{\Phi}_1^{-1}(x,y,z)^\top \\ \mathbf{\Psi}_1^{0}(x,y,z)^\top \\ \mathbf{\Phi}_1^{0}(x,y,z)^\top \\ \mathbf{\Psi}_1^{1}(x,y,z)^\top \\ \mathbf{\Phi}_1^{1}(x,y,z)^\top \end{pmatrix},$$

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

$$A_l := \begin{pmatrix} A_{x,l} \\ A_{y,l} \\ A_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+3)}, \quad C_l := \begin{pmatrix} C_{x,l} \\ C_{y,l} \\ C_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l-1)} \quad (n \neq 0), \tag{2.31}$$

$$B_l := \begin{pmatrix} B_{x,l} \\ B_{y,l} \\ B_{z,l} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+1)}, \quad G_l(x,y,z) := \begin{pmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{pmatrix} \in \mathbb{C}^{6(2l+1)\times 2(2l+1)}. \tag{2.32}$$

Just like for the scalar case, for each $l = 0, 1, 2\ldots$ 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 [22, p.78], which can be expanded to obtain the recurrence:

$$\begin{cases} \tilde{\mathbb{T}}_0(x,y,z) := 0_{2,3}, \\ \tilde{\mathbb{T}}_{l+1}(x,y,z) = -D_l^\top (B_l - G_l(x,y,z))\tilde{\mathbb{T}}_l(x,y,z) - D_l^\top C_l\, \tilde{\mathbb{T}}_{l-1}(x,y,z), \quad l \in \mathbb{N}. \end{cases}$$

For $l \in \mathbb{N}$, we can set

$$D_l^\top = \begin{pmatrix} & \boldsymbol{\eta}_0^\top & \\ & \boldsymbol{\eta}_1^\top & \\ 0_{2(2l+1)} & 0_{2(2l+1)} & \mathcal{D}_l \\ & \boldsymbol{\eta}_2^\top & \\ & \boldsymbol{\eta}_3^\top & \end{pmatrix} \in \mathbb{R}^{2(2l+3)\times 6(2l+1)}, \tag{2.33}$$

where $\mathcal{D}_l \in \mathbb{R}^{2(2l+1)\times 2(2l+1)}$ is the matrix

$$\mathcal{D}_l := \begin{pmatrix} \frac{1}{\Gamma_{l,-l,2}} & & & & \\ & \frac{1}{\Gamma_{l,-l,2}} & & & \\ & & \ddots & & \\ & & & \frac{1}{\Gamma_{l,l,2}} & \\ & & & & \frac{1}{\Gamma_{l,l,2}} \end{pmatrix}$$

and where $\boldsymbol{\eta}_0, \boldsymbol{\eta}_1, \boldsymbol{\eta}_2, \boldsymbol{\eta}_3 \in \mathbb{R}^{6(2l+1)}$ are vectors with entries given by

$$\left(\boldsymbol{\eta}_0\right)_j = \begin{cases} \frac{1}{A_{l,-l,3}} & j = 1 \\ \frac{-A_{l,-l,4}}{A_{l,-l,3}\,\Gamma_{l,1-l,2}} & j = 4(2n+1)+3 \\ 0 & \text{otherwise,} \end{cases}$$

$$\left(\boldsymbol{\eta}_1\right)_j = \begin{cases} \left(\boldsymbol{\eta}_0\right)_{j-1} & j = 2, 4(2l+1)+4 \\ 0 & \text{otherwise,} \end{cases}$$

$$\left(\boldsymbol{\eta}_2\right)_j = \begin{cases} \frac{1}{A_{l,l,4}} & j = 2(2l+1)-1 \\ \frac{-A_{l,l,3}}{A_{l,l,4}\,\Gamma_{l,l-1,2}} & j = 6(2l+1)-3 \\ 0 & \text{otherwise,} \end{cases}$$

$$\left(\boldsymbol{\eta}_3\right)_j = \begin{cases} \left(\boldsymbol{\eta}_2\right)_{j-1} & j = 2(2l+1), 6(2l+1)-2 \\ 0 & \text{otherwise.} \end{cases}$$

2.5.3 Computational aspects

It will be useful to be able to describe the coefficients of a vector-valued function in the tangent bundle of Ω in multiple ways, and as such we will introduce some more notation for the "splitting" of the basis vectors into the two groups stemming from the gradient and perpendicular gradient directions. Let us explain what we mean by this.

Define $\mathbb{T}^{\boldsymbol{\Psi}}, \mathbb{T}^{\boldsymbol{\Phi}}$ by

$$\mathbb{T}^{\boldsymbol{\Psi}} := \begin{pmatrix} \mathbb{T}_0^{\boldsymbol{\Psi}} \\ \mathbb{T}_1^{\boldsymbol{\Psi}} \\ \vdots \end{pmatrix}, \quad \text{where} \quad \mathbb{T}_l^{\boldsymbol{\Psi}} := \begin{pmatrix} (\boldsymbol{\Psi}_l^{-l})^\top \\ \vdots \\ (\boldsymbol{\Psi}_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0, \tag{2.34}$$

$$\mathbb{T}^{\boldsymbol{\Phi}} := \begin{pmatrix} \mathbb{T}_0^{\boldsymbol{\Phi}} \\ \mathbb{T}_1^{\boldsymbol{\Phi}} \\ \vdots \end{pmatrix}, \quad \text{where} \quad \mathbb{T}_l^{\boldsymbol{\Phi}} := \begin{pmatrix} (\boldsymbol{\Phi}_l^{-l})^\top \\ \vdots \\ (\boldsymbol{\Phi}_l^{l})^\top \end{pmatrix} \in \mathbb{C}^{(2l+1)\times 3} \quad \forall\, l \in \mathbb{N}_0. \tag{2.35}$$

If $\boldsymbol{u}$ is a vector-valued function on the tangent bundle of Ω, it will have the coefficients vectors $\boldsymbol{u}^c, \boldsymbol{u}^{\boldsymbol{\Psi}c}, \boldsymbol{u}^{\boldsymbol{\Phi}c}$ for its expansion in the VSH basis up to order $N \in \mathbb{N}$, defined such that

$$\begin{aligned} \boldsymbol{u}(x,y,z) &\approx \tilde{\mathbb{T}}(x,y,z)^\top \, \boldsymbol{u}^c \\ &\equiv \mathbb{T}^{\boldsymbol{\Psi}}(x,y,z)^\top \, \boldsymbol{u}^{\boldsymbol{\Psi}c} + \mathbb{T}^{\boldsymbol{\Phi}}(x,y,z)^\top \, \boldsymbol{u}^{\boldsymbol{\Phi}c} \\ &:= \sum_{l=0}^{N} \sum_{m=-l}^{l} \big[u^{\boldsymbol{\Psi}}_{l,m} \, \boldsymbol{\Psi}_l^m(x,y,z) + u^{\boldsymbol{\Phi}}_{l,m} \, \boldsymbol{\Phi}_l^m(x,y,z) \big]. \end{aligned}$$

Of course, just like for the scalar case, we can use transforms to compute the coefficients of such a known function, and further evaluate, and apply differential operators to, a function knowing just its coefficients.

Obtaining coefficients

As eluded to, we would like to be able to obtain the coefficients for the expansion of a vector valued function in the VSH basis up to a given degree, similar to how we approach the scalar case. To do this, we can use a vector spherical harmonic transform. The development of vector spherical harmonic transforms is well established [82], and continues today (see [28]).

Function evaluation

The Clenshaw algorithm presented in Section 2.4.2 can also be used to evaluate a vector-valued function in the tangent bundle of Ω, where the matrices $C_n, B_n, D_n^\top, G_n(x,y,z)$ are all defined in Section 2.5.2:

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

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

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

$$= (\boldsymbol{\xi}_1)_1 \boldsymbol{\Psi}_1^{-1} + (\boldsymbol{\xi}_1)_2 \boldsymbol{\Phi}_1^{-1} + (\boldsymbol{\xi}_1)_3 \boldsymbol{\Psi}_1^{0} + (\boldsymbol{\xi}_1)_4 \boldsymbol{\Phi}_1^{0} + (\boldsymbol{\xi}_1)_5 \boldsymbol{\Psi}_1^{1} + (\boldsymbol{\xi}_1)_6 \boldsymbol{\Phi}_1^{1}.$$

Here, at each iteration, the vector $\boldsymbol{u}_n^c$ is given by the merging of the two order n subvector of $\boldsymbol{u}^c$:

$$\boldsymbol{u}_n^c := \begin{pmatrix} u_{n,-n}^{\boldsymbol{\Psi}} \\ u_{n,-n}^{\boldsymbol{\Phi}} \\ \vdots \\ u_{n,n}^{\boldsymbol{\Psi}} \\ u_{n,n}^{\boldsymbol{\Phi}} \end{pmatrix}.$$

Notice how the iteration also ends at $n = 1$ (not $n = 0$) here, since the VSHs for order $n = 0$ are zero.

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. Of course, not all PDEs can be sparsely represented, however we can do this for key operators such as the spherical gradient, divergence and Laplace–Beltrami, as well as other operators found in examples such as the linearised shallow water equations. These operators will take coefficients of a function's expansion in either the SH or VSH basis, to coefficients in either basis.

Let $\boldsymbol{u}$ be a vector-valued function on the tangent bundle of Ω with coefficients vectors $\boldsymbol{u}^{\boldsymbol{\Psi}c}, \boldsymbol{u}^{\boldsymbol{\Phi}c}$ 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 SH basis also up to order N, i.e.

$$\begin{aligned}
\boldsymbol{u}(x,y,z) &\approx \tilde{\mathbb{T}}(x,y,z)^\top\, \boldsymbol{u}^c \\
&\equiv \mathbb{T}^{\boldsymbol{\Psi}}(x,y,z)^\top\, \boldsymbol{u}^{\boldsymbol{\Psi}c} + \mathbb{T}^{\boldsymbol{\Phi}}(x,y,z)^\top\, \boldsymbol{u}^{\boldsymbol{\Phi}c} \\
&:= \sum_{l=0}^{N} \sum_{m=-l}^{l} \big[u^{\boldsymbol{\Psi}}_{l,m}\, \boldsymbol{\Psi}_l^m(x,y,z) + u^{\boldsymbol{\Phi}}_{l,m}\, \boldsymbol{\Phi}_l^m(x,y,z)\big], \\
f(x,y,z) &\approx \mathbb{P}(x,y,z)^\top\, \boldsymbol{f}^c := \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l,m}\, Y_l^m(x,y,z).
\end{aligned}$$

In order to fully exploit the sparsity of the relationships and ensure we are using banded-block-banded operators, in problems where we have an interdependency of scalar and vector-valued functions it can be useful to "expand" the scalar function's coefficients vector $\boldsymbol{f}^c$ to be the length of the vector-valued one $\boldsymbol{u}^c$, with zeros being inserted after each entry, i.e. define the *expanded co-*

efficients for a scalar function on Ω *in the SH basis* by

$$\tilde{\boldsymbol{f}}^c := \begin{pmatrix} \tilde{\boldsymbol{f}}^c{}_0 \\ \vdots \\ \tilde{\boldsymbol{f}}^c{}_N \end{pmatrix} \in \mathbb{R}^{2(N+1)^2}, \quad \tilde{\boldsymbol{f}}^c{}_l := \begin{pmatrix} f_{l,-l} \\ 0 \\ f_{l,-l+1} \\ 0 \\ \vdots \\ f_{l,l} \\ 0 \end{pmatrix} \in \mathbb{R}^{4(l+1)}.$$

To help with the definitions of the operators we will discuss, let $\mathcal{E}_s, \mathcal{E}_v$ be (severely) rectangular matrices defined such that $\mathcal{E}_s \tilde{\boldsymbol{f}}^c = \boldsymbol{f}^c$ and $\mathcal{E}_v \boldsymbol{f}^c = \tilde{\boldsymbol{f}}^c$. We are now in a position to derive the sparse differential operators that can be applied to the functions $\boldsymbol{u}, f$.

Definition 4. *We define the operator matrices* $\mathcal{D}, \tilde{\mathcal{D}}, \mathcal{G}, \tilde{\mathcal{G}}, \mathcal{L}$ *according to:*

$$\begin{aligned}
\nabla \cdot \boldsymbol{u}(x,y,z) &= \mathbb{P}(x,y,z)^\top \, \mathcal{D} \, \boldsymbol{u}^{\boldsymbol{\Psi} c}, \\
\nabla \cdot \boldsymbol{u}(x,y,z) &= \mathbb{P}(x,y,z)^\top \, \mathcal{E}_s \left(\tilde{\mathcal{D}} \, \boldsymbol{u}^c\right), \\
\nabla_{\mathrm{S}} f(x,y,z) &= \mathbb{T}^{\boldsymbol{\Psi}}(x,y,z)^\top \, \mathcal{G} \, \boldsymbol{f}^c, \\
\nabla_{\mathrm{S}} f(x,y,z) &= \tilde{\mathbb{T}}(x,y,z)^\top \, \tilde{\mathcal{G}} \, \tilde{\boldsymbol{f}}^c, \\
\Delta_{\mathrm{S}} f(x,y,z) &= \mathbb{P}(x,y,z)^\top \, \mathcal{L} \, \boldsymbol{f}^c.
\end{aligned}$$

Remark: The operators $\tilde{\mathcal{D}}, \tilde{\mathcal{G}}$ would be used when vectors of the resulting length are required for the problem you are wishing to solve.

For clarity, we note that Δ_{S} is defined in equation (2.1), and the spherical gradient and divergence operators are given by

$$\begin{aligned}
\nabla_{\mathrm{S}} &= \frac{\partial}{\partial\varphi} + \frac{1}{\sin\varphi}\frac{\partial}{\partial\theta}, \\
\nabla\cdot\boldsymbol{u} &= \frac{1}{\sin\varphi}\frac{\partial}{\partial\varphi}\big(\sin\varphi u_\varphi\big) + \frac{1}{\sin\varphi}\frac{\partial}{\partial\theta}u_\theta,
\end{aligned}$$

where $\boldsymbol{u} \equiv \hat{\boldsymbol{\phi}}\, u_\varphi + \hat{\boldsymbol{\theta}}\, u_\theta$.

Theorem 1. *The operator matrices defined in Definition 4 are diagonal, and are given by:*

$$\mathcal{G} = I_{(N+1)^2}, \quad \tilde{\mathcal{G}} = \begin{pmatrix} 1 &&&&&& \\ & 0 &&&&& \\ && 1 &&&& \\ &&& 0 &&& \\ &&&& \ddots && \\ &&&&& 1 & \\ &&&&&& 0 \end{pmatrix} \in \mathbb{R}^{2(N+1)^2\times 2(N+1)^2},$$

$$\mathcal{D} \equiv \mathcal{L} := \begin{pmatrix} \mathcal{L}_0 && \\ & \ddots & \\ && \mathcal{L}_N \end{pmatrix} \in \mathbb{R}^{(N+1)^2\times(N+1)^2},$$

$$\tilde{\mathcal{D}} = \begin{pmatrix} \tilde{\mathcal{D}}_0 && \\ & \ddots & \\ && \tilde{\mathcal{D}}_N \end{pmatrix} \in \mathbb{R}^{2(N+1)^2\times 2(N+1)^2},$$

where

$$\mathcal{L}_l := -l(l+1)\, I_{2l+1}, \quad \tilde{\mathcal{D}}_l := \begin{pmatrix} -l(l+1) & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & -l(l+1) & \\ & & & & 0 \end{pmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)}.$$

.

Proof. The arguments for $\mathcal{G}$ and $\tilde{\mathcal{G}}$ are trivial by definition. The spherical harmonics, as the name eludes to, satisfy a harmonic relationship $\Delta_{\mathrm{S}} Y_l^m = l(l+1)Y_l^m$ (see e.g. [35]). Thus, for the proof for $\mathcal{D}$ and $\tilde{\mathcal{D}}$, consider

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

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

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

□

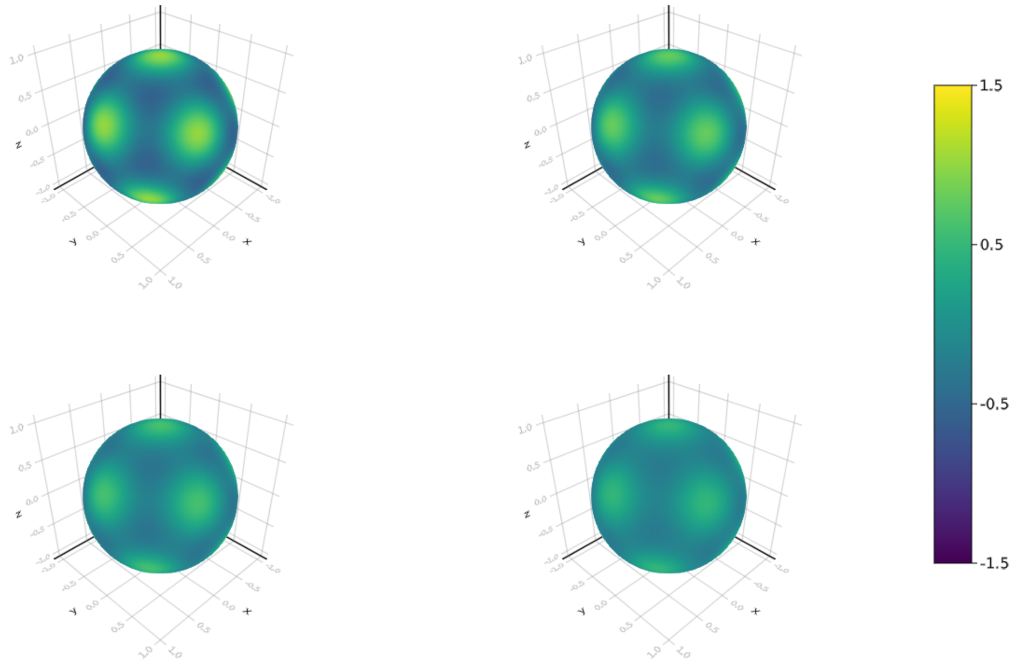


Figure 2.3: Four snapshots of the solution u of the heat equation with $\alpha = 1/42$ and a step size of $\Delta t = 0.01$, solved using the BDF2 timestepping method and order $N = 20$. Top Left: Initial conditions (0 timesteps). Top Right: After 25 timesteps. Bottom Left: After 50 timesteps. Bottom Right: After 75 timesteps.

2.6 Examples

Now that we have our differential operators, let us apply them in some examples.

2.6.1 Heat equation

To demonstrate proof of concept, we can apply the framework we have proposed to modelling the heat equation on the unit sphere. In doing so, we can demonstrate how our method allows us to expand and evaluate functions, and turn the differential equation into a matrix-vector problem at each timestep.

Let $u : \Omega \to \mathbb{C}$ represent the temperature at a point (x, y, z) on the sphere and suppose that it is modelled by the equation

$$\frac{\partial}{\partial t} u = \alpha \Delta_{\mathrm{S}} u \tag{2.36}$$

for some $\alpha \in \mathbb{R}$. A simple timestepping method we can use to iterate with is the BDF2 method [37, §2.3]. Let u_n for $n = 0, 1, 2, \dots$ be the solution at time $n\Delta t$ where Δt is the timestep. The timestepping method is

$$\begin{aligned} \frac{u_1 - u_0}{\Delta t} &= \alpha \Delta_{\mathrm{S}} u_1 \\ \frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} &= \alpha \Delta_{\mathrm{S}} u_{n+1}, \quad n = 1, 2, \dots \end{aligned}$$

$\iff$

$$\begin{aligned} [1 - \Delta t \alpha \Delta_{\mathrm{S}}] u_1 - &= u_0 \\ [3 - 2\Delta t \alpha \Delta_{\mathrm{S}}] u_{n+1} &= 4u_n - u_{n-1}, \quad n = 1, 2, \dots . \end{aligned}$$

Let us write this in coefficient space. Firstly, our coefficients vectors for the function u we will denote $\boldsymbol{u}^c$ – that is:

$$u(x, y, z) \approx \mathbb{P}(x, y, z)^\top \, \boldsymbol{u}^c.$$

Our system then becomes

$$\begin{aligned} [I - \Delta t \alpha \boldsymbol{\mathcal{L}}] \boldsymbol{u}_1^c - &= u_0 \\ [3I - 2\Delta t \alpha \boldsymbol{\mathcal{L}}] \boldsymbol{u}_{n+1}^c &= 4\boldsymbol{u}_n^c - \boldsymbol{u}_{n-1}^c, \quad n = 1, 2, \dots . \end{aligned}$$

From here, it is clear that at each timestep we simply have a fairly trivial linear system to solve, with the matrices $I - \Delta t \alpha \mathcal{L}$, $3I - 2\Delta t \alpha \mathcal{L}$ being banded-block-banded (in fact, simply diagonal here). We demonstrate this theory in Figure 2.3, where we see four snapshots of the solution to the heat equation in equation (2.36) on the unit sphere with our order N set large enough (here, $N = 20$). We set $\alpha = \frac{1}{42}$ and a step size of $\Delta t = 0.01$, and take the initial condition for the heat u to be a "football function"[4] – that is we take

$$u_0 := Y_6^0 + \sqrt{\frac{14}{11}} Y_6^6.$$

The snapshots of the solution u in Figure 2.3 are taken of the initial conditions, plus after 25, 50 and 75 timesteps respectively.

2.6.2 Linearised shallow water equations

The linearised shallow water equations (SWEs) allow us to showcase more of the differential operators that we defined in Definition 4 (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

[4] These initial conditions are taken from an example found at https://www.chebfun.org/examples/sphere/SphereHeatConduction.html

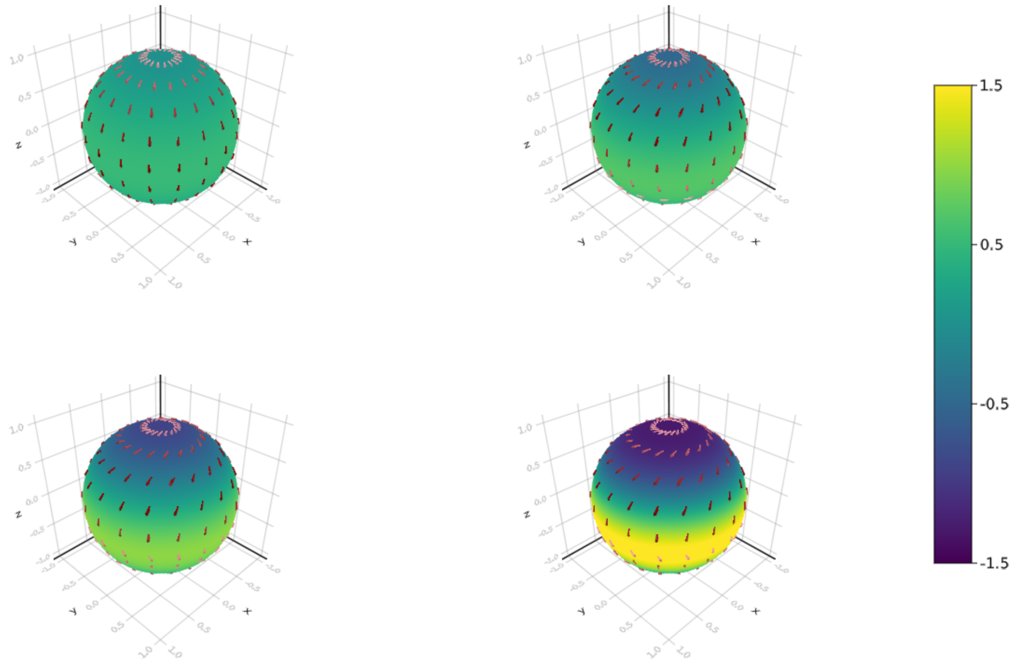


Figure 2.4: Four snapshots of the solution for the height h (surface colour) and the wave velocity u (red arrows) of the linearised shallow water equations with $\tilde{\Omega} = \mathcal{H} = 1$ and a step size of $\Delta t = 0.01$, solved using the backwards Euler timestepping method (BDF1) and order $N = 20$. The initial conditions are given in equation (2.38). Top Left: Initial conditions (0 timesteps). Top Right: After 50 timesteps. Bottom Left: After 75 timesteps. Bottom Right: After 100 timesteps.

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

$$\begin{cases} \frac{\partial \boldsymbol{u}}{\partial t} + f\hat{\boldsymbol{r}} \times \boldsymbol{u} - \nabla_{\mathrm{S}} h = \boldsymbol{0} \\ \frac{\partial h}{\partial t} + \mathcal{H} \nabla_{\mathrm{S}} \cdot \boldsymbol{u} = 0 \end{cases} \tag{2.37}$$

where $f = 2\tilde{\Omega}\cos(\varphi) = 2\tilde{\Omega}z$ is the Coriolis parameter[5], and $\tilde{\Omega}$ is the rotation rate of the sphere surface (that is, the amount the body rotates per unit time)[6].

A keen eye may notice that – while we have operators for the multiplication by z, the spherical gradient and divergence – we require one more operator not yet defined for the unit vector cross product $\hat{\boldsymbol{r}} \times \boldsymbol{u}$.

Definition 5. *Define the operator matrix $\mathcal{R}$ according to:*

$$\hat{\boldsymbol{r}}(x,y,z) \times \boldsymbol{u}(x,y,z) = \tilde{\mathbb{T}}(x,y,z)^\top \, \mathcal{R}\boldsymbol{u}^c.$$

Lemma 4. *The operator $\mathcal{R}$ defined in Definition 5 is sparse with banded-block-banded structure. More specifically, $\mathcal{R}$ has block-bandwidths $(0,0)$, and sub-block-bandwidths $(1,1)$ (i.e. is tridiagonal).*

Proof. Using the relations that $\boldsymbol{\Psi}_l^m = \nabla_{\mathrm{S}} Y_l^m$ and $\boldsymbol{\Phi}_l^m = \hat{\boldsymbol{r}} \times \nabla_{\mathrm{S}} Y_l^m$ for each $l \in \mathbb{N}$, $m \in \mathbb{Z}$ s.t. $-l \leq m \leq l$, we have that:

$$\begin{aligned}
\hat{\boldsymbol{r}} \times \boldsymbol{u} &= \hat{\boldsymbol{r}} \times \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m}^{\boldsymbol{\Psi}} \boldsymbol{\Psi}_l^m + u_{l,m}^{\boldsymbol{\Phi}} \boldsymbol{\Phi}_l^m] \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m}^{\boldsymbol{\Psi}} \hat{\boldsymbol{r}} \times \boldsymbol{\Psi}_l^m + u_{l,m}^{\boldsymbol{\Phi}} \hat{\boldsymbol{r}} \times (\hat{\boldsymbol{r}} \times \boldsymbol{\Psi}_l^m)] \\
&= \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m}^{\boldsymbol{\Psi}} \, \boldsymbol{\Phi}_l^m - u_{l,m}^{\boldsymbol{\Phi}} \, \boldsymbol{\Psi}_l^m)].
\end{aligned}$$

[5]Normally, the Coriolis parameter is expressed in terms of the latitude: latitude $= \frac{\pi}{2} - \varphi$
[6]On a full scale Earth, the rotation rate is $\tilde{\Omega} = 7.292110^{-5}$ rad s^{-1}.

We can then write down the operator $\mathcal{R}$ as follows:

$$\mathcal{R} = \begin{pmatrix} R & & \\ & R & \\ & & \ddots \end{pmatrix} \in \mathbb{R}^{2(N+1)^2 \times 2(N+1)^2},$$

where the blocks R are simply given by

$$R := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in \mathbb{R}^{2\times 2}.$$

□

For simplicity, we will implement a backward Euler timestepping method to solve the linear SWEs with timestep Δt. Of course, other timestepping methods are equally implementable (for example, the method used in the IFS model that ECMWF uses is a semi-implicit, semi-Lagrangian (SISL) timestepping method [18]), but we simplify things here to show proof of concept. Using $\boldsymbol{u}_n, h_n$ to represent the solution at time $n\Delta t$:

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

Let us write this in coefficient space. Firstly, our coefficients vectors for the functions $\boldsymbol{u}, h$ we will denote $\boldsymbol{u}^c, \boldsymbol{h}^c$ – that is:

$$\begin{aligned} \boldsymbol{u}(x,y,z) &\approx \tilde{\mathbb{T}}(x,y,z)^\top \boldsymbol{u}^c \\ h(x,y,z) &\approx \mathbb{P}(x,y,z)^\top \boldsymbol{h}^c. \end{aligned}$$

As eluded to earlier, we will "extend" the scalar function's coefficients vector, writing $\tilde{\boldsymbol{h}}^c = \mathcal{E}_v \boldsymbol{h}^c$, as described in Section 2.5.4. Thus, our system can be written as a matrix-vector system:

$$\begin{aligned}
\boldsymbol{u}^c_{n+1} &= \boldsymbol{u}^c_n + \Delta t\, (\tilde{\mathcal{G}} \tilde{\boldsymbol{h}}^c_{n+1} - 2\tilde{\Omega}^T J_z \mathcal{R} \boldsymbol{u}^c_{n+1}) \\
\tilde{\boldsymbol{h}}^c_{n+1} &= \tilde{\boldsymbol{h}}^c_n - \Delta t\, \mathcal{H} \tilde{\mathcal{D}} \boldsymbol{u}^c_{n+1}
\end{aligned}$$

$\iff$

$$\begin{aligned}
\boldsymbol{u}^c_{n+1} &= \boldsymbol{u}^c_n + \Delta t\, (\tilde{\mathcal{G}} \tilde{\boldsymbol{h}}^c_n - \Delta t\, \mathcal{H} \tilde{\mathcal{G}} \tilde{\mathcal{D}} \boldsymbol{u}^{\boldsymbol{\Psi}c}_{n+1} - 2\tilde{\Omega}^T J_z \mathcal{R} \boldsymbol{u}^c_{n+1}) \\
\tilde{\boldsymbol{h}}^c_{n+1} &= \tilde{\boldsymbol{h}}^c_n - \Delta t\, \mathcal{H} \tilde{\mathcal{D}} \boldsymbol{u}^c_{n+1}
\end{aligned}$$

$\iff$

$$\begin{aligned}
\left[I + \Delta t^2 \mathcal{H} \tilde{\mathcal{G}} \tilde{\mathcal{D}} + 2\tilde{\Omega} \Delta t\, {}^T J_z \mathcal{R} \right] \boldsymbol{u}^c_{n+1} &= \boldsymbol{u}^c_n + \Delta t \tilde{\mathcal{G}} \tilde{\boldsymbol{h}}^c_n \\
\tilde{\boldsymbol{h}}^c_{n+1} &= \tilde{\boldsymbol{h}}^c_n - \Delta t\, \mathcal{H} \tilde{\mathcal{D}} \boldsymbol{u}^c_{n+1}.
\end{aligned}$$

Here, it is clear that the matrix $I + \Delta t^2 \mathcal{H} \tilde{\mathcal{G}} \tilde{\mathcal{D}} + 2\tilde{\Omega} \Delta t^T J_z \mathcal{R}$ 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 $\boldsymbol{u}^c_{n+1}, \tilde{\boldsymbol{h}}^c_{n+1}$ if we know $\boldsymbol{u}^c_n, \tilde{\boldsymbol{h}}^c_n$. Of course, when evaluating the function h, we can simply gather back the coefficients vector $\boldsymbol{h}^c$ by $\boldsymbol{h}^c = \mathcal{E}_s \tilde{\boldsymbol{h}}^c$.

As a demonstration, in Figure 2.4 we see four snapshots of the solution to the system in equation (2.37) on the unit sphere, with $\tilde{\Omega} = \mathcal{H} = 1$ and initial conditions given by

$$\boldsymbol{u}_0 := \hat{\boldsymbol{\phi}}\mu \sin\varphi, \quad h_0 := \mu \sin^2\varphi, \tag{2.38}$$

where $\mu = \frac{\pi}{6}$, with the solution order N set large enough (here, $N = 20$). This example is very similar to "test case 2" in the well-known standard test set for shallow water equations in spherical geometries [92]. The snapshots of the wave height h are taken of the initial conditions, plus after 50, 75 and 100 timesteps respectively, using a step size of $\Delta t = 0.01$.

2.7 Conclusion

Spherical harmonics have been widely used to solve PDEs, in particular a spherical harmonics approach is used as part of the Integrated Forecasting System (IFS) that ECMWF uses for their forecasts. In this chapter, we have chosen to view the spherical harmonics as orthogonal (in fact orthonormal) polynomials in x, y and z in order to illustrate and understand more about how the framework presented here for using multivariate OPs in a spectral method translate to the sphere. We have derived the entries of Jacobi matrices that represent multiplication by the coordinates, showing how they are banded-block-banded in structure. We have set out how one can find coefficients for the expansion of a function in the spherical harmonics basis using established transforms, and how one can evaluate a function given its coefficients vector using a multidimensional version of the Clenshaw algorithm. We extended our framework to include the tangent bundle of the sphere – that is, the space of vectors orthogonal to the unit outward normal for each point on the sphere –

where we can use the vector spherical harmonics as vector-valued orthogonal polynomials to be a basis, demonstrating how similar such Jacobi matrices, function expansion and evaluation can be derived. Further, by exploiting the natural sparsity of the relationships between the OPs in the bases, we have shown how matrices for differential and other operators will be sparse and banded-block-banded in structure too. In fact, for the spherical harmonics, these are simply diagonal. Finally, we presented a couple of simple examples of how one can put this all into practice, namely solving the heat equation and the linearised shallow water equations on the unit sphere.

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 us first achieve a foundation in two-dimensions by looking at a special class of geometries that includes disk slices and trapeziums.

In recent years, there has been some interesting work in the area of multivariate orthogonal polynomials in two-dimensional domains (see [22]), such as for a Chebyshev-based spectral method on the rectangle [39]. In particular, spectral methods have been established on the disk [11, 86] and the triangle [59]. Examples of applications for the disk include use in optics [47], astrophysics [65], and fluid dynamics [23, 54, 40], and for the triangle include solving Volterra integral equations [31].

A review of spectral methods on the disk for solving the Poisson equation has been completed [11], that looks at methods involving various bases for expanding functions in the disk including Zernike polynomials and Chebyshev polynomials. It was concluded that using Chebyshev polynomials yields mixed results, but that there was also no single advised basis to use, due to Zernike polynomials having a lack of radial fast transform at the time despite being found to yield accurate results. In the years since however, such radial fast transforms have been developed [74, 68, 90]. The Zernike disk OPs can be written in terms of Jacobi polynomials [11]:

$$Z_n^m(r,\theta) := R_n^m(r)\sin(m\theta), \quad Z_n^{-m}(r,\theta) := R_n^m(r)\cos(m\theta),$$

where the radial part is

$$R_n^m(r) := r^m P^{(0,m)}_{(n-m)/2}(2r^2-1),$$

for $n-m$ even, while it is defined as 0 for $n-m$ odd. A generalisation of the Zernike polynomials has been used for the development of a sparse spectral method on the disk [86]. These radial OPs are:

$$Q_n^{k,m}(r) := C_n^{k,m} r^m P_n^{(k,m)}(2r^2-1), \tag{3.1}$$

where $C_n^{k,m}$ is some normalising constant so that they are orthonormal with respect to the inner product $\int_0^1 p(r)\ q(r)\ (1-r^2)^k\ r\ \mathrm{d}r$. These OPs constitute a one-parameter family of orthogonal polynomials on the unit disk, with the classical Zernike polynomials being retrieved via setting the parameter $k=0$. The use of polar coordinates allows for radially symmetric partial differential operators, while the incorporation of a parameter means they can be represented as banded matrices by exploiting the relations of the Jacobi polynomials. Jacobi polynomials are extremely useful for solving a number of problems in both 1D and 2D, since one can utilise the sparsity of the relations that they hold to yield operator matrices that are efficient to solve [20].

In a similar vein to the ultraspherical method for the unit interval [58, 19], a choice of OPs for the triangle are the *Jacobi polynomials on the triangle*, which are a three-parameter family of polynomials in (x, y) with differential operators acting in such a way so as to increment or decrement the parameter values [22, 41, 59]:

$$P_{n,k}^{(a,b,c)}(x, y) := \tilde{P}_{n-k}^{(2k+b+c+1,a)}(x)\ (1-x)^k\ \tilde{P}_k^{(c,b)}\left(\frac{y}{1-x}\right), \tag{3.2}$$

for $(x, y) \in \{(x, y) \in \mathbb{R}^2 \quad | \quad 0 < x < 1,\ 0 < y < 1 - x\}$, where $\tilde{P}_k^{(a,b)}$ is the degree k *shifted Jacobi polynomial*[1] with a, b, c being parameter values. Since there is no radial symmetry, differential operators for the triangle (as will be the case for the domains we investigate in this chapter) will be more complex than those for the disk.

In this chapter, we aim to present a basis and develop a sparse spectral method on generalisations of these domains, namely the disk-slice and trapezium. The full unit disk and triangle cases can be viewed as special cases of the spectral methods we investigate here too. We will show that the operators for multiplication by x and y, as well as differential and parameter conversion, will be banded-block-banded.

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

[1]The shifted Jacobi polynomials are orthogonal on the interval $[0, 1]$ and given by $\tilde{P}_k^{(a,b)}(x) = P_k^{(a,b)}(2x - 1)$ where $P_k^{(a,b)}$ is the standard degree k Jacobi polynomial.

on the domain

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

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 ≤ 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, by choosing the function ρ and constants $\alpha, \beta, \gamma, \delta$ appropriately (for example, choosing $\rho(x) = 1 - \xi x$ and $(\alpha, \beta) = (\gamma, \delta) = (0, 1)$ for some constant $\xi > 0$ returns the trapezium case). Moreover, one should be able to see that the full disk and triangle can also be obtained in such a way.

We will show that partial differential equations become sparse linear systems when viewed as acting on expansions involving a family of orthogonal polynomials that generalise Jacobi polynomials, mirroring the ultraspherical spectral method for ordinary differential equations on the interval [58], and its analogues on the disk [86] and triangle [60, 59]. On the disk-slice the family of weights we consider are of the form

$$W^{(a,b,c)}(x,y) = (\beta - x)^a\,(x-\alpha)^b\,(1-x^2-y^2)^c,$$

for $\alpha \le x \le \beta$, $-\rho(x) \le y \le \rho(x)$. The corresponding OPs are denoted

$H_{n,k}^{(a,b,c)}(x,y)$, where n denotes the polynomial degree, and $0 \leq k \leq n$. We define these to be orthogonalised lexicographically, that is,

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

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 we will see in Definition 6.

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 for equations on the triangle [60, 59] and for equations on the disk [86] with the frameworks discussed earlier both result 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 [55, (18.2.12)] 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 [6], see also work by Li and Shen [43].

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 $H^{(a,b,c,d)}_{n,k}(x,y)$. 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 ([22, p.55–56]). *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, for $n = 0,1,2,\ldots$, $k = 0,\ldots,n$, the 2D polynomials defined on Ω given by*

$$H_{n,k}(x,y) := p_{n-k,k}(x)\,\rho(x)^k\,q_k\left(\frac{y}{\rho(x)}\right),$$

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 1 in the following definitions. First we introduce notation for two families of univariate OPs.

Definition 6. *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:

$$\langle p, \, q \rangle_{w_R^{(a,b,c)}} := \frac{1}{\omega_R^{(a,b,c)}} \int_\alpha^\beta p(x) \, q(x) \, w_R^{(a,b,c)}(x) \, \mathrm{d}x, \tag{3.3}$$

$$\langle p, q \rangle_{w_P^{(a,b)}} := \frac{1}{\omega_P^{(a,b)}} \int_\gamma^\delta p(y) \, q(y) \, w_P^{(a,b)}(y) \, \mathrm{d}y, \tag{3.4}$$

where

$$\omega_R^{(a,b,c)} := \int_\alpha^\beta w_R^{(a,b,c)}(x) \, \mathrm{d}x, \quad \omega_P^{(a,b)} := \int_\gamma^\delta w_P^{(a,b)}(y) \, \mathrm{d}y. \tag{3.5}$$

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 equation (3.3), 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 equation (3.4).

We can now write down our 2D OP family.

Definition 7. *For parameters $a, b, c, d \in \mathbb{R}$, define the four-parameter 2D* *orthogonal polynomials as the set* $\{H_{n,k}^{(a,b,c,d)}\}$ *where:*

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

The comparison with the construction of the 3D spherical harmonics is evident here (the R_n OPs are in place of the Jacobi polynomials, and the P_n 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 holds, or Condition 2 holds with $w_P^{(a,b)}$ being an even function (i.e. $a = b$, and we can hence denote the weight as $w_P^{(a)}(x) = w_P^{(a,a)}(x) = (\delta - x^2)^a$). That is,

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

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

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

We can see that they are indeed orthogonal using the change of variable $t =$

$\frac{y}{\rho(x)}$, for the following normalisation:

$$
\begin{aligned}
&\left\langle H^{(a,b,c,d)}_{n,k},\, H^{(a,b,c,d)}_{m,j} \right\rangle_{H^{(a,b,c,d)}} \qquad (3.6)\\
&= \iint_\Omega \Big[R^{(a,b,c+d+2k+1)}_{n-k}(x)\, R^{(a,b,c+d+2j+1)}_{m-j}(x)\, \rho(x)^{k+j} \\
&\qquad \cdot\, P^{(d,c)}_k\left(\frac{y}{\rho(x)}\right)\, P^{(d,c)}_j\left(\frac{y}{\rho(x)}\right)\, W^{(a,b,c,d)}(x,y)\Big]\, \mathrm{d}y\, \mathrm{d}x \\
&= \Big(\int_\alpha^\beta R^{(a,b,c+d+2k+1)}_{n-k}(x)\, R^{(a,b,c+d+2j+1)}_{m-j}(x)\, w_R^{(a,b,c+d+k+j+1)}(x)\, \mathrm{d}x \Big) \\
&\qquad \cdot\, \Big(\int_\gamma^\delta P^{(d,c)}_k(t)\, P^{(d,c)}_j(t)\, w_P^{(d,)}(t)\, \mathrm{d}t \Big) \\
&= \omega_P^{(d,c)}\, \delta_{k,j} \int_\alpha^\beta R^{(a,b,c+d+2k+1)}_{n-k}(x)\, R^{(a,b,c+d+2k+1)}_{m-k}(x)\, w_R^{(a,b,c+d+2k+1)}(x)\, \mathrm{d}x \\
&= \omega_R^{(a,b,c+d+2k+1)}\, \omega_P^{(d,c)}\, \delta_{n,m}\, \delta_{k,j}. \qquad (3.7)
\end{aligned}
$$

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:

$$H_{n,k}^{(a,b,c)}(x,y) := R_{n-k}^{(a,b,2c+2k+1)}(x)\,\rho(x)^k\,P_k^{(c,c)}\left(\frac{y}{\rho(x)}\right), \quad (x,y) \in \Omega. \tag{3.8}$$

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 [46, §5]).

Remark: We should note at this stage that hereon we will continue to use the notation $P_n^{(a,b)}$ to refer to the univariate OPs orthonormal with respect to the weight $w_P^{(a,b)}$. For the disk-slice case, this means they are the orthonormal Jacobi polynomials, which is why we choose this notation. We stress that this is in difference to the spherical harmonic framework in Chapter 2, where conventionally they are defined using the un-normalized (i.e. simply orthogonal) classical Jacobi polynomials, and for which we also used the notation $P_n^{(a,b)}$.

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 their entries, 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:

$$xR_n^{(a,b,c)}(x) = \beta_n^{(a,b,c)} R_{n+1}^{(a,b,c)}(x) + \alpha_n^{(a,b,c)} R_n^{(a,b,c)}(x) + \beta_{n-1}^{(a,b,c)} R_{n-1}^{(a,b,c)}(x), \tag{3.9}$$

$$yP_n^{(d,c)}(y) = \delta_n^{(d,c)} P_{n+1}^{(d,c)}(y) + \gamma_n^{(d,c)} P_n^{(d,c)}(y) + \delta_{n-1}^{(d,c)} P_{n-1}^{(d,c)}(y). \tag{3.10}$$

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 equations (3.9–3.10) 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. *$H_{n,k}^{(a,b,c,d)}(x, y)$ satisfy the following relations:*

$$
\begin{aligned}
xH_{n,k}^{(a,b,c,d)}(x, y) &= \alpha_{n,k,1}^{(a,b,c,d)} H_{n-1,k}^{(a,b,c,d)}(x, y) + \alpha_{n,k,2}^{(a,b,c,d)} H_{n,k}^{(a,b,c,d)}(x, y) \\
&\quad + \alpha_{n+1,k,1}^{(a,b,c,d)} H_{n+1,k}^{(a,b,c)}(x, y), \\
yH_{n,k}^{(a,b,c,d)}(x, y) &= \beta_{n,k,1}^{(a,b,c,d)} H_{n-1,k-1}^{(a,b,c,d)}(x, y) + \beta_{n,k,2}^{(a,b,c,d)} H_{n-1,k}^{(a,b,c,d)}(x, y) \\
&\quad + \beta_{n,k,3}^{(a,b,c,d)} H_{n-1,k+1}^{(a,b,c,d)}(x, y) + \beta_{n,k,4}^{(a,b,c,d)} H_{n,k-1}^{(a,b,c,d)}(x, y) \\
&\quad + \beta_{n,k,5}^{(a,b,c,d)} H_{n,k}^{(a,b,c,d)}(x, y) + \beta_{n,k,6}^{(a,b,c,d)} H_{n,k+1}^{(a,b,c,d)}(x, y) \\
&\quad + \beta_{n,k,7}^{(a,b,c,d)} H_{n+1,k-1}^{(a,b,c,d)}(x, y) + \beta_{n,k,8}^{(a,b,c,d)} H_{n+1,k}^{(a,b,c,d)}(x, y) \\
&\quad + \beta_{n,k,9}^{(a,b,c,d)} H_{n+1,k+1}^{(a,b,c,d)}(x, y),
\end{aligned}
$$

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

$$\begin{aligned}
\alpha_{n,k,1}^{(a,b,c,d)} &:= \beta_{n-k-1}^{(a,b,c+d+2k+1)}, \qquad \alpha_{n,k,2}^{(a,b,c,d)} := \alpha_{n-k}^{(a,b,c+d+2k+1)}, \\
\beta_{n,k,1}^{(a,b,c,d)} &:= \delta_{k-1}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ R_{n-k}^{(a,b,c+d+2k-1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,2}^{(a,b,c,d)} &:= \gamma_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x) R_{n-k-1}^{(a,b,c+d+2k+1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,3}^{(a,b,c,d)} &:= \delta_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)}, R_{n-k-2}^{(a,b,c+d+2k+3)} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}, \\
\beta_{n,k,4}^{(a,b,c,d)} &:= \delta_{k-1}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ R_{n-k+1}^{(a,b,c+d+2k-1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,5}^{(a,b,c,d)} &:= \gamma_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x) R_{n-k}^{(a,b,c+d+2k+1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,6}^{(a,b,c,d)} &:= \delta_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)}, R_{n-k-1}^{(a,b,c+d+2k+3)} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}, \\
\beta_{n,k,7}^{(a,b,c,d)} &:= \delta_{k-1}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ R_{n-k+2}^{(a,b,c+d+2k-1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,8}^{(a,b,c,d)} &:= \gamma_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)},\ \rho(x) R_{n-k+1}^{(a,b,c+d+2k+1)} \right\rangle_{w_R^{(a,b,c+d+2k+1)}}, \\
\beta_{n,k,9}^{(a,b,c,d)} &:= \delta_{k}^{(d,c)} \left\langle R_{n-k}^{(a,b,c+d+2k+1)}, R_{n-k}^{(a,b,c+d+2k+3)} \right\rangle_{w_R^{(a,b,c+d+2k+3)}}.
\end{aligned}$$

Proof. The relation for multiplication by x follows from equation (3.9). 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

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

Recall from equation (3.7) that $\left\| H_{m,j}^{(a,b,c,d)} \right\|_{H^{(a,b,c,d)}}^{2} = \omega_R^{(a,b,c+d+2j+1)}\, \omega_P^{(d,c)}$. Then for $m = 0, \ldots, n+1$, $j = 0, \ldots, m$, using the change of variable $t = \frac{y}{\rho(x)}$:

$$
\begin{aligned}
&\left\langle y H^{(a,b,c,d)}_{n,k}, H^{(a,b,c,d)}_{m,j} \right\rangle_{H^{(a,b,c,d)}} \\
&= \iint_\Omega H^{(a,b,c,d)}_{n,k}(x,y)\, H^{(a,b,c,d)}_{m,j}(x,y)\, y\, W^{(a,b,c,d)}(x,y)\, dy\, dx \\
&= \Big(\int_\alpha^\beta R^{(a,b,c+d+2k+1)}_{n-k}(x)\, R^{(a,b,c+d+2j+1)}_{m-j}(x)\, \rho(x)^{k+j+2}\, w_R^{(a,b,c+d)}(x)\, \mathrm{d}x \Big) \\
&\qquad \cdot \Big(\int_\gamma^\delta P^{(d,c)}_k(t)\, P^{(d,c)}_j(t)\, t\, w_P^{(d,c)}(t)\, \mathrm{d}t \Big) \\
&= \Big(\int_\alpha^\beta R^{(a,b,c+d+2k+1)}_{n-k}(x)\, R^{(a,b,c+d+2j+1)}_{m-j}(x)\, w_R^{(a,b,c+d+k+j+2)}(x)\, \mathrm{d}x \Big) \\
&\qquad \cdot \Big(\int_\gamma^\delta P^{(d,c)}_k(t)\, P^{(d,c)}_j(t)\, t\, w_P^{(d,c)}(t)\, \mathrm{d}t \Big) \\
&= \begin{cases}
\delta^{(d,c)}_k\, \omega_P^{(d,c)}\, \omega_R^{(a,b,c+d+2k+3)} \left\langle R^{(a,b,c+d+2k+1)}_{n-k}, R^{(a,b,c+d+2k+3)}_{m-k-1} \right\rangle_{w_R^{(a,b,c+d+2k+3)}} & \\
 & \text{if } j = k+1 \\
\gamma^{(d,c)}_k\, \omega_P^{(d,c)}\, \omega_R^{(a,b,c+d+2k+1)} \left\langle R^{(a,b,c+d+2k+1)}_{n-k},\ \rho(x) R^{(a,b,c+d+2k+1)}_{m-k} \right\rangle_{w_R^{(a,b,c+d+2k+1)}} & \\
 & \text{if } j = k \\
\delta^{(d,c)}_{k-1}\, \omega_P^{(d,c)}\, \omega_R^{(a,b,c+d+2k-1)} \left\langle R^{(a,b,c+d+2k-1)}_{n-k},\ \rho(x)^2 R^{(a,b,c+d+2k-1)}_{m-k+1} \right\rangle_{w_R^{(a,b,c+d+2k-1)}} & \\
 & \text{if } j = k-1 \\
0 & \text{otherwise,}
\end{cases}
\end{aligned}
$$

where, by orthogonality,

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

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.

□

These relations lead to Jacobi operators that correspond to multiplication by x and y. Define, for $n = 0, 1, 2, \dots$:

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

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

$$J_x^{(a,b,c,d)}\, \mathbb{H}^{(a,b,c,d)}(x,y) = x\, \mathbb{H}^{(a,b,c,d)}(x,y), \tag{3.11}$$

$$J_y^{(a,b,c,d)}\, \mathbb{H}^{(a,b,c,d)}(x,y) = y\, \mathbb{H}^{(a,b,c,d)}(x,y). \tag{3.12}$$

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 $f(x,y) = \mathbb{H}^{(a,b,c,d)}(x,y)^\top \boldsymbol{f}$. Then $x\,f(x,y)$ is approximated by $\mathbb{H}^{(a,b,c,d)}(x,y)^\top J_x^{(a,b,c,d)\top} \boldsymbol{f}$. In other words, $J_x^{(a,b,c,d)\top} \boldsymbol{f}$ 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 $(1,1)$):

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

For $J_x^{(a,b,c,d)}$, the blocks are diagonal (sub-block-bandwidths $(0,0)$) for $n = 0, 1, 2, \ldots$:

$$A_{x,n} := \begin{pmatrix} \alpha_{n+1,0,1}^{(a,b,c,d)} & 0 & \dots & 0 \\ & \ddots & & \vdots \\ & & \alpha_{n+1,n,1}^{(a,b,c,d)} & 0 \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+2)},$$

$$B_{x,n} := \begin{pmatrix} \alpha_{n,0,2}^{(a,b,c,d)} & & \\ & \ddots & \\ & & \alpha_{n,n,2}^{(a,b,c,d)} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)},$$

$$C_{x,n} := \left(A_{n-1}^x\right)^\top \in \mathbb{R}^{(n+1)\times n}, \quad (n \neq 0)$$

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

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

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

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

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 equations (3.11–3.12) into a block-tridiagonal system:

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

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 $n = 0, 1, 2\dots$,

$$A_n := \begin{pmatrix} A_{x,n} \\ A_{y,n} \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+2)}, \quad C_n := \begin{pmatrix} C_{x,n} \\ C_{y,n} \end{pmatrix} \in \mathbb{R}^{2(n+1)\times n} \quad (n \neq 0), \tag{3.13}$$

$$B_n := \begin{pmatrix} B_{x,n} \\ B_{y,n} \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+1)}, \quad G_n(x,y) := \begin{pmatrix} xI_{n+1} \\ yI_{n+1} \end{pmatrix} \in \mathbb{R}^{2(n+1)\times(n+1)}. \tag{3.14}$$

For each $n = 0, 1, 2\dots$ let $D_n^\top$ be any matrix that is a left inverse of A_n, i.e. such that $D_n^\top A_n = I_{n+2}$. 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 [22, p.78], which can be expanded to obtain the recurrence for $n = 0, 1, 2, \dots$:

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

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

$$D_n^\top := \begin{pmatrix} \frac{1}{\alpha_{n+1,0,1}^{(a,b,c,d)}} & & & & & & & \\ & \ddots & & & & & & \\ & & \ddots & & & & & \\ & & & \frac{1}{\alpha_{n+1,n,1}^{(a,b,c,d)}} & & & & \\ \eta_0 & 0 & \dots & 0 & \eta_1 & \dots & \dots & \eta_{n+1} \end{pmatrix}, \tag{3.15}$$

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.

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

Definition 8. *The matrices $-D_n^\top(B_n - G_n(x,y,z))$, $D_n^\top C_n$ defined via equa-*

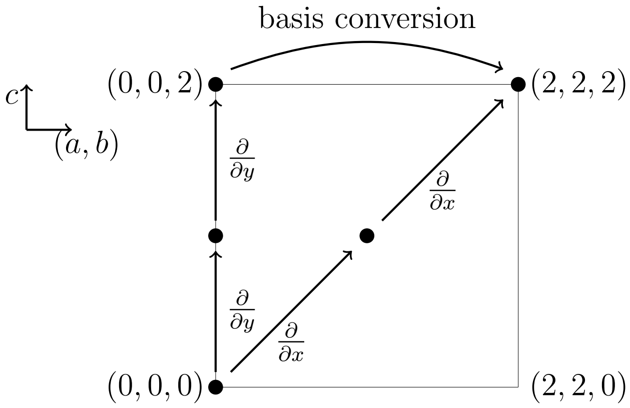


Figure 3.1: The Laplace operator acting on vectors of $H_{n,k}^{(0,0,0)}$ coefficients has a sparse matrix representation if the range is represented as vectors of $H_{n,k}^{(2,2,2)}$ coefficients. Here, the arrows indicate that the corresponding operation has a sparse matrix representation when the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

tions (3.13–3.15) are the recurrence coefficient matrices associated with the OPs $\{H_{n,k}^{(a,b,c,d)}\}$.

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 orthonormal 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 orthonormal 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 $f(x,y) = \mathbb{H}^{(a,b,c)}(x,y)^\top \boldsymbol{f}$.

Definition 9. *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:

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

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 [55, (18.9.3)], and on the triangle [60]. 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 9 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:

$$w_R^{(a,b,c)\,\prime}(x) = -a\, w_R^{(a-1,b,c)}(x) + b\, w_R^{(a,b-1,c)}(x) + c\,\rho(x)\,\rho'(x)\, w_R^{(a,b,c-2)}(x), \tag{3.16}$$

$$w_P^{(c)\,\prime}(y) = -2c\, y\, w_P^{(c-1)}(y), \tag{3.17}$$

$$\rho(x)\,\rho'(x) = -x. \tag{3.18}$$

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 $m = 0, \ldots, n-1$, $j = 0, \ldots, m$ 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

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

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

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

Now, using equation (3.17), 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

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

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 $\frac{\partial}{\partial x} H^{(a,b,c)}_{n,k} = \sum_{m=0}^{n-1} \sum_{j=0}^{m} c^x_{m,j}\, H^{(a+1,b+1,c+1)}_{m,j}$. 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

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

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

$$\begin{aligned}
&\left\langle \frac{\partial}{\partial x} H^{(a,b,c)}_{n,k}, H^{(a+1,b+1,c+1)}_{m,j} \right\rangle_{H^{(a+1,b+1,c+1)}} \\
&= \Big(\int_\alpha^\beta R^{(a,b,2c+2k+1)\,\prime}_{n-k}\, R^{(a+1,b+1,2c+2j+3)}_{m-j}\, \rho^{k+j+1}\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad \cdot \Big(\int_\gamma^\delta P^{(c,c)}_k\, P^{(c+1,c+1)}_j\, w_P^{(c+1)}\, \mathrm{d}t \Big) \\
&\quad + k \Big(\int_\alpha^\beta R^{(a,b,2c+2k+1)}_{n-k}\, R^{(a+1,b+1,2c+2j+3)}_{m-j}\, \rho^{k+j}\, \rho'\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad \cdot \Big(\int_\gamma^\delta P^{(c,c)}_k\, P^{(c+1,c+1)}_j\, w_P^{(c+1)}\, \mathrm{d}t \Big) \\
&\quad - \Big(\int_\alpha^\beta R^{(a,b,2c+2k+1)}_{n-k}\, R^{(a+1,b+1,2c+2j+3)}_{m-j}\, \rho^{k+j}\, \rho'\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \Big) \\
&\qquad \cdot \Big(\int_\gamma^\delta t\, P^{(c,c)\,\prime}_k\, P^{(c+1,c+1)}_j\, w_P^{(c+1)}\, \mathrm{d}t \Big).
\end{aligned} \tag{3.19}$$

We will first show that the second factor of each term in equation (3.19) 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 $P^{(c,c)}_k$ is an even polynomial for even k, and an odd polynomial for odd k. Thus, $P^{(c,c)}_k\, P^{(c+1,c+1)}_{k-1}$ 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, equation (3.19) is zero for $j \notin \{k-2, k\}$.

Now, using equation (3.16), 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

$$
\begin{aligned}
&\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)\,\prime}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, \rho^{k+j+1}\, w_R^{(a+1,b+1,2c+2)}\, \mathrm{d}x \\
&= \int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)\,\prime}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\, w_R^{(a+1,b+1,2c+k+j+3)}\, \mathrm{d}x \\
&= -\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)}\, \frac{\mathrm{d}}{\mathrm{d}x}\Big[R_{m-j}^{(a+1,b+1,2c+2j+3)}\, w_R^{(a+1,b+1,2c+k+j+3)}\Big]\, \mathrm{d}x \\
&= -\int_\alpha^\beta R_{n-k}^{(a,b,2c+2k+1)}\, \Big\{R_{m-j}^{(a+1,b+1,2c+2j+3)\,\prime}\, w_R^{(a+1,b+1,2c+k+j+3)} \\
&\qquad\qquad + (2c+k+j+3)\, \rho\, \rho'\, w_R^{(a+1,b+1,2c+k+j+1)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)} \\
&\qquad\qquad + (b+1)\, w_R^{(a+1,b,2c+k+j+3)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)} \\
&\qquad\qquad - (a+1)\, w_R^{(a,b+1,2c+k+j+3)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)}\Big\}\, \mathrm{d}x \\
&= -\,\omega_R^{(a,b,2c+2k+1)}\, \Big\{ \Big\langle R_{n-k}^{(a,b,2c+2k+1)},\, w_R^{(1,1,j-k+2)}\, R_{m-j}^{(a+1,b+1,2c+2j+3)\,\prime}\Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad + (2c+k+j+3)\Big\langle R_{n-k}^{(a,b,2c+2k+1)},\, \rho\rho'\, w_R^{(1,1,j-k)} R_{m-j}^{(a+1,b+1,2c+2j+3)}\Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad + (b+1)\Big\langle R_{n-k}^{(a,b,2c+2k+1)},\, w_R^{(1,0,j-k+2)} R_{m-j}^{(a+1,b+1,2c+2j+3)}\Big\rangle_{w_R^{(a,b,2c+2k+1)}} \\
&\quad - (a+1)\Big\langle R_{n-k}^{(a,b,2c+2k+1)},\, w_R^{(0,1,j-k+2)} R_{m-j}^{(a+1,b+1,2c+2j+3)}\Big\rangle_{w_R^{(a,b,2c+2k+1)}} \Big\}.
\end{aligned}
\tag{3.20}
$$

By recalling equation (3.18) 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 equation (3.20) is is zero for $m-j+3+j-k < n-k \iff m < n-3$.

Finally,

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

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

$$\left\langle \frac{\partial}{\partial x} H_{n,k}^{(a,b,c)}, H_{m,j}^{(a+1,b+1,c+1)} \right\rangle_{H^{(a+1,b+1,c+1)}} = 0,$$

for $m < n-3$, $j \notin \{k-2, k\}$, 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

$$\frac{\partial}{\partial x} W^{(a,b,c)}(x,y) = -aW^{(a-1,b,c)}(x,y) + bW^{(a,b,c)}(x,y) + 2c\rho(x)\, \rho'(x)\, W^{(a,b,c-1)}, \tag{3.21}$$

$$\frac{\partial}{\partial y} W^{(a,b,c)}(x,y) = -2c\, y\, W^{(a,b,c-1)}(x,y), \tag{3.22}$$

and also that

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

□

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

Definition 10. *Define the operator matrices*

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

for conversion between non-weighted spaces, and

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

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 10 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* $(2,0)$.

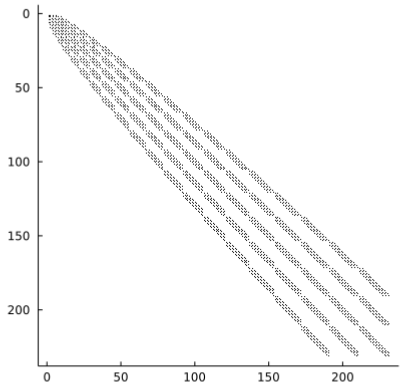
Proof. We proceed with the case for the non-weighted operators $T^{(a,b)\to(a+\tilde{a},b+\tilde{b},c+\tilde{c})}$, where $\tilde{a},\tilde{b},\tilde{c}\in\{0,1\}$. Since $\{H_{m,j}^{(a+\tilde{a},b+\tilde{b},c+\tilde{c})}\}$ for $m=0,\dots,n$, $j=0,\dots,m$ is an orthogonal basis for any degree n polynomial, 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

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

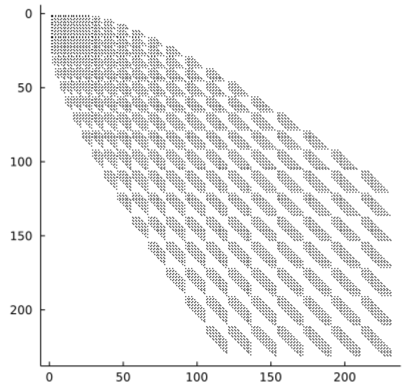
Then, using the change of variable $t=\frac{y}{\rho(x)}$, we have that

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

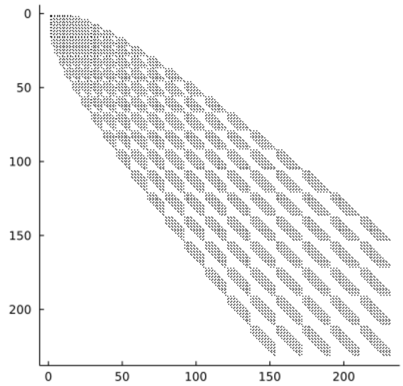
Since $w_P^{(\tilde{c})}$ is a polynomial degree $2\tilde{c}$, we have that the above is then zero for $j<k-2\tilde{c}$. Further, since $w_R^{(\tilde{a},\tilde{b},\,2\tilde{c}+j-k)}$ is a polynomial of degree $\tilde{a}+\tilde{b}+2\tilde{c}+j-k$,



(a)



(b)



(c)

Figure 3.2: "Spy" plots of (differential) operator matrices, showing their sparsity. (a) The Laplacian operator $\Delta_W^{(1,1,1)\to(1,1,1)}$. (b) The 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 $k = 200$. (c) The biharmonic operator ${}_2\Delta_W^{(2,2,2)\to(2,2,2)}$

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

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

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 3.2.

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 $\mathbb{W}^{(2,2,2)}$ to coefficients in the space $\mathbb{H}^{(0,0,0)}$. Note that a function expanded in the $\mathbb{W}^{(2,2,2)}$ 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 3.2.

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 equation (3.9), by careful application of the Christoffel–Darboux formula [55, (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 11. *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:*

$$\langle p,\, q\rangle_{w_{\tilde{R}}^{(a,b,c,d)}} := \frac{1}{\omega_{\tilde{R}}^{(a,b,c,d)}} \int_\alpha^\beta p(x)\, q(x)\, w_{\tilde{R}}^{(a,b,c,d)}(x)\,\mathrm{d}x, \tag{3.23}$$

where

$$\omega_{\tilde{R}}^{(a,b,c,d)} := \int_\alpha^\beta w_{\tilde{R}}^{(a,b,c,d)}(x)\,\mathrm{d}x. \tag{3.24}$$

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 equation (3.23).*

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:

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

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

$$\tilde{R}_n^{(a,b,c+1,d)}(x) = \mathcal{C}_n^{(a,b,c,d)} \sum_{k=0}^n \tilde{R}_k^{(a,b,c,d)}(1)\,\tilde{R}_k^{(a,b,c,d)}(x), \tag{3.26}$$

$$\tilde{R}_n^{(a,b,c,d+1)}(x) = \mathcal{D}_n^{(a,b,c,d)} \sum_{k=0}^n \tilde{R}_k^{(a,b,c,d)}(-1)\,\tilde{R}_k^{(a,b,c,d)}(x). \tag{3.27}$$

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

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

$$\mathcal{C}_n^{(a,b,c,d)} = \left(\frac{\omega_{\tilde{R}}^{(a,b,c+1,d)}}{\omega_{\tilde{R}}^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(1)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1)\,\tilde{\beta}_n^{(a,b,c,d)}}\right)^{\frac{1}{2}}, \tag{3.28}$$

$$\mathcal{D}_n^{(a,b,c,d)} = (-1)^n\left(\frac{-\omega_{\tilde{R}}^{(a,b,c,d+1)}}{\omega_{\tilde{R}}^{(a,b,c,d)}\,\tilde{R}_n^{(a,b,c,d)}(-1)\,\tilde{R}_{n+1}^{(a,b,c,d)}(-1)\,\tilde{\beta}_n^{(a,b,c,d)}}\right)^{\frac{1}{2}}. \tag{3.29}$$

Now, by the Christoffel–Darboux formula [55, (18.2.12)], we have that for any $x, y \in \mathbb{R}$,

$$\sum_{k=0}^{n} \tilde{R}_k^{(a,b,c,d)}(y)\,\tilde{R}_k^{(a,b,c,d)}(x)$$
$$= \tilde{\beta}_n^{(a,b,c,d)}\,\frac{\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(y) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(y)}{y-x}. \tag{3.30}$$

Then,

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

using equation (3.28) and equation (3.30), showing that the RHS and LHS of equation (3.26) are equivalent. Further,

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

using equation (3.29) and equation (3.30), showing that the RHS and LHS of equation (3.27) are also equivalent. □

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

$$\tilde{\alpha}_n^{(a,b,c+1,d)} = \frac{\tilde{R}_{n+2}^{(a,b,c,d)}(1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}\,\tilde{\beta}_{n+1}^{(a,b,c,d)} - \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}{\tilde{R}_{n}^{(a,b,c,d)}(1)}\,\tilde{\beta}_{n}^{(a,b,c,d)} + \tilde{\alpha}_{n+1}^{(a,b,c,d)}, \tag{3.31}$$

$$\tilde{\beta}_n^{(a,b,c+1,d)} = \frac{\mathcal{C}_n^{(a,b,c,d)}}{\mathcal{C}_{n+1}^{(a,b,c,d)}}\,\frac{\tilde{R}_n^{(a,b,c,d)}(1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(1)}\,\tilde{\beta}_n^{(a,b,c,d)}. \tag{3.32}$$

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

$$\tilde{\alpha}_n^{(a,b,c,d+1)} = \frac{\tilde{R}_{n+2}^{(a,b,c,d)}(-1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_{n+1}^{(a,b,c,d)} - \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}{\tilde{R}_{n}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_{n}^{(a,b,c,d)} + \tilde{\alpha}_{n+1}^{(a,b,c,d)}, \tag{3.33}$$

$$\tilde{\beta}_n^{(a,b,c,d+1)} = \frac{\mathcal{D}_n^{(a,b,c,d)}}{\mathcal{D}_{n+1}^{(a,b,c,d)}}\,\frac{\tilde{R}_n^{(a,b,c,d)}(-1)}{\tilde{R}_{n+1}^{(a,b,c,d)}(-1)}\,\tilde{\beta}_n^{(a,b,c,d)}. \tag{3.34}$$

Proof. First, using equation (3.26) and equation (3.30) we have that

$$\begin{aligned}
&(1-x)\,x\,\tilde{R}_n^{(a,b,c+1,d)}(x)\\
&= \mathcal{C}_n^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c,d)}\,x\left[\tilde{R}_n^{(a,b,c,d)}(x)\,\tilde{R}_{n+1}^{(a,b,c,d)}(1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\,\tilde{R}_n^{(a,b,c,d)}(1)\right]\\
&= \mathcal{C}_n^{(a,b,c,d)}\,\tilde{\beta}_n^{(a,b,c,d)}\\
&\quad\cdot\Big\{\tilde{R}_{n+1}^{(a,b,c,d)}(1)\,\Big(\tilde{\beta}_n^{(a,b,c,d)}\tilde{R}_{n+1}^{(a,b,c,d)}(x) + \tilde{\alpha}_n^{(a,b,c,d)}\tilde{R}_n^{(a,b,c,d)}(x)\\
&\qquad\qquad + \tilde{\beta}_{n-1}^{(a,b,c,d)}\tilde{R}_{n-1}^{(a,b,c,d)}(x)\Big)\\
&\qquad - \tilde{R}_n^{(a,b,c,d)}(1)\,\Big(\tilde{\beta}_{n+1}^{(a,b,c,d)}\tilde{R}_{n+2}^{(a,b,c,d)}(x) + \tilde{\alpha}_{n+1}^{(a,b,c,d)}\tilde{R}_{n+1}^{(a,b,c,d)}(x)\\
&\qquad\qquad + \tilde{\beta}_n^{(a,b,c,d)}\tilde{R}_n^{(a,b,c,d)}(x)\Big)\Big\}.
\end{aligned} \tag{3.35}$$

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

$$
\begin{aligned}
&(1-x)\, x\, \tilde{R}_n^{(a,b,c+1,d)}(x) \\
&= (1-x)\Big\{\tilde{\beta}_n^{(a,b,c+1,d)}\tilde{R}_{n+1}^{(a,b,c+1,d)}(x) + \tilde{\alpha}_n^{(a,b,c+1,d)}\tilde{R}_n^{(a,b,c+1,d)}(x) \\
&\qquad\qquad + \tilde{\beta}_{n-1}^{(a,b,c+1,d)}\tilde{R}_{n-1}^{(a,b,c+1,d)}(x)\Big\} \\
&= \mathcal{C}_{n+1}^{(a,b,c,d)}\tilde{\beta}_n^{(a,b,c+1,d)}\tilde{\beta}_{n+1}^{(a,b,c,d)}\left(\tilde{R}_{n+1}^{(a,b,c,d)}(x)\tilde{R}_{n+2}^{(a,b,c,d)}(1) - \tilde{R}_{n+2}^{(a,b,c,d)}(x)\tilde{R}_{n+1}^{(a,b,c,d)}(1)\right) \\
&\quad + \mathcal{C}_{n}^{(a,b,c,d)}\tilde{\alpha}_n^{(a,b,c+1,d)}\tilde{\beta}_{n}^{(a,b,c,d)}\left(\tilde{R}_{n}^{(a,b,c,d)}(x)\tilde{R}_{n+1}^{(a,b,c,d)}(1) - \tilde{R}_{n+1}^{(a,b,c,d)}(x)\tilde{R}_{n}^{(a,b,c,d)}(1)\right) \\
&\quad + \mathcal{C}_{n-1}^{(a,b,c,d)}\tilde{\beta}_{n-1}^{(a,b,c+1,d)}\tilde{\beta}_{n-1}^{(a,b,c,d)}\left(\tilde{R}_{n-1}^{(a,b,c,d)}(x)\tilde{R}_{n}^{(a,b,c,d)}(1) - \tilde{R}_{n}^{(a,b,c,d)}(x)\tilde{R}_{n-1}^{(a,b,c,d)}(1)\right).
\end{aligned}
\tag{3.36}
$$

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 equation (3.35) and equation (3.36) 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:*

$$
\tilde{\alpha}_n^{(a,b,c+1,d)} = \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(1)} - \frac{\tilde{\beta}_{n}^{(a,b,c,d)}}{\chi_{n}^{(a,b,c,d)}(1)} + \tilde{\alpha}_n^{(a,b,c,d)}, \tag{3.37}
$$

$$
\tilde{\beta}_n^{(a,b,c+1,d)} = \left(\frac{1-\tilde{\alpha}_{n+1}^{(a,b,c,d)} - \frac{\tilde{\beta}_{n}^{(a,b,c,d)}}{\chi_{n}^{(a,b,c,d)}(1)}}{1-\tilde{\alpha}_{n}^{(a,b,c,d)} - \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(1)}}\right)^{\frac{1}{2}} \tilde{\beta}_n^{(a,b,c,d)}. \tag{3.38}
$$

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

$$\tilde{\alpha}_n^{(a,b,c,d+1)} = \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(-1)} - \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(-1)} + \tilde{\alpha}_n^{(a,b,c,d)}, \tag{3.39}$$

$$\tilde{\beta}_n^{(a,b,c,d+1)} = \left(\frac{-1 + \tilde{\alpha}_{n+1}^{(a,b,c,d)} + \frac{\tilde{\beta}_n^{(a,b,c,d)}}{\chi_n^{(a,b,c,d)}(-1)}}{-1 + \tilde{\alpha}_n^{(a,b,c,d)} + \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(-1)}} \right)^{\frac{1}{2}} \tilde{\beta}_n^{(a,b,c,d)}. \tag{3.40}$$

where

$$\chi_n^{(a,b,c,d)}(y) := \frac{\tilde{R}_{n+1}^{(a,b,c,d)}(y)}{\tilde{R}_n^{(a,b,c,d)}(y)} \tag{3.41}$$

$$= \frac{1}{\tilde{\beta}_n^{(a,b,c,d)}} \left(y - \tilde{\alpha}_n^{(a,b,c,d)} - \frac{\tilde{\beta}_{n-1}^{(a,b,c,d)}}{\chi_{n-1}^{(a,b,c,d)}(y)} \right), \quad y \in \{-1, 1\}. \tag{3.42}$$

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 $H^{(a,b,c)}_{n,k}(x,y)$ 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 $(s_k, w^{(s)}_k)$, and on $[-1,1]$ with weight $(1-t^2)^c$ as $(t_k, w^{(t)}_k)$. Define*

$$\begin{aligned}
x_{i+(j-1)N} &:= s_j, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2}\right\rceil, \\
y_{i+(j-1)N} &:= \rho(s_j)\, t_i, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2}\right\rceil, \\
w_{i+(j-1)N} &:= w^{(s)}_j w^{(t)}_i, \quad i,j = 1,\dots,\left\lceil \frac{N+1}{2}\right\rceil.
\end{aligned}$$

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

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

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 $\le N$.

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

$$\begin{aligned}
&\iint_\Omega f_e(x,y)\, W^{(a,b,c)}(x,y)\,\mathrm{d}y\,\mathrm{d}x \\
&\qquad = \int_\alpha^\beta \int_{-1}^1 f_e\big(s,\rho(s)t\big)\, V^{(a,b,c)}(s,t)\,\rho(s)\,\mathrm{d}t\,\mathrm{d}s \\
&\qquad = \int_\alpha^\beta w_R^{(a,b,2c+1)}(s)\,\Big(\int_{-1}^1 f_e\big(s,\rho(s)t\big)\, w_P^{(c)}(t)\,\mathrm{d}t\Big)\,\mathrm{d}s \\
&\qquad \approx \int_\alpha^\beta w_R^{(a,b,2c+1)}(s)\,\sum_{i=1}^{M_2}\Big(w_i^{(t)} f_e\big(s,\rho(s)t_i\big)\Big)\,\mathrm{d}s \quad (\star) \\
&\qquad \approx \sum_{j=1}^{M_1}\left(w_j^{(s)}\sum_{i=1}^{M_2}\Big(w_i^{(t)} f_e\big(s_j,\rho(s_j)t_i\big)\Big)\right) \quad (\star\star) \\
&\qquad = \sum_{k=1}^{M_1M_2} w_k\, f_e(x_k,y_k).
\end{aligned}$$

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

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

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

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

for N sufficiently large, where

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

for all $n = 0, 1, 2, \dots, N$, and where

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

Recall from equation (3.7) that $\left\| H_{n,k}^{(a,b,c)} \right\|^2_{H^{(a,b,c)}} = \omega_R^{(a,b,2c+2k+1)}\, \omega_P^{(c)}$. Using the quadrature rule detailed in Section 4.2 for the inner product, we can calculate the coefficients $f_{n,k}$ for each $n = 0, \dots, N$, $k = 0, \dots, n$:

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

where $\lambda_k^{(a,b,c)} := \frac{1}{2\, \omega_R^{(a,b,2c+2k+1)}\, \omega_P^{(c)}}$ and $M = \left\lceil \frac{1}{2}(N+1) \right\rceil^2$.

3.3.4 Calculating non-zero entries of the operator matrices

The proofs of Theorem 2 and Lemma 6 provide a way to calculate the non-zero entries of the operator matrices given in Definition 9 and Definition 10. 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 the Poisson equation, an inhomogeneous variable coefficient Helmholtz equation and the Biharmonic equation, demonstrating the versatility of the approach.

As mentioned earlier, we can handle these boundary conditions by incorporating them into the chosen basis OP family. The weight $W^{(1,1,1)}(x,y)$ is of course zero on the boundary of Ω, and in fact any polynomial that vanishes on the boundary will have $W^{(1,1,1)}(x,y)$ as a factor. Hence, any function expanded in the $\mathbb{W}^{(1,1,1)}$ basis will satisfy zero Dirichlet conditions. The same argument can be used to see why any function expanded in the $\mathbb{W}^{(2,2,2)}$ basis will satisfy zero Neumann conditions too.

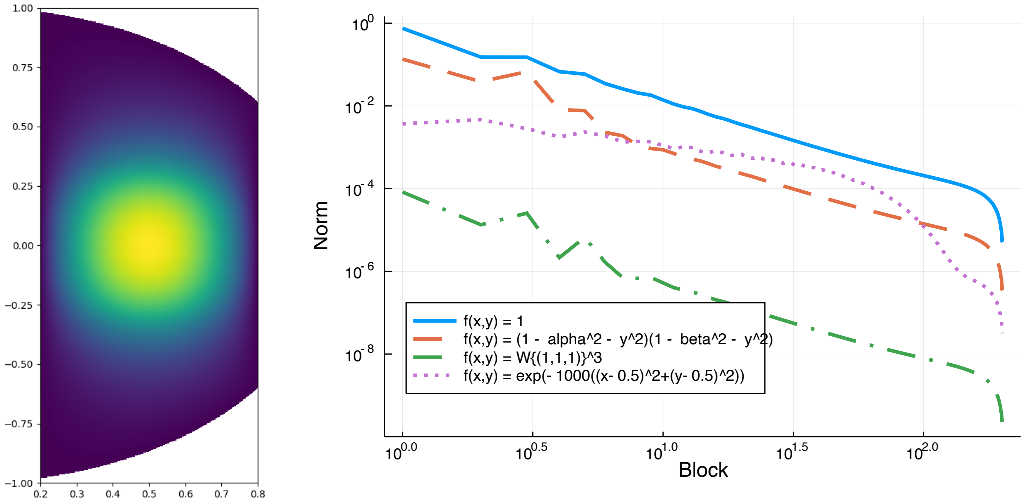


Figure 3.3: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y) = 1 + \mathrm{erf}(5(1 - 10((x - 0.5)^2 + y^2)))$. Right: The norms of each block of the computed solution of the Poisson equation with the given right hand side functions. This demonstrates algebraic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

$$\begin{cases} \Delta u(x,y) = f(x,y) & \text{in } \Omega \\ u(x,y) = 0 & \text{on } \partial\Omega \end{cases}. \tag{3.43}$$

noting the imposition of zero Dirichlet boundary conditions on u.

We can tackle the problem as follows. Since u vanishes on the boundary, any polynomial expansion will have $W^{(1,1,1)}(x, y)$ as a factor, and so we can denote the coefficient vector for expansion of u in the $\mathbb{W}^{(1,1,1)}$ OP basis up to degree N

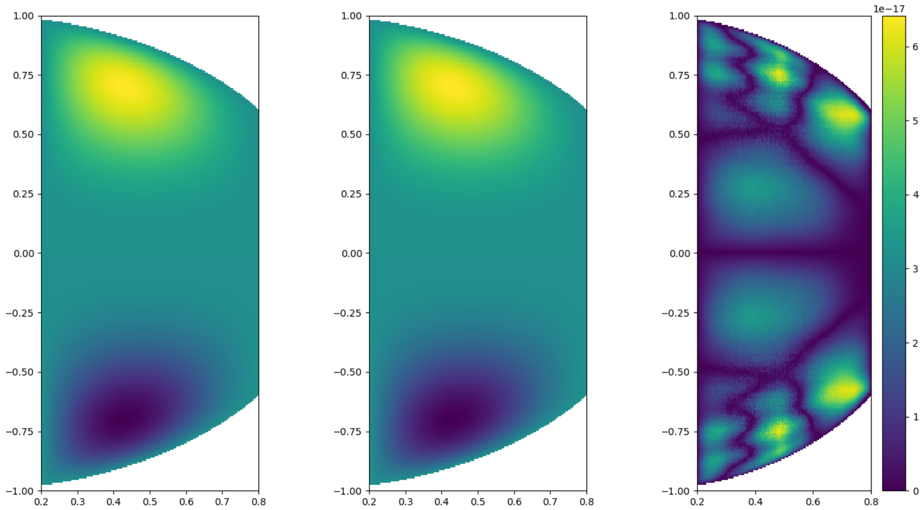


Figure 3.4: The computed solution to $\Delta u = f$ with zero boundary conditions compared with the exact solution $u(x,y) = W^{(1,1,1)}(x,y)y^3 \exp(x)$. Left: Computed. Centre: Exact. Right: Plot of the error (colourbar is shown to demonstrate magnitude of the error is of the order 10^{-17})

by $\boldsymbol{u}$, while the coefficient vector for expansion of f in the $\mathbb{H}^{(1,1,1)}$ OP basis up to degree N we can denote by $\boldsymbol{f}$. Since f is known, we can obtain $\boldsymbol{f}$ using the quadrature rule above. In matrix-vector notation, our system hence becomes:

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

which can be solved to find $\boldsymbol{u}$. In Figure 3.3 we see the solution to the Poisson equation with zero boundary conditions given in equation (3.43) in the disk-slice Ω. In Figure 3.3 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

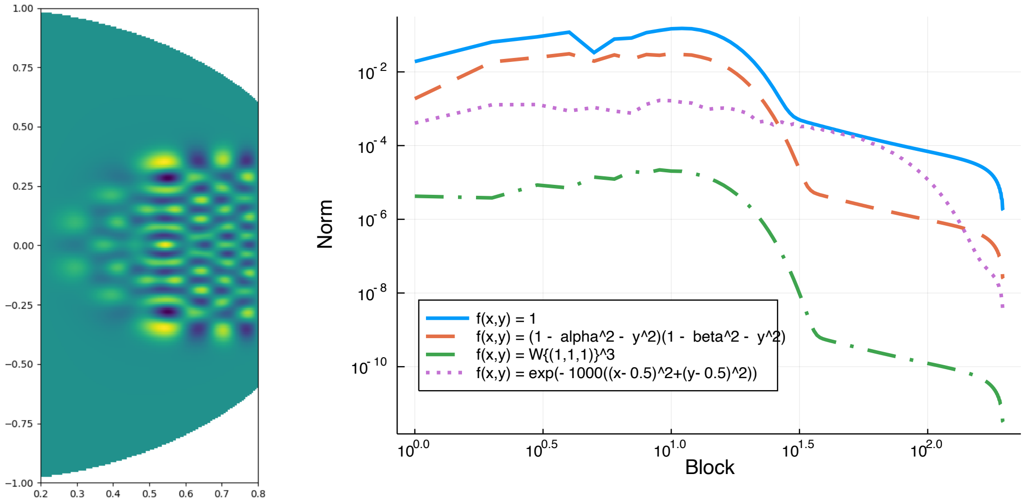


Figure 3.5: Left: The computed solution to $\Delta u + k^2\, v\, u = f$ with zero boundary conditions with $f(x, y) = x(1 - x^2 - y^2)e^x$, $v(x, y) = 1 - (3(x - 1)^2 + 5y^2)$ and $k = 100$. Right: The norms of each block of the computed solution of the Helmholtz equation with the given right hand side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

at the same rate as the coefficients 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. We see that the computed solution is almost exact. 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 $f(x, y) = \Delta\big[W^{(1,1,1)}(x, y)\, y^3\, \exp(x)\big]$.

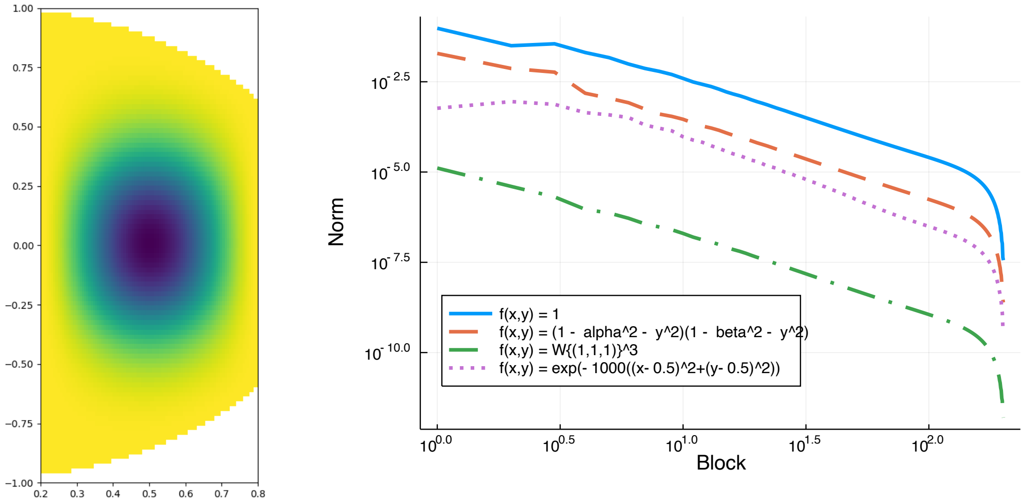


Figure 3.6: Left: The computed solution to $\Delta^2 u = f$ with zero Dirichlet and Neumann boundary conditions with $f(x,y) = 1+\mathrm{erf}(5(1-10((x-0.5)^2+y^2)))$. Right: The norms of each block of the computed solution of the biharmonic equation with the given right hand side functions.

3.4.2 Inhomogeneous variable-coefficient Helmholtz

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

$$\begin{cases} \Delta u(x,y) + k^2\, v(x,y)\, u(x,y) = f(x,y) & \text{in } \Omega, \\ u(x,y) = 0 \quad \text{on } \partial\Omega. \end{cases} \tag{3.44}$$

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 $\boldsymbol{u}$, and the coefficient vector for expansion of f in the $\mathbb{H}^{(1,1,1)}$ OP basis up to degree N by $\boldsymbol{f}$. Since f is known, we can obtain the coefficients $\boldsymbol{f}$ 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 à la the procedure introduced in [59]. 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:

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

which can be solved to find $\boldsymbol{u}$. We can see the sparsity and structure of this matrix system in Figure 3.2 with $v(x, y) = xy^2$ as an example. In Figure 3.5 we see the solution to the inhomogeneous variable-coefficient Helmholtz equation with zero boundary conditions given in equation (3.44) 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 3.5 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

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

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

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

3.4.3 Biharmonic equation

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

$$\begin{cases} \Delta^2 u(x,y) = f(x,y) & \text{in } \Omega, \\ u(x,y) = 0, \quad \frac{\partial u}{\partial n}(x,y) = 0 & \text{on } \partial\Omega. \end{cases} \tag{3.45}$$

where Δ^2 is the Biharmonic operator, noting the imposition of zero Dirichlet and Neumann boundary conditions on u. In Figure 3.6 we see the solution to the Biharmonic equation (3.45) in the disk-slice Ω. In Figure 3.6 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.

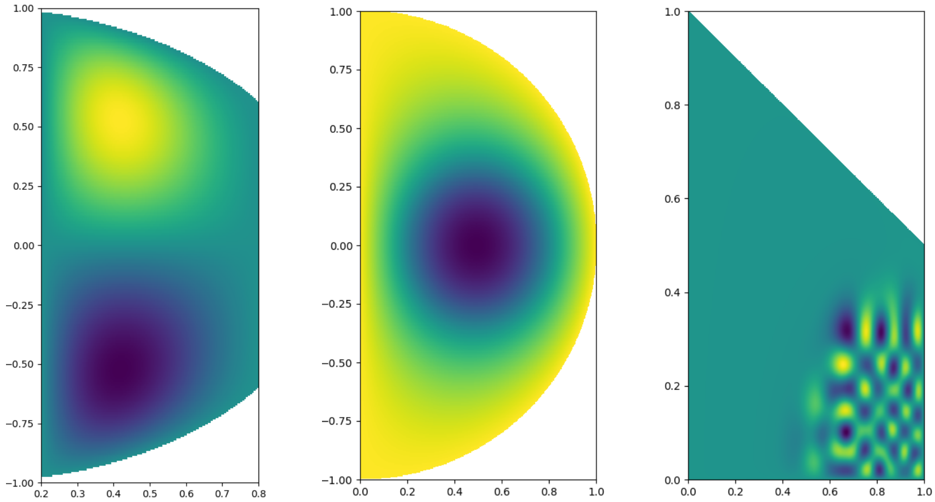


Figure 3.7: Left: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y) = W^{(1,1,1)}(x, y)y\cos(x)$ in the disk-slice using the p-FEM approach with a single element. Centre: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x, y) = 1 + \mathrm{erf}(5(1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

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 a 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

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

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 Theorem 2, 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 $n = 0,1,2,\dots$ 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 $0 \le k \le n$, $n = 0,1,2,\dots,$

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

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 [6] to construct a sparse p-finite element method in terms of the operators constructed above, with the benefit of ensuring that the resulting discretisation is symmetric. Consider the 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 $v \in V := H_0^1(\Omega) = \{v \in H^1(\Omega) \quad | \quad v|_{\partial\Omega} = 0\}$,

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

As eluded to, in general we would discretise our domain Ω with a mesh $\mathcal{T}$

consisting of elements τ, where each $\tau \in \mathcal{T}$ 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.

$$L(v_p) = a(u_p, v_p) \quad \forall\, v_p \in V_p. \tag{3.46}$$

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 $\Lambda^{(a,b,c)} := \left\langle \mathbb{H}^{(a,b,c)},\, \mathbb{H}^{(a,b,c)\top} \right\rangle_{H^{(a,b,c)}}$. 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 $a = b = c = 1$

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

and rewrite equation (3.46) in matrix form:

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

$$
\begin{aligned}
&= \int_\tau \Big(\boldsymbol{v}^\top W_x^{(1,1,1)^\top} \mathbb{H}^{(0,0,0)} \mathbb{H}^{(0,0,0)^\top} W_x^{(1,1,1)} \boldsymbol{u} \\
&\qquad + \boldsymbol{v}^\top (T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)})^\top \mathbb{H}^{(0,0,0)} \mathbb{H}^{(0,0,0)^\top} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \boldsymbol{u} \Big) \, \mathrm{d}\boldsymbol{x} \\
&= \boldsymbol{v}^\top \Big(W_x^{(1,1,1)^\top} \Lambda^{(0,0,0)} W_x^{(1,1,1)} \\
&\qquad + (T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)})^\top \Lambda^{(0,0,0)} T_W^{(1,1,0)\to(0,0,0)} W_y^{(1,1,1)} \Big) \, \boldsymbol{u},
\end{aligned}
$$

where $\boldsymbol{u}, \boldsymbol{v}$ 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

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

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

Since equation (3.46) is equivalent to stating that

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

(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:

$$
A\boldsymbol{u} = \tilde{\boldsymbol{f}},
$$

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 $\tilde{\boldsymbol{f}}$ is given by

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

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.

3.7 Conclusions

In this chapter we have shown that bivariate orthogonal polynomials can lead to sparse discretizations of general linear PDEs on specific domains whose boundary is specified by an algebraic curve – notably here the disk-slice – with Dirichlet boundary conditions. This work extends the triangle case [6, 43, 59] and whole disk case [11, 86] to non-classical geometries, and forms a building block in developing an $hp-$finite element method to solve PDEs on other polygonal domains by using suitably shaped elements (for example, by dividing the disk or a section of the disk into disk-slice elements, which has applications in turbulent pipe flow [23, 40, 86]).

We have demonstrated how one can construct the three-or-four-parameter OP families (depending on the domain) that form the basis for our sparse spectral methods, and presented a procedure, utilising the Christoffel-Darboux formula

[55, (18.2.12)], of explicitly calculating the recurrence coefficients for the univariate OPs that are part of the construction. These coefficients contribute to calculations of the entries in the Jacobi matrices and other differential operators. Moreover, we have defined a quadrature rule that can be used for expanding functions in our OP basis and for calculating said entries of important operators. We have looked at a few mathematical examples including the Poisson, variable coefficient Helmholtz, and biharmonic equations and shown that our method performs well. Importantly, all operator matrices used are shown to be sparse, and in fact banded-block-banded in structure.

Looking ahead, this work serves as a stepping stone to constructing similar methods to solve partial differential equations on sub-domains of the 2-sphere surface, such as spherical caps that we will discuss in the next chapter.

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. 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 with discretisations that can be made well-conditioned using a simple preconditioner.

Our aim in this chapter is to develop a sparse spectral method 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 *spherical cap* Ω defined 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 $\beta := 1$. Simply put, the region of the surface of the 2-sphere where the z-coordinate range is limited to the interval $[\alpha, 1]$ is what we refer to as the spherical cap.

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 construction more involved, but the approach is essentially the same which is why they are omitted here.

For the spherical cap, 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 [61]. Equivalently, we can think of these as polynomials modulo the vanishing ideal $\{(x, y, z) \in \mathbb{R}^3 \quad | \quad x^2+y^2+z^2 = 1\}$, 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 avoid the singular nature at the poles or as α approaches 0 that such a projection may give, since our new approach yields a smooth polynomial basis for all $\alpha \in [-1, 1)$.

There are of course other approaches for solving PDEs on surfaces, such as the closest point method [45, 44]. This involves recasting the PDE as one involving a "closest point" operator in a 3D volume that acts as a "shell" for the surface. While such an approach is useful for other geometries, it is of low order and does not achieve spectral convergence with sparse discretisations. Further, for our domain of interest, the closest point method does not take advantage of any rotational symmetry, and so is unable to achieve optimal complexity with a direct solver.

On the spherical cap, the family of weights we will 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 that we will see in Definition 13.

Just as for the spherical harmonics framework for the whole sphere in Chapter 2, we consider partial differential operators involving the spherical Laplacian (the Laplace–Beltrami operator). Recall that we write the spherical coordinates as

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

where $\rho(z) := \sqrt{1-z^2}$, and that the Laplace–Beltrami operator is then

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

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, à la the ultraspherical spectral method we investigated in Chapter 3 for disk-slices and trapeziums (see also [78]), as well as for intervals [58], triangles [59], and the related work on sparse discretisations involving Jacobi polynomials on disks [86] and spheres [87, 42]. Just as we proceeded in Chapter 3 for the disk-slice case in 2D (see also [78]), we will 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 [46, §5]) 1D OPs as those outlined for the disk-slice, and so methods for calculating these 1D OP recurrence coefficients and integrals have already been outlined in Chapter 3 (see also [78]). 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 $\Delta_S + v(x, y, z)$ where v is first approximated by a polynomial. A nice feature 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 4.5 with $v(x, y, z) = \cos z$.

The code that allows one to produce the numerical examples in this chapter is publicly available as a Julia package[1] to partner the ApproxFun package [57] – however, this package is purely experimental at this stage.

4.1 The circle arc

The spherical cap can be thought of as a higher dimensional version of the circle arc (a one-dimensional "surface" in two-dimensional space). Recently, a procedure for defining OPs in two variables on quadratic curves, such as ellipses and parabolas, has been presented [62], where the unit circle is one of

[1] https://github.com/snowball13/OrthogonalPolynomialFamilies.jl

the five classes of curve that can be generalised to give any curve in the plane $\mathbb{R}^2$. One can define OPs on the circle in terms of Fourier series, which we write here as orthogonal polynomials in x and y.

Definition 12 ([62]). *Define the unit circle $\omega := \{\boldsymbol{x} = (x, y) \in \mathbb{R}^2 \quad | \quad x^2 + y^2 = 1\}$, and define the parameter θ for each $(x, y) \in \omega$ by $x = \cos\theta$, $y = \sin\theta$. Define the polynomials $\{Y_{k,i}\}$ for $k = 0, 1, \ldots,$ $i = 0, 1$ on $(x, y) \in \omega$ by*

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

for $k = 1, 2, 3, \ldots$ 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 Y_0 is defined so as to ensure orthonormality.

However, for an arc of the unit circle $\{\boldsymbol{x} = (x, y) \in \mathbb{R}^2 \quad | \quad x \geq h,\, x^2 + y^2 = 1\}$ for some $h \in (-1, 1)$ (note we can orientate the arc as we please without loss of generality), we would need to make a modification so that the polynomials are orthonormal with respect to a different inner product accounting for the truncated domain of the arc:

$$\begin{aligned}\langle p,\, q\rangle_{Y^h} &:= c^h \int_{-\arccos h}^{\arccos h} p(\mathbf{x}(\theta))\, q(\mathbf{x}(\theta))\, \mathrm{d}\theta \\ &= c^h \int_h^1 \Big\{ p(x, \sqrt{1-x^2})\, q(x, \sqrt{1-x^2}) \\ &\qquad\qquad + p(x, -\sqrt{1-x^2})\, q(x, -\sqrt{1-x^2}) \Big\} \frac{\mathrm{d}x}{\sqrt{1-x^2}},\end{aligned}$$

for some normalising constant c^h. In the same vein, we can choose to construct the arc OPs in the same way as the whole circle OPs – that is, define $\{T_k^h\}$, $\{U_k^h\}$ as two sets of univariate orthogonal polynomials on the interval $[h, 1]$, orthogonal with respect to the weight functions $(1-x^2)^{-\frac{1}{2}}$ and $(1-x^2)^{\frac{1}{2}}$ respectively, and then define

$$\begin{aligned}Y_{0,0}^h(\mathbf{x}) &\equiv Y_{0,0}^h(x, y) := Y_0^h =: Y_{0,0}^h(\theta), \\ Y_{k,0}^h(\mathbf{x}) &\equiv Y_{k,0}^h(x, y) := T_k^h(x) =: Y_{k,0}^h(\theta), \\ Y_{k,1}^h(\mathbf{x}) &\equiv Y_{k,1}^h(x, y) := y\, U_{k-1}^h(x) =: Y_{k,1}^h(\theta),\end{aligned}$$

where Y_0^h is chosen so that $\left\langle Y_0^h,\, Y_0^h \right\rangle_{Y^h} = 1$.

4.2 Orthogonal polynomials on spherical caps

4.2.1 Explicit construction

A continuation to the procedure for defining OPs on quadratic curves (see [62]) has also been presented [61], where OPs are defined on quadratic surfaces of revolution in higher dimensions (specifically, surfaces in $\mathbb{R}^{d+1}$ for $d \geq 2$).

The authors describe their technique as modelled on the structure of the unit sphere, by approaching the construction as a generalisation of spherical harmonics.

Using this approach, we can construct the 3D orthogonal polynomials on the spherical cap or band Ω from 1D orthogonal polynomials on the interval $[\alpha, \beta]$, and from Fourier series written as orthogonal polynomials in x and y. Recall that the spherical cap is defined by

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

Proposition 4 ([61]). *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 given by*

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

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

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

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. The univariate OPs that we will choose for the $r_{n,k}$ polynomials above will be the non-classical $R^{(a,b)}$ OPs that we defined in Definition 6. Since there is only one boundary for the spherical cap, we will only need to use a two-parameter version[2]). For reference, the family of orthonormal polynomials on $[\alpha, \beta]$ denoted $\{R_n^{(a,b)}\}$ are defined such that they are orthonormal with respect to the inner product

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

where

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

is the weight function and

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

is a normalising constant.

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

Definition 13. *Define the one-parameter 3D orthogonal polynomials via:*

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

[2]For a spherical band with two boundaries, we would need the three-parameter version

By construction, $\{Q^{(a)}_{n,k,i}\}$ 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

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

A method for obtaining explicit recurrence coefficients and evaluating integrals for the weight function $w_R^{(a,b)}(x)$ was established in Chapter 3 (see also [78]). The weight is in fact semi-classical, and is equivalent to a generalized Jacobi weight [46, §5].

4.2.2 Jacobi matrices

Recall that 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 calculable (see Chapter 3). We can use equation (4.5) to determine the 3D recurrences for $Q^{(a)}_{n,k,i}(x, y, z)$. Importantly, we can deduce sparsity in the recurrence relationships. We first require the following lemma.

Lemma 7. *The following identities hold for* $k = 2, 3, \ldots,$ $j = 0, 1, \ldots$ *and*

$i, h \in \{0, 1\}$:

$$1) \quad \int_0^{2\pi} Y_0\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = Y_0\, \pi\, \delta_{0,h}\, \delta_{1,j}$$

$$2) \quad \int_0^{2\pi} Y_0\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = Y_0\, \pi\, \delta_{1,h}\, \delta_{1,j}$$

$$3) \quad \int_0^{2\pi} Y_{1,i}(\theta)\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = \pi\, \delta_{i,h}\, (Y_0\, \delta_{0,j} + \frac{1}{2}\delta_{2,j})$$

$$4) \quad \int_0^{2\pi} Y_{1,i}(\theta)\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = \pi\, \delta_{|i-1|,h}\, ((-1)^{i+1}\, Y_0\, \delta_{0,j} + (-1)^i\, \frac{1}{2}\, \delta_{2,j})$$

$$5) \quad \int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\ \cos\theta\, \mathrm{d}\theta = \frac{1}{2}\, \pi\, \delta_{i,h}\, (\delta_{k-1,j} + \delta_{k+1,j})$$

$$6) \quad \int_0^{2\pi} Y_{k,i}(\theta)\, Y_{j,h}(\theta)\ \sin\theta\, \mathrm{d}\theta = \frac{1}{2}\, \pi\, \delta_{|i-1|,h}\, ((-1)^{i+1}\, \delta_{k-1,j} + (-1)^i\, \delta_{k+1,j}).$$

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

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

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

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

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

□

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:*

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

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

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

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

$$\begin{aligned} \alpha^{(a)}_{n,k,1} &:= \eta_{k-1} \left\langle R^{(a,2k)}_{n-k},\ R^{(a,2(k-1))}_{n-k} \right\rangle_{w_R^{(a,2k)}}, \\ \alpha^{(a)}_{n,k,2} &:= \eta_{k} \left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k-2} \right\rangle_{w_R^{(a,2(k+1))}}, \\ \alpha^{(a)}_{n,k,3} &:= \eta_{k-1} \left\langle R^{(a,2k)}_{n-k},\ R^{(a,2(k-1))}_{n-k+1} \right\rangle_{w_R^{(a,2k)}}, \\ \alpha^{(a)}_{n,k,4} &:= \eta_{k} \left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k-1} \right\rangle_{w_R^{(a,2(k+1))}}, \\ \alpha^{(a)}_{n,k,5} &:= \eta_{k-1} \left\langle R^{(a,2k)}_{n-k},\ R^{(a,2(k-1))}_{n-k+2} \right\rangle_{w_R^{(a,2k)}}, \\ \alpha^{(a)}_{n,k,6} &:= \eta_{k} \left\langle R^{(a,2k)}_{n-k}, R^{(a,2(k+1))}_{n-k} \right\rangle_{w_R^{(a,2(k+1))}}, \end{aligned}$$

$$\beta^{(a)}_{n,k,i,j} := \begin{cases} -\alpha^{(a)}_{n,k,j} & \textit{if } (i = 0 \textit{ and } j \textit{ is odd}) \textit{ or } (i = 1 \textit{ and } j \textit{ is even}) \\ \alpha^{(a)}_{n,k,j} & \textit{otherwise,} \end{cases}$$

$$\gamma^{(a)}_{n,k,1} := \beta^{(a,2k)}_{n-k-1}, \qquad \gamma^{(a)}_{n,k,2} := \alpha^{(a,2k)}_{n-k}, \qquad \gamma^{(a)}_{n,k,3} := \beta^{(a,2k)}_{n-k}.$$

Remark: For z multiplication, note that different Fourier modes do not interact. This is because multiplication by z is invariant with respect to rotation around the z-axis.

Proof. The 3-term recurrence for multiplication by z follows from equation (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 $\left\| Q^{(a)}_{m,j,h} \right\|^{2}_{Q^{(a)}} = \pi\, \omega^{(a,2j)}_{R}$. Using a change of variables

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

we have that, for $m = 0, \dots, n+1$, $j = 0, \dots, m$,

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

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 $\beta^{(a)}_{n,k,1}, \dots, \beta^{(a)}_{n,k,6}$ as stated in the Lemma:

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

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

□

The recurrences in Lemma 8 lead to (block) Jacobi matrices 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, 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 $J_x^{(a)}, J_y^{(a)}, J_z^{(a)}$ as the Jacobi matrices corresponding to

$$\begin{aligned} J_x^{(a)}\,\tilde{\mathbb{Q}}^{(a)}(x,y,z) &= x\,\tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ J_y^{(a)}\,\tilde{\mathbb{Q}}^{(a)}(x,y,z) &= y\,\tilde{\mathbb{Q}}^{(a)}(x,y,z), \\ J_z^{(a)}\,\tilde{\mathbb{Q}}^{(a)}(x,y,z) &= z\,\tilde{\mathbb{Q}}^{(a)}(x,y,z), \end{aligned} \tag{4.7}$$

where

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

The Jacobi matrices are once again in fact banded-block-banded matrices – see Definition 1. More specifically, each Jacobi matrix is block-tridiagonal (block-bandwidths $(1,1)$).

For $J_x^{(a)}$, the sub-blocks have sub-block-bandwidths $(2,2)$:

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

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

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

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

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

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

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

For $J_y^{(a)}$, the sub-blocks have sub-block-bandwidths $(3,3)$:

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

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

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

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

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

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

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

For $J_z^{(a)}$, the sub-blocks are diagonal, i.e. have sub-block-bandwidths $(0, 0)$:

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

$$B_{z,n}^{(a)} := \begin{pmatrix} \Gamma_{n,0,2}^{(a)} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \Gamma_{n,n,2}^{(a)} \end{pmatrix} \in \mathbb{R}^{(2n+1)\times(2n+1)},$$

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

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

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

$$\Gamma_{n,0,j}^{(a)} := \gamma_{n,0,j}^{(a)}. \tag{4.9}$$

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

Just as we saw for the spherical harmonics and the disk-slice, one can obtain a recursive method of calculating point evaluations for the OPs by gaining a multidimensional three-term recurrence relation. Combining each system in equation (4.7) into a block-tridiagonal system, for any $(x, y, z) \in \Omega$, yields:

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

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

$$A_n := \begin{pmatrix} A_{x,n}^{(a)} \\ A_{y,n}^{(a)} \\ A_{z,n}^{(a)} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n+3)}, \quad C_n := \begin{pmatrix} C_{x,n}^{(a)} \\ C_{y,n}^{(a)} \\ C_{z,n}^{(a)} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n-1)} \quad (n \neq 0), \tag{4.10}$$

$$B_n := \begin{pmatrix} B_{x,n}^{(a)} \\ B_{y,n}^{(a)} \\ B_{z,n}^{(a)} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(2n+1)}, \quad G_n(x,y,z) := \begin{pmatrix} xI_{2n+1} \\ yI_{2n+1} \\ zI_{2n+1} \end{pmatrix} \in \mathbb{R}^{3(2n+1)\times(n+1)}. \tag{4.11}$$

For each $n = 0, 1, 2 \dots$ let $D_n^\top$ be any matrix that is a left inverse of A_n, i.e. such that $D_n^\top A_n = I_{2n+3}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the $D_n^\top$'s, we obtain a lower triangular system [22, p.78], which can be expanded to obtain the recurrence for $n = 0, 1, 2, \ldots$:

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

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

$$D_n^\top := \begin{pmatrix} 0 & & 0 & & (\Gamma_{n,0,3}^{(a)})^{-1} & & \\ & \ddots & & \ddots & & \ddots & \\ & & 0 & & 0 & & (\Gamma_{n,n,3}^{(a)})^{-1} \\ & & & & \boldsymbol{\eta}_0^\top & & \\ & & & & \boldsymbol{\eta}_1^\top & & \end{pmatrix} \in \mathbb{R}^{(2n+3)\times 3(2n+1)}, \tag{4.12}$$

for $n = 1, 2, \ldots$ where again $\Gamma_{n,k,3}^{(a)}$ are defined in equation (4.8) and equation

(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

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

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

For $n = 0$, we can simply take

$$D_0^\top := \begin{pmatrix} 0 & 0 & \frac{1}{\gamma^{(a)}_{0,0,3}} \\ \frac{1}{\alpha^{(a)}_{0,0,6}} & 0 & 0 \\ 0 & \frac{1}{\beta^{(a)}_{0,0,6}} & 0 \end{pmatrix} \in \mathbb{R}^{3\times 3}. \tag{4.13}$$

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

Definition 14. *The matrices $-D_n^\top(B_n - G_n(x,y,z))$, $D_n^\top C_n$ defined via equations (4.10–4.13) are the recurrence coefficient matrices associated with the OPs $\{Q^{(a)}_{n,k,i}\}$.*

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:

$$\mathbb{Q}^{(a)}_{N,k} := \begin{pmatrix} Q^{(a)}_{k,k,0}(x,y,z) \\ Q^{(a)}_{k,k,1}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,k,0}(x,y,z) \\ Q^{(a)}_{N,k,1}(x,y,z) \end{pmatrix} \in \mathbb{R}^{2(N-k+1)}, \quad k = 1, \dots, N, \tag{4.14}$$

$$\mathbb{Q}^{(a)}_{N,0} := \begin{pmatrix} Q^{(a)}_{0,0,0}(x,y,z) \\ \vdots \\ Q^{(a)}_{N,0,0}(x,y,z) \end{pmatrix} \in \mathbb{R}^{N+1}, \tag{4.15}$$

$$\mathbb{Q}^{(a)}_{N} := \begin{pmatrix} \mathbb{Q}^{(a)}_{N,0} \\ \vdots \\ \mathbb{Q}^{(a)}_{N,N} \end{pmatrix} \in \mathbb{R}^{(N+1)^2}. \tag{4.16}$$

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:

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

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 an 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:*

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

The incrementing and decrementing of parameters as seen here is analogous to other to that seen in Chapter 3 (see also [78]), and we further reiterate that it is also seen for other well known orthogonal polynomial families' derivatives – for example the Jacobi polynomials on the interval (as seen in the NIST Digital Library of Mathematical Functions [55, (18.9.3)]) and on the triangle [60]. 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 (4.14–4.16) 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:*

- $D_\varphi^{(a)}$ *is block-diagonal with sub-block-bandwidths* $(2,4)$.
- $W_\varphi^{(a)}$ *is block-diagonal with sub-block-bandwidths* $(4,2)$.
- D_θ *is block-diagonal with sub-block-bandwidths* $(1,1)$.
- $\mathcal{L}^{(a)\to(a+\tilde{a})}$ *is block-diagonal with sub-block-bandwidths* $(0,4)$.
- $\mathcal{L}_W^{(a)\to(a-\tilde{a})}$ *is block-diagonal with sub-block-bandwidths* $(4,0)$.
- $\Delta_W^{(1)}$ *is block-diagonal with 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* $n = 0, 1, \ldots,$ $k = 0, \ldots, n$ *we have that*

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

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

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

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:

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

Then,

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

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

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

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

Now,

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

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 $Q^{(a)}_{n,k,i}$ yields

$$
\begin{aligned}
&\Delta_{\mathrm{S}}\, Q^{(a)}_{n,k,i} \\
&= \frac{1}{\rho} \frac{\partial}{\partial \varphi} \Big(\rho \frac{\partial}{\partial \varphi} [R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^k \varphi] \Big) Y_{k,i}(\theta) + R^{(a,2k)}_{n-k}(\cos\varphi)\ \sin^{k-2}\varphi \frac{\partial^2}{\partial \theta^2} Y_{k,i}(\theta) \\
&= Y_{k,i}(\theta)\, \rho(z)^k \Big\{ -k(k+1) R^{(a,2k)}_{n-k}(z) - 2(k+1) z\, R^{(a,2k)}_{n-k}{}'(z) \\
&\qquad + \rho(z)^2 R^{(a,2k)}_{n-k}{}''(z) \Big\},
\end{aligned} \tag{4.17}
$$

and

$$\begin{aligned}
&\Delta_{\mathrm{S}}\big(w_R^{(a,0)}\, Q_{n,k,i}^{(a)}\big) \\
&= \frac{1}{\rho}\frac{\partial}{\partial\varphi}\Big(\rho\frac{\partial}{\partial\varphi}[w_R^{(a,0)}(\cos\varphi)\, R_{n-k}^{(a,2k)}(\cos\varphi)\, \sin^k\varphi]\Big)Y_{k,i}(\theta) \\
&\qquad\qquad + w_R^{(a,0)}(\cos\varphi)\, R_{n-k}^{(a,2k)}(\cos\varphi)\, \sin^{k-2}\varphi\frac{\partial^2}{\partial\theta^2}Y_{k,i}(\theta) \\
&= Y_{k,i}(\theta)\Big\{R_{n-k}^{(a,2k)}(z)\big[-k(k+1)w_R^{(a,k)}(z) - 2a(k+1)z\, w_R^{(a-1,k)}(z)\big] \\
&\qquad\qquad + a(a-1)R_{n-k}^{(a,2k)}(z)\, w_R^{(a-2,k+1)}(z) \\
&\qquad\qquad + R_{n-k}^{(a,2k)\,\prime}(z)\big[-2(k+1)z\, w_R^{(a,k)}(z) + 2a\, w_R^{(a-1,k+2)}(z)\big] \\
&\qquad\qquad + R_{n-k}^{(a,2k)\,\prime\prime}(z)\, w_R^{(a,k+2)}(z)\Big\}. \qquad (4.18)
\end{aligned}$$

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

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

where the coefficients are

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

Using equation (4.17), and integrating by parts twice, we then have that

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

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

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

Using equation (4.18), and integrating by parts thrice, we then have that

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

$$
\begin{aligned}
&= \pi\, \delta_{k,j}\, \delta_{i,h} \int_{\alpha}^{1} \Big\{ R^{(a-\tilde{a},2k)}_{m-k}\, R^{(a,2k)}_{n-k}\, w_R^{(a-2,2k)} \big[- k(k+1) w_R^{(2,0)} - 2a(k+1) z\, w_R^{(1,0)} \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + a(a-1)\rho^2 \big] \\
&\qquad\qquad + R^{(a,2k)}_{n-k}\, w_R^{(a-1,2k+2)} \big[R^{(a-\tilde{a},2k)}_{m-k}{}'' \rho^2 - 2(k+1) z\, R^{(a-\tilde{a},2k)}_{m-k}{}' \big] \\
&\qquad\qquad - a R^{(a,2k)}_{n-k}\, R^{(a-\tilde{a},2k)}_{m-k}\, w_R^{(a-2,2k)} \big[(a-1)\rho^2 - 2(k+1) z\, w_R^{(1,0)} \big] \Big\}\, \mathrm{d}z \\
&= \pi\, \delta_{k,j}\, \delta_{i,h} \int_{\alpha}^{1} R^{(a,2k)}_{n-k}\, w_R^{(a,2k)}\, r_{m-k}\, \mathrm{d}z,
\end{aligned}
$$

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

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

Using equation (4.18) with $a = 1$, and Lemma 9, we then have that

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

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

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 conversion operators, transforming the OPs from one (weighted or non-weighted) parameter space to another.

Definition 16. *Define the operator matrices* $T^{(a)\to(a+\tilde{a})}$, $T_W^{(a)\to(a-\tilde{a})}$ *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 $m = 0,\dots,n$, $j = 0,\dots,m$, $h = 0,1$ 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

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

where

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

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

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 $\mathbb{W}_N^{(1)}(x,y,z) = w_R^{(1,0)}(z)\,\mathbb{Q}_N^{(1)}(x,y,z)$ to coefficients in the non-weighted space $\mathbb{Q}_N^{(1)}(x,y,z)$. Note that this construction will ensure the imposition of the Dirichlet zero boundary conditions on Ω, similar to how the Dirichlet zero boundary conditions would be imposed for the operator $\Delta_W^{(1)}$ in Definition 15. The matrix operator for this ρ^2-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 Δ_{S}^2, for which we assume zero Dirichlet and Neumann conditions. That is,

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

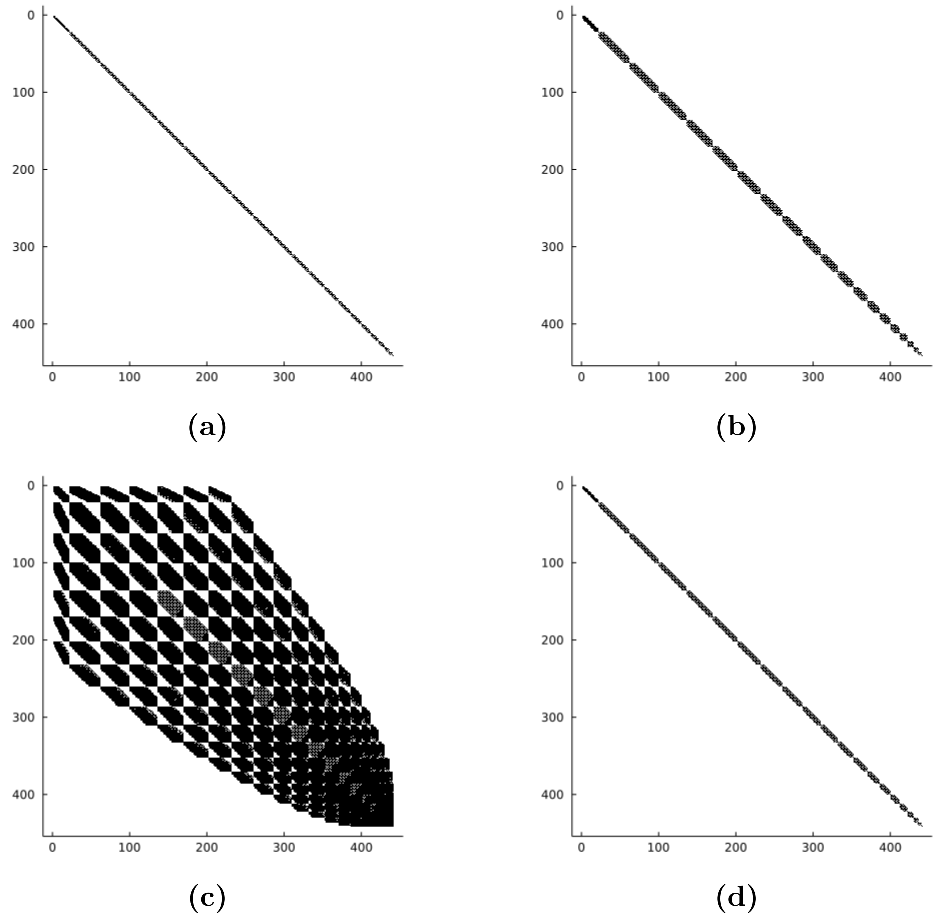


Figure 4.1: "Spy" plots of (differential) operator matrices, showing their sparsity, plotted for $N = 20$. Note that here each block corresponds to the order k and not the degree n. (a) The Laplace-Beltrami operator $\Delta_W^{(1)}$. (b) The ρ^2-factored Laplace-Beltrami operator $D_\varphi^{(0)}\, W_\varphi^{(1)} + T^{(0)\to(1)}\, T_W^{(1)\to(0)}\, (D_\theta)^2$. (c) The variable coefficient Helmholtz operator $\Delta_W^{(1)} + k^2\, T^{(0)\to(1)}\, V({J_x^{(0)}}^\top, {J_y^{(0)}}^\top, {J_z^{(0)}}^\top)\, T_W^{(1)\to(0)}$ 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 $k = 200$. (d) The biharmonic operator $\mathcal{B}_W^{(2)}$.

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. For the spherical cap Ω, this is simply $\hat{\boldsymbol{\phi}}(x, y, z)$. Hence,

$$\nabla_{\mathrm{S}} u(x, y, z) \cdot \hat{\boldsymbol{n}}(x, y, z) = \nabla_{\mathrm{S}} u(x, y, z) \cdot \hat{\boldsymbol{\phi}}(x, y, z) = -\rho(z) \frac{\partial u}{\partial z}(x, y, z),$$

and the boundary conditions simplify to

$$u(x, y, z) = 0, \quad \frac{\partial u}{\partial z}(x, y, z) = 0 \quad \text{for } (x, y, z) \in \partial\Omega.$$

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 $u(x, y, z) = w_R^{(2,0)}(z)\, \tilde{u}(x, y, z)$. 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.

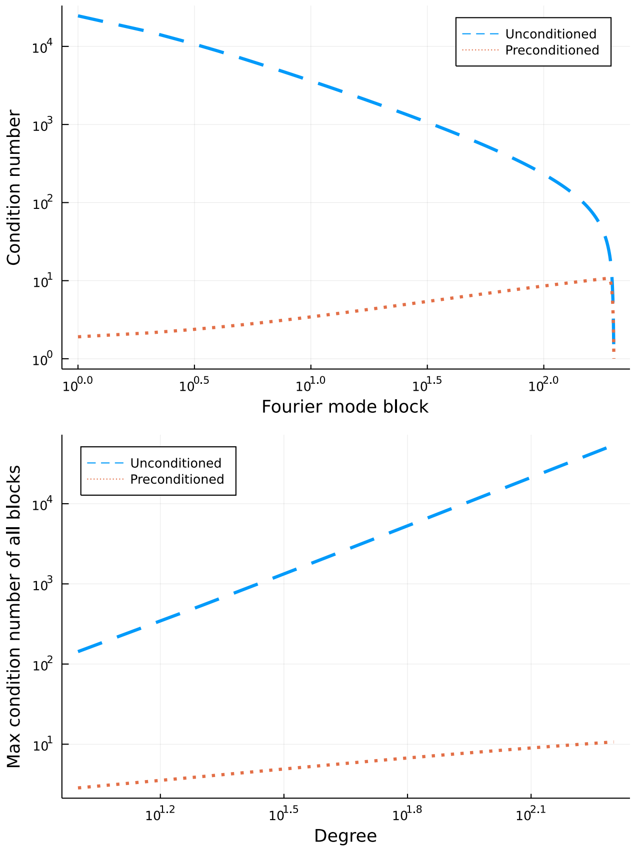


Figure 4.2: Plots of the condition number for the Laplacian operator matrix $\Delta_W^{(1)}$ and the preconditioned matrix $P^{-1}\Delta_W^{(1)}$ where P is the matrix of the diagonal of $\Delta_W^{(1)}$. Top: The condition numbers of each diagonal block of $\Delta_W^{(1)}$ for $N = 200$, as well as those for $P^{-1}\Delta_W^{(1)}$. Bottom: The maximum condition number of all diagonal blocks of the Laplacian and the preconditioned Laplacian operators, as the degree N increases.

4.3.2 Stability of the Laplacian operator

Denote the condition number of the matrix A:

$$\kappa(A) := \|A\|_2 \left\|A^{-1}\right\|_2,$$

which encodes how accurate the solution to $A\boldsymbol{x} = \boldsymbol{b}$ is under perturbation. Since the Laplacian is block-diagonal one can determine the condition number from the condition numbers of each block on the diagonal, and hence deduce the accuracy in solving the Poisson equation, where graphical representations are seen in Figure 4.2 for the $\Delta_W^{(1)}$ operator matrix. As the degree N increases, the condition numbers of these blocks grows algebraically fast (at least, the condition number for the first block where $m = 0$ does, which will be the largest for each N). Fortunately however, by applying a trivial diagonal preconditioning matrix similar to that seen for the ultraspherical method [58], we can significantly bound this growth of the condition numbers – this is also seen in Figure 4.2. The preconditioning matrix chosen is P^{-1}, where P is the matrix of the diagonal of $\Delta_W^{(1)}$.

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 [78], by careful application of the Christoffel–Darboux formula [55, (18.2.12)].

4.4.2 Quadrature rule on the spherical cap

In this section we construct a quadrature rule that is 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 $j = 1, \dots, M_1$, $l = 1, \dots, M_2$:*

$$
\begin{aligned}
x_{l+(j-1)M_2} &:= \rho(t_j)\, s_l, \\
y_{l+(j-1)M_2} &:= \rho(t_j)\, \sqrt{1-s_l^2}, \\
z_{l+(j-1)M_2} &:= t_j, \\
w_{l+(j-1)M_2} &:= w_j^{(t)} w_l^{(s)}.
\end{aligned}
$$

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

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

where $M = M_1 M_2$, and the quadrature rule is exact if $f(x,y,z)$ is a polynomial *of degree* $\leq N$ *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 [55, (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

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

for any function g, using a change of variables $x \to -x$ for the second term in the integral. Then, integrating the even function f_e we have

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

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

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

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 $\mathbb{Q}^{(a)}_{N,k}, \mathbb{Q}^{(a)}_{N}$ is defined in equations (4.14–4.16) and where

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

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

Recall from equation (4.4) that $\left\| Q^{(a)}_{n,k,i} \right\|^2_{Q^{(a)}} = \omega^{(a,2k)}_R\, \pi$. 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 $n = 0, \ldots, N$, $k = 0, \ldots, n$, $i = 0, 1$:

$$\begin{aligned} f_{n,k,i} &= \frac{1}{\omega^{(a,2k)}_R\, \pi} \sum_{j=1}^{M} w_j \big[f(x_j, y_j, z_j) Q^{(a)}_{n,k,i}(x_j, y_j, z_j) \\ &\qquad\qquad + f(-x_j, -y_j, z_j) Q^{(a)}_{n,k,i}(-x_j, -y_j, z_j) \big] \\ &= \frac{1}{M_2\, \omega^{(a,2k)}_R} \sum_{j=1}^{M_1} w^{(t)}_j \sum_{l=1}^{M_2} \big[f(x_j, y_j, z_j) Q^{(a)}_{n,k,i}(x_j, y_j, z_j) \\ &\qquad\qquad + f(-x_j, -y_j, z_j) Q^{(a)}_{n,k,i}(-x_j, -y_j, z_j) \big], \end{aligned}$$

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 $M_1 := \lceil \frac{N+1}{2} \rceil$).

Remark: While it may be possible to leverage fast transforms, as in [74, 75], to speed up the calculation of the coefficients, this remains an open question.

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, as we have seen for the spherical harmonics and disk-slice in Chapter 2 and Chapter 3 respectively. 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

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

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

The trivariate Clenshaw algorithm works similar to the bivariate Clenshaw algorithm introduced in [59] for expansions in the triangle:

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

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

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

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

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

i.e. $\tilde{V}\tilde{\boldsymbol{f}}$ is the coefficients vector for the function $v(x,y,z)\, f(x,y,z)$ in the $\tilde{\mathbb{Q}}^{(a)}$ basis.

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 $X := (J_x^{(a)})^\top$, $Y := (J_y^{(a)})^\top$, and $Z := (J_z^{(a)})^\top$. The operator $\tilde{V}$ is then the result of the following:

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

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

$$\text{set } \boldsymbol{\xi}_n^T = \tilde{\boldsymbol{v}}_n^T - \boldsymbol{\xi}_{n+1}^T D_n^T \big(B_n - G_n(X,Y,Z)\big) - \boldsymbol{\xi}_{n+2}^T D_{n+1}^T C_{n+1}$$

3) Output: $\tilde{V} = v(X,Y,Z) \approx \boldsymbol{\xi}_0\, \tilde{\mathbb{Q}}_0^{(a)} = \xi_0\, Q_0^{(a)}$,

where at each iteration, $\boldsymbol{\xi}_n$ is a vector of matrices[3]. Of course, by using rearranged versions of the Jacobi matrices (that act on coefficients $\boldsymbol{f}$ that expand the function f in the $\mathbb{Q}^{(a)}$ basis), the same algorithm would return the operator V so that

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

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

[3]It may help to think of this symbolically. At each iteration, the entries of $\boldsymbol{\xi}_n$ are polynomials in X, Y, and Z. On the final step, $\boldsymbol{\xi}_0 = \xi_0$ is hence some polynomial expression in X, Y, and Z, which we can then evaluate by inserting the Jacobi matrices.

basis.

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, an inhomogeneous variable coefficient Helmholtz equation, and the biharmonic equation, as well as a time dependent heat equation, demonstrating the versatility of the approach.

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:

$$\begin{cases} \Delta_{\mathbb{S}} u(x,y,z) = f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = 0 & \text{on } \partial\Omega, \end{cases} \tag{4.19}$$

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 $\boldsymbol{u}$, and the coefficient vector for expansion of f in the $\mathbb{Q}_N^{(1)}$ OP basis up to degree N by $\boldsymbol{f}$. Since f is known, we can obtain $\boldsymbol{f}$ using the quadrature rule in Section 4.4.3. In matrix-vector notation, our system

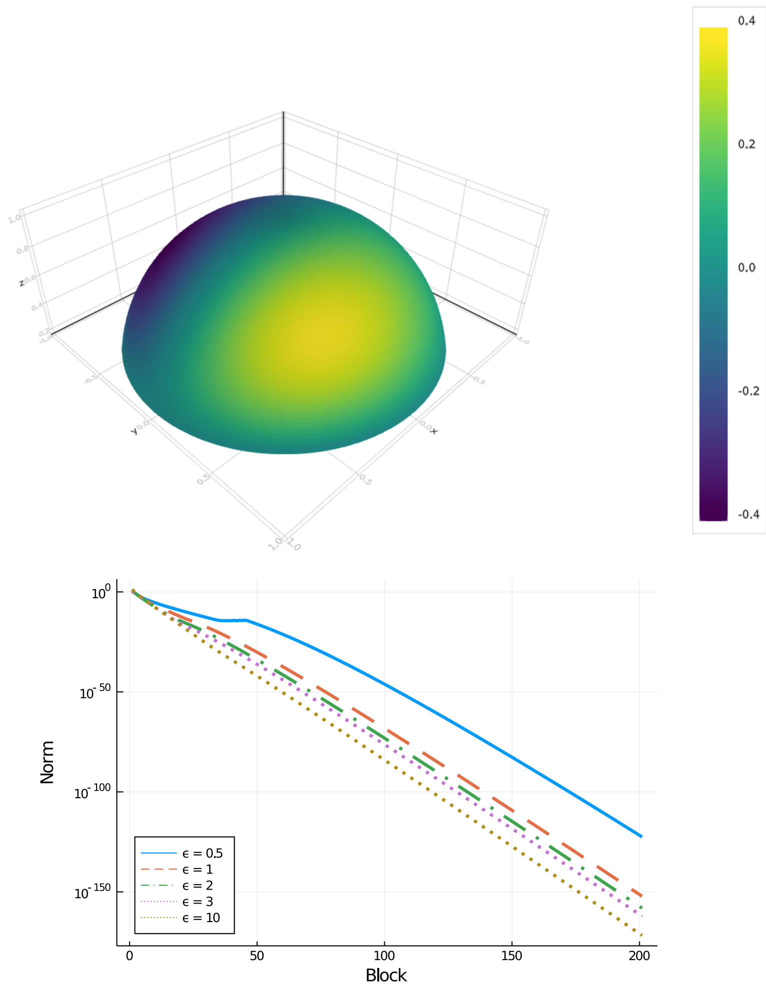


Figure 4.3: Top: The computed solution to $\Delta u = f$ with zero boundary conditions with $f(x,y,z) = -2e^x yz(2+x) + w_R^{(1,0)}(z)e^x(y^3 + z^2 y - 4xy - 2y)$. Bottom: The norms of each block of the computed solution of the Poisson equation with right hand side function $f(x,y,z) = \left\| \mathbf{x} - (\epsilon + 1/\sqrt{3})\,(1,1,1)^\top \right\|$ for different ϵ values. This indicates spectral convergence.

hence becomes:

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

which can be solved to find $\boldsymbol{u}$. In Figure 4.3 we see the solution to the Poisson equation with zero boundary conditions given in equation (4.19) in the disk-slice Ω. 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 Poisson equation with $N = 200$, that is, $(N+1)^2 = 40,401$ unknowns. The right hand sides we choose here are given by

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

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 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.

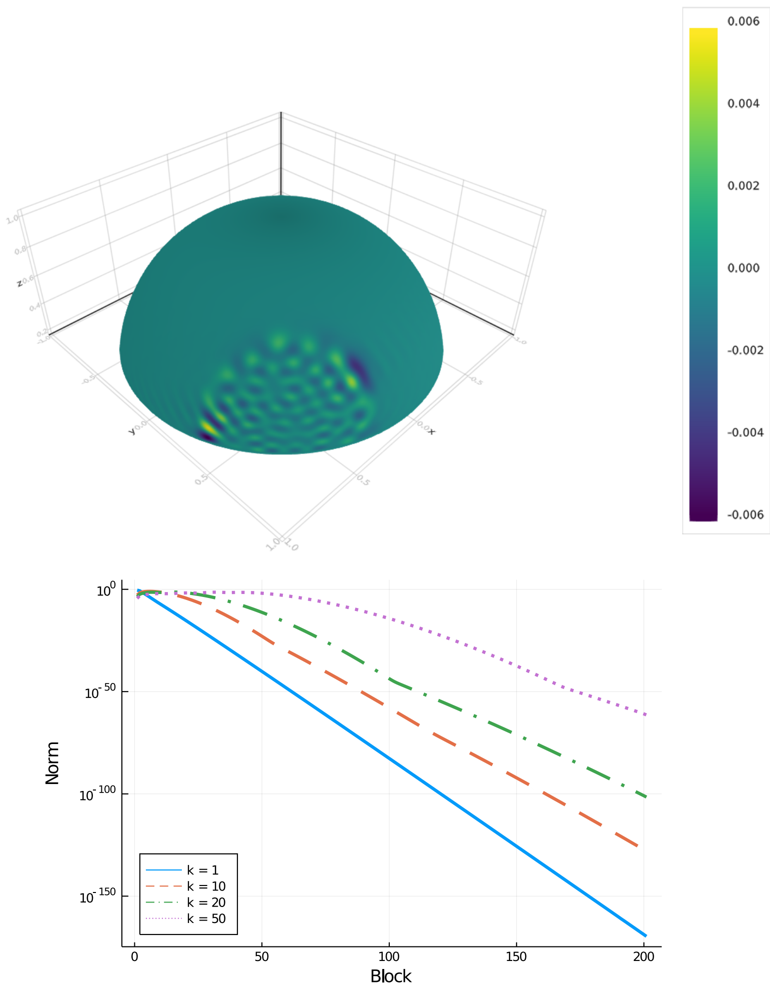


Figure 4.4: Top: The computed solution to $\Delta u + k^2\ v\ u = f$ with zero boundary conditions with $f(x, y, z) = ye^x(z-\alpha)$, $v(x, y, z) = 1-(3(x-x_0)^2+5(y-y_0)^2+2(z-z_0)^2)$ where $(x_0, z_0) := (0.7, 0.2)$, $y_0 := \sqrt{1 - x_0^2 - z_0^2}$ and $k = 100$. Bottom: The norms of each block 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.

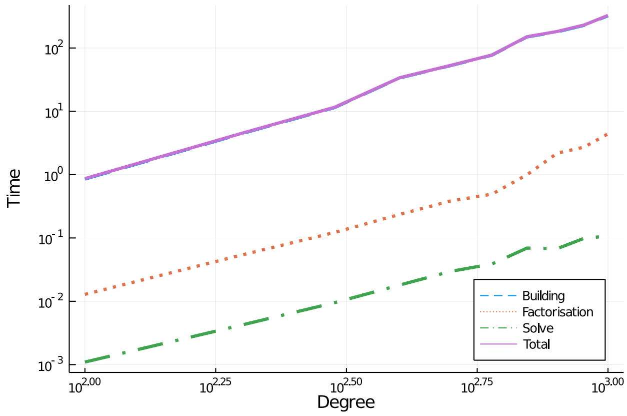


Figure 4.5: Time in seconds to build and solve the system $\left[\Delta_S + v(x,y,z)\right] u(x,y,z) = f(x,y,z)$, for a rotationally invariant $v(x,y,z) = v(z)$. This demonstrates that the approach is roughly of order $\mathcal{O}(N^2)$, where N is the degree to which we approximate the solution (the number of unknowns is then $(N+1)^2$). Here, we used $f = -2e^x yz(2+x) + (z-\alpha)e^x(y^3 + z^2 y - 4xy - 2y)$ and $v(x,y,z) = v(z) = \cos(z)$.

4.5.2 Inhomogeneous variable-coefficient Helmholtz

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

$$\begin{cases} \Delta_S u(x,y,z) + k^2\, v(x,y,z)\, u(x,y,z) = f(x,y,z) & \text{in } \Omega \\ u(x,y,z) = 0 & \text{on } \partial\Omega, \end{cases} \tag{4.20}$$

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 $\boldsymbol{u}$, and the coefficient vector for expansion of f in the $\mathbb{Q}_N^{(1)}$ OP basis up to degree N by $\boldsymbol{f}$. Since f is known, we can obtain the coefficients $\boldsymbol{f}$ 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 à la the procedure introduced in [59]. 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:

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

which can be solved to find $\boldsymbol{u}$. 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 4.4 we see the solution to the inhomogeneous variable-coefficient Helmholtz equation with zero boundary conditions given in equation (4.20) 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 4.4 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 4.5 we plot the time taken[4] to construct the operator for $\Delta_S + v(x, y, z)$, with a rotationally invariant $v(x, y, z) = v(z) = \cos z$, 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

[4]measured using the "@belapsed" macro from the BenchmarkTools.jl package [14] in Julia.

optimal $\mathcal{O}(N^2)$.

4.5.3 Biharmonic equation

Our last example is the biharmonic equation. Find $u(x, y, z)$ given a function $f(x, y, z)$ such that:

$$\begin{cases} \Delta_{\mathrm{S}}^2 u(x, y, z) = f(x, y, z) & \text{in } \Omega \\ u(x, y, z) = 0, \quad \frac{\partial u}{\partial n}(x, y, z) = \nabla_S\, u(x, y, z) \cdot \hat{\boldsymbol{n}}(x, y, z) = 0 & \text{on } \partial\Omega, \end{cases} \tag{4.21}$$

where Δ_{S}^2 is the biharmonic operator, noting the imposition of zero Dirichlet and Neumann boundary conditions on u. Recall from Section 4.3.1 that for the spherical cap, the boundary conditions here simplify to $u = \frac{\partial u}{\partial z} = 0$ on $\partial\Omega$ (since the normal vector of the boundary is simply $\hat{\boldsymbol{\phi}}(x, y, z)$). In Figure 4.6 we see the solution to the biharmonic equation (4.21) in the spherical cap Ω. In Figure 4.6 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 exponential convergence for these more complex functions.

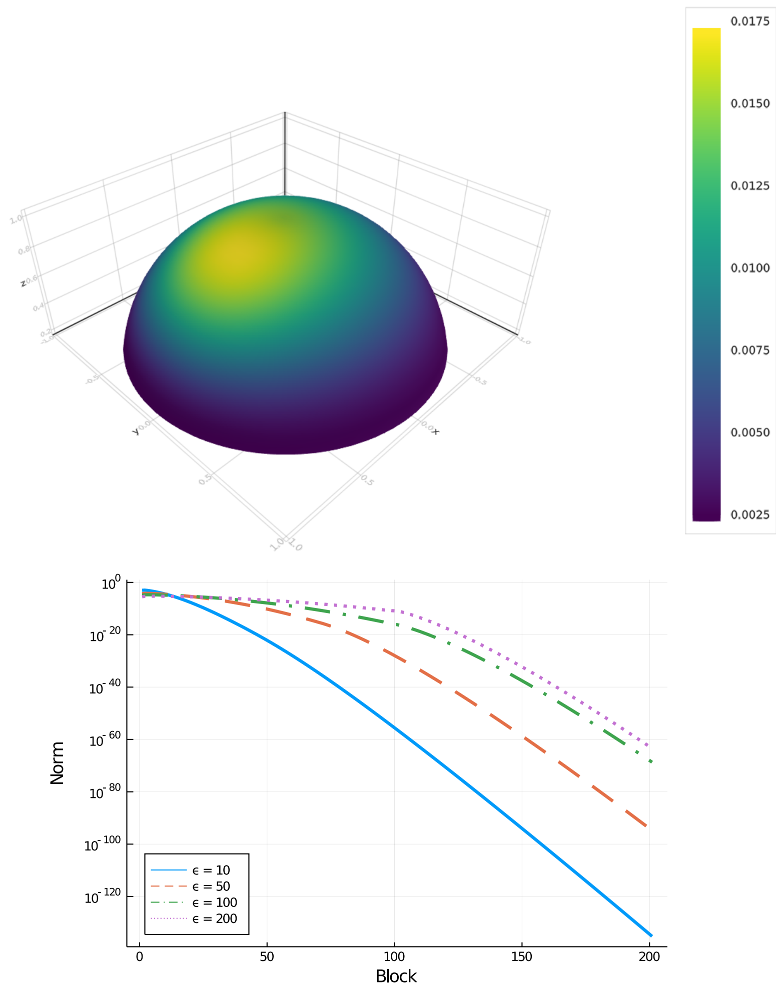


Figure 4.6: Left: The computed solution to $\Delta^2 u = f$ with zero Dirichlet and Neumann boundary conditions with $f(x, y, z) = (1 + \text{erf}(5(1 - 10((x - 0.5)^2 + y^2))))\rho(z)^2$. Right: The norms of each block of the computed solution of the biharmonic equation with the right hand side function $f(x, y, z) = \exp(-\epsilon((x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2))$ 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 spectral convergence.

4.5.4 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 Helmholtz problem

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

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

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

for $\tilde{u}$, where

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

for $(x,y,z) \in \Omega$. This new problem is then a zero boundary condition Helmholtz problem with right hand side g. 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

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

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, which are precisely the Fourier coefficients of $c(\cos\theta, \sin\theta)$. 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 manner.

Other boundary conditions aside from those already presented here are beyond the scope of this thesis. However, the approach established for the case of a triangle domain in 2D shows how Neumann conditions can be considered as a system of equations in partial derivatives involving Dirchlet conditions [59]. This approach may also work here for the spherical cap. Ideally, one would properly tackle the tangent bundle (that is defined in Definition 3) which would lower the degrees of freedom, but this is future work – see Appendix A.

4.6 Conclusions

We have shown that trivariate orthogonal polynomials can lead to sparse discretizations of general linear PDEs on spherical cap domains, with Dirichlet boundary conditions on the $z = \alpha \in (0, 1)$ boundary. We have provided a detailed practical framework for the application of the methods described for quadratic surfaces of revolution [61], by utilising the non-classical 1D OPs on the interval $[\alpha, 1]$ with the weight $(z - \alpha)^a\,(1 - z^2)^{b/2}$ defined for the disk-slice case [78]. Generalisation to spherical bands ($\alpha \leq z \leq \beta$) is straightforward. This work thus forms a building block in developing an $hp-$finite element method to solve PDEs on the sphere by using spherical band and spherical cap shaped elements.

This work also serves as a stepping stone to constructing similar methods to solve partial differential equations on other 3D sub-domains of the sphere such as spherical triangles. It is clear from the construction in this chapter that discretizations of the spherical Laplacian and other partial differential operators are sparse on other suitable sub-components of the sphere. The resulting sparsity in high-polynomial degree discretizations presents an attractive alternative to methods based on bijective mappings (e.g., [8, 72, 10]). Constructing these sparse spectral methods for surface PDEs on spherical triangles is future work, and has applications in weather prediction [80], though it is not yet clear how to directly construct, or perhaps *compute*, the necessary orthogonal polynomials.

The next stage is to develop an orthogonal basis for the tangent bundle of the spherical cap (or band), and obtain sparse differential operators for the spherical gradient, divergence etc. On the complete sphere, the vector spherical harmonics that form the orthogonal basis are simply the gradients and perpendicular gradients of the scalar spherical harmonics [2] which has been used effectively for solving PDEs on the sphere [87, 42] – however, we do not have that luxury for the spherical cap or band, and hence the construction of a basis will not be as straightforward.

Chapter 5

Summary and future directions

5.1 Summary

In this thesis, we have developed sparse spectral methods for solving partial differential equations on disk-slices and trapeziums in 2D, and spherical caps as a surface in 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 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).

A further avenue to take the framework for scalar functions is to construct a vector polynomial basis for functions whose values lie on the tangent bundle of the sphere. In Appendix A, we provide a summary for how one needs to approach this. The motivation for such is so as to be able to derive similarly sparsely structured operators for the spherical gradient and divergence. The main observation however is that, while the vector spherical harmonics are already established as being such an orthogonal and complete basis for the whole sphere, a similar construction for the spherical cap would not yield the same result.

Ideally, we would like to pair the framework presented in Chapter 4 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.

Discretizations of partial differential operators are sparse on other suitable sub-domains of the sphere, as evidenced by the construction presented for the spherical cap. Hence, using the techniques learnt here, one could also look to constructing similar methods for solving PDEs on spherical triangles, with a view to using these sub-domains as elements for a spherical spectral element method. Moreover, one could use this framework to also develop sparse spectral methods on more general domains defined by an algebraic surface – in particular those defined by non-uniform rational B-splines (NURBS). However, it is not obvious how one would derive or compute the OPs for such domains.

Appendices

A Tangent bundle of the spherical cap

One desired goal is to be able to extend the methodology detailed in Chapter 4 to the tangent bundle of the spherical cap Ω (see Definition 3). By creating a basis of orthogonal vector polynomials (OVPs) for the spherical cap Ω, we can expand vector-valued functions that lie in the tangent bundle in this basis. Such functions that are useful for the sphere are gradients and perpendicular-gradients of scalar functions, as we have seen in Section 2.6 where we solved the linearised shallow water equations on the whole sphere.

Any function in the tangent bundle of Ω can be written as

$$\boldsymbol{F} = \hat{\boldsymbol{\phi}} F_\varphi + \hat{\boldsymbol{\theta}} F_\theta$$

for some scalar functions F_φ, F_θ on Ω. Of course, we can expand these functions in our spherical cap scalar OPs $\mathbb{Q}^{(a)}$ (or $\mathbb{W}^{(a)}$ if they satisfy zero boundary conditions). Gradients and perpendicular gradients of scalar functions also take the form of $\boldsymbol{F}$.

For the whole sphere, recall from Section 2.5 that we simply chose the vector spherical harmonics as our tangent bundle basis, defined as the gradient and perpendicular gradients of the scalar spherical harmonics. We could make that choice because the vector spherical harmonics as defined were naturally orthogonal, and formed a complete basis for such functions $\boldsymbol{F}$. Unfortunately, we do not have the same luxury here, with the sets $\{\nabla_{\mathrm{S}}\Big(w_R^{(a,0)}\, Q_{n,k,i}^{(a)}\Big),\ \hat{\boldsymbol{r}} \times \nabla_{\mathrm{S}}\Big(w_R^{(a,0)}\, Q_{n,k,i}^{(a)}\Big)\}$ and $\{\nabla_{\mathrm{S}} Q_{n,k,i}^{(a)},\ \hat{\boldsymbol{r}} \times \nabla_{\mathrm{S}} Q_{n,k,i}^{(a)}\}$ not being orthogonal for any parameter a, and with the same observation for the non-weighted OPs. As such, one would need to find an orthogonal basis that spans the tangent bundle of the spherical cap Ω, such that we can sparsely expand, either analytically or numerically, the spherical gradients of our scalar basis polynomials and other vector fields of the form $\boldsymbol{F}$.

Index of Notation

a, b, c, d Lower case letters a, b, c, d refer to OP family parameters (unless otherwise stated)

$|m|$ The absolute value of a scalar m

$\alpha_{l,m,j}$ Lower case greek letters with subscripts refer to coefficients in scalar OP relations (unless otherwise stated)

$A_{l,m,j}$ Capital greek letters with subscripts refer to coefficients in vector OP (VSH) relations (unless otherwise stated)

$\mathbb{C}$ The complex numbers

c_l^m The normalising constant for the spherical harmonic Y_l^m

a^* The complex conjugate of $a \in \mathbb{C}$

Δt A timestep for a simulation

Δ The Laplacian operator in $\mathbb{R}^2$

Δ^2 The biharmonic operator in $\mathbb{R}^2$

Δ_{S} The Laplace–Beltrami operator

$\boldsymbol{f}, \boldsymbol{\xi}$ Lower case bold letters refer to vectors

∇_{S} The spherical gradient operator

$H^{(a,b,c,d)}_{n,k}$ Four-parameter bivariate OP of degree n and order k defined on the given domain and by the given inner product

$\mathbb{H}^{(a,b,c,d)}$ Vector of the disk-slice/trapezium OPs ordered by degree, with parameters a, b, c, d

$\mathbb{H}^{(a,b,c,d)}_n$ (Sub-)Vector of the disk-slice/trapezium OPs of degree n, with parameters a, b, c, d

I, I_d The identity matrix (in $\mathbb{R}^{d\times d}$)

$\langle u, v\rangle$ An inner product (defined by the context)

$\langle p,\ q\rangle_{H^{(a,b,c,d)}}$ A multidimensional inner product over Ω with the weight $W^{(a,b,c,d)}$ associated with the OPs $\{H^{(a,b,c,d)}_{n,k}\}$

$\langle p,\ q\rangle_{Q^{(a)}}$ A multidimensional inner product over Ω with the weight $W^{(a)}$ associated with the OPs $\{Q^{(a)}_{n,k,i}\}$

$\langle p,\ q\rangle_w$ A one-dimensional inner product with weight w

J_x, J_y, J_z Jacobi operator matrices

${}^TJ_x, {}^TJ_y, {}^TJ_z$ The Jacobi matrices for the tangent bundle VSH basis

$\delta_{n,n'}$ The Kronecker delta function; 1 if $n = n'$, else 0

$\mathbb{N}$ The natural numbers (positive integers)

$\mathbb{N}_0$ The set $\mathbb{N} \cup \{0\}$

$\|f\|$ The norm of a function f, defined by the square root of the relevant inner product

$\|f\|_{H^{(a,b,c,d)}}$ The norm of a function f, defined by the square root of the inner product over Ω given by the weight $W^{(a,b,c,d)}$ associated with the OPs $\{H^{(a,b,c,d)}_{n,k}\}$

$\|f\|_{Q^{(a)}}$ The norm of a function f, defined by the square root of the inner product over Ω given by the weight $W^{(a)}$ associated with the OPs $\{Q^{(a)}_{n,k,i}\}$

ω_R, ω_P Normalising constants for inner products

Ω The domain of interest

$\hat{\boldsymbol{\phi}}$, $\hat{\boldsymbol{\theta}}$ The standard spherical coordinate angular basis vectors

φ The polar angle in spherical coordinates

$\boldsymbol{\Phi}_l^m$ The vector spherical harmonic $\nabla_{\mathrm{S}}^{\perp} Y_l^m = \hat{\boldsymbol{r}} \times \nabla_{\mathrm{S}} Y_l^m$

P_l The degree l Legendre polynomial

P_l^m The Associated Legendre polynomial of degree l and order m

$P_n^{(a,b)}$ The degree n Jacobi polynomial (context determines normalized or not) unless otherwise stated

$\boldsymbol{\Psi}_l^m$ The vector spherical harmonic $\nabla_{\mathrm{S}} Y_l^m$

$\mathbb{P}$ Vector of the SH OPs

$\mathbb{P}_l$ (Sub-)Vector of the degree l SH OPs

$\tilde{\mathbb{Q}}^{(a)}$ Vector of the spherical cap OPs ordered by degree, with parameter a

$\tilde{\mathbb{Q}}_n^{(a)}$ (Sub-)Vector of the spherical cap OPs of degree n, with parameter a

$\mathbb{Q}_N^{(a)}$ Vector of the spherical cap OPs up to degree N, grouped by order k, with parameter a

$\mathbb{Q}_{N,k}^{(a)}$ (Sub-)Vector of the spherical cap OPs of order k up to degree N, with parameter a

$R_n^{(a,b,c)}$ Non-classical three-parameter univariate OP of degree n

$\mathbb{R}$ The real numbers

$\hat{\boldsymbol{r}}$ The unit normal vector at the point (x, y, z)

$\mathbb{R}^d$ The d-dimensional coordinate space over the real numbers

$\tilde{\mathbb{T}}$ Vector of the VSHs

θ The azimuthal angle in spherical coordinates

$\tilde{\mathbb{T}}_l$ (Sub)-Vector of the VSHs of order l

$\boldsymbol{v}^\top, A^\top$ Transpose of the vector $\boldsymbol{v}$ or matrix A (non complex conjuagate)

$W^{(a)}, W^{(a,b,c)}, W^{(a,b,c,d)}$ Weight function for relevant multidimensional OPs, with the given parameters

$w_R^{(a,b,c)}$, $w_P^{(a,b)}$ Weight functions for the one-dimensional OPs $\{R_n^{(a,b,c)}\}$ and $\{P_n^{(a,b)}\}$ respectively

$\mathbb{W}^{(a,b,c,d)}$ Vector of the weighted disk-slice/trapezium OPs ordered by degree, with parameters a, b, c, d

$\mathbb{W}_N^{(a)}$ Vector of the weighted spherical cap OPs up to degree N, grouped by order k, with parameter a

x, y, z Lower case non-bold x, y, z represents cartesian coordinates

Y_l^m The degree l and order m spherical harmonic

$\mathbb{Z}$ The integers

0_d The zero matrix in $\mathbb{R}^{d \times d}$

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