Spherical harmonics as orthogonal polynomials in three variables

Ben Snowball

June 29, 2018

1 Introduction

Give outline

Mention shallow water equation. Include plot.

1.1 On the Unit Interval (1D)

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

$$\frac{\mathrm{d}}{\mathrm{d}x} P_l^{(a,b)}(x) = \text{const.} \times P_{l-1}^{(a+1,b+1)}(x) \tag{1}$$

$$\implies \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) = \text{const.} \times P_{l-m}^{(m,m)}(x) \tag{2}$$

where $P_l^{(a,b)}(x)$ is the l degree Jacobi polynomial, orthogonal with weight $w(x) = (1 - x)^a(1 + x)^b$, and $P_l(x) := P_l^{(0,0)}(x)$ is the Legendre polynomial of degree l.

Further, we can define associated Legendre polynomials that are also orthogonal:

$$P_l^m(x) := (-1)^m(1 - x^2)^{\frac{m}{2}} \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) = \hat{c}_l^m (1 - x^2)^{\frac{m}{2}} P_{l-m}^{(m,m)}(x) \tag{3}$$

$$P_l^{-m}(x) := \tilde{c}_l^m P_l^m(x), \tag{4}$$

for $m \in \mathbb{N}_0$ where

I prefer to write $m = 0, 1, 2, \ldots$ to avoid any ahance of confusion

$$\hat{c}_l^m := \frac{\Gamma(l+m+1)}{(-2)^m \Gamma(l+1)} \tag{5}$$

$$\tilde{c}_l^m := \frac{(-1)^m \Gamma(l-m+1)}{\Gamma(l+m+1)} \tag{6}$$

using the gamma function $\Gamma(n) := (n-1)!$ for $n \in \mathbb{N}$.

1.2 On the Unit Sphere (3D)

Let (x, y, z) be a point on the unit sphere such that $x^2 + y^2 + z^2 = 1$. Let θ, φ denote the angles such that

$$x = \sin\theta \cos\varphi \tag{7}$$

$$y = \sin\theta \sin\varphi \tag{8}$$

$$z = \cos\theta. \tag{9}$$

Further, define

$$c_l^m := \left(\frac{(2l+1)\Gamma(l-m+1)}{4\pi\Gamma(l+m+1)} \right)^{\frac{1}{2}}, \tag{10}$$

and

$$\alpha_l^m := \begin{cases} c_l^m \hat{c}_l^{|m|} & \text{if } m \geq 0 \\ c_l^m \hat{c}_l^{|m|} \tilde{c}_l^{|m|} & \text{if } m < 0 \end{cases}. \tag{11}$$

We can the define the spherical harmonics, orthogonal on the unit sphere as:

$$Y_l^m(\theta, \varphi) := c_l^m e^{im\varphi} P_l^m(\cos\theta) \tag{12}$$

$$= \alpha_l^m (1 - (\cos\theta)^2)^{\frac{|m|}{2}} e^{im\varphi} P_{l-|m|}^{(|m|,|m|)}(\cos\theta), \quad \text{where } 0 \leq |m| \leq l,\ l \in \mathbb{N}_0. \tag{13}$$

Note that we can then express Y_l^m in terms of x, y, z instead of θ, φ by noting that $\cos\theta = z$ and that $e^{im\varphi}$ can be expressed in terms of x, y, z for any $m \in \mathbb{Z}$. Indeed, they are polynomials in x, y, z which we denote $Y_l^m(x, y, z)$. They span all polynomials modulo the ideal generated by $x^2 + y^2 + z^2 - 1$.

2 Surface of the sphere

2.1 Deriving expressions for the multiplication by x, y, z of the spherical harmonics

We start by expressing $x\,Y_l^m(x,y,z)$, $y\,Y_l^m(x,y,z)$, and $z\,Y_l^m(x,y,z)$ in terms of $Y_{l'}^{m'}(x,y,z)$ for any point (x,y,z) on the unit circle.

Move the derivations to an appendix to make the text flow better

Using (7)–(9), we can write

Add references to the DLMF. Be precise about which equation as it makes it easier for yourself to look up.

$$Y_l^m(x,y,z) = \alpha_l^m (1-z^2)^{\frac{|m|}{2}} e^{im\varphi} P_{l-|m|}^{(|m|,|m|)}(z), \quad \text{where } 0 \le |m| \le l,\ l \in \mathbb{N}_0. \tag{14}$$

Note that the recurrence relationship for the Jacobi polynomials satisfies

$$zP_k^{(m,m)}(z) = \frac{1}{\kappa_{k,m}}\left[P_{k+1}^{(m,m)}(z) - \lambda_{k,m}P_k^{(m,m)}(z) + \mu_{k,m}P_{k-1}^{(m,m)}(z)\right], \tag{15}$$

for $k \ge 0$, $m \in \mathbb{Z}$, where

$$\kappa_{k,m} := \frac{(2k+2m+1)(k+m+1)}{(k+1)(k+2m+1)}, \tag{16}$$

$$\lambda_{k,m} := 0 \tag{17}$$

$$\mu_{k,m} := \frac{k+m+1}{(k+1)(k+2m+1)}. \tag{18}$$

Thus,

$$zP_{l-m}^{(m,m)}(z) = \tilde{F}_{l,m}P_{l-m+1}^{(m,m)}(z) + \tilde{G}_{l,m}P_{l-m-1}^{(m,m)}(z), \tag{19}$$

for $k \ge 0$, $m \in \mathbb{Z}$, where

$$\tilde{F}_{l,m} := \frac{(l-m+1)(l+m+1)}{(2l+1)(l+1)}, \tag{20}$$

$$\tilde{G}_{l,m} := \begin{cases} \frac{l}{2l+1} & \text{if } l-m \ge 1 \\ 0 & \text{otherwise.} \end{cases}. \tag{21}$$

Further, note that

$$\cos\varphi\, e^{im\varphi} = \frac{1}{2}(e^{i\varphi} + e^{-i\varphi})e^{im\varphi} = \frac{1}{2}(e^{i(m+1)\varphi} + e^{i(m-1)\varphi}) \tag{22}$$

$$\sin\varphi\, e^{im\varphi} = \frac{1}{2i}(e^{i\varphi} - e^{-i\varphi})e^{im\varphi} = \frac{-i}{2}(e^{i(m+1)\varphi} - e^{i(m-1)\varphi}) \tag{23}$$

Finally, note the relationship between the Jacobi polynomials $P_l^{(a,b)}(z)$ and the ultraspherical polynomials $C_n^{(\lambda)}(z)$, as well as the three-term recurrence relation for the ultraspherical polynomials, i.e. for $m \in \mathbb{N}_0$:

$$\nu_{l,m} C_{l-m}^{(m+1/2)}(z) = P_{l-m}^{(m,m)}(z), \tag{24}$$

and

$$C_n^{(\lambda)}(z) = \xi_{n,\lambda}^{(1)} \left[C_n^{(\lambda+1)}(z) - C_{n-2}^{(\lambda+1)}(z) \right] \tag{25}$$

$$(1 - z^2)\, C_n^{(\lambda)}(z) = \frac{1}{\xi_{n,\lambda}^{(2)}} \left[\xi_{n,\lambda}^{(3)} C_n^{(\lambda-1)}(z) - \xi_{n,\lambda}^{(4)} C_{n+2}^{(\lambda-1)}(z) \right], \tag{26}$$

where

$$\nu_{l,m} := \frac{\Gamma(l+1)\Gamma(2m+1)}{\Gamma(l+m+1)\Gamma(m+1)} \tag{27}$$

$$\xi_{n,\lambda}^{(1)} := \frac{\lambda}{n+\lambda} \tag{28}$$

$$\xi_{n,\lambda}^{(2)} := 4(\lambda - 1)(n + \lambda) \tag{29}$$

$$\xi_{n,\lambda}^{(3)} := (n + 2\lambda - 2)(n + 2\lambda - 1) \tag{30}$$

$$\xi_{n,\lambda}^{(4)} := (n+1)(n+2). \tag{31}$$

Thus, we can write three-term recurrences for the Jacobi polynomials as:

$$P_{l-m}^{(m,m)}(z) = \tilde{A}_{l,m} P_{l-m}^{(m+1,m+1)}(z) + \tilde{B}_{l,m} P_{l-m-2}^{(m+1,m+1)}(z) \tag{32}$$

$$(1 - z^2)\, P_{l-m}^{(m,m)}(z) = \tilde{D}_{l,m} P_{l-m+2}^{(m-1,m-1)}(z) + \tilde{E}_{l,m} P_{l-m}^{(m-1,m-1)}(z), \tag{33}$$

for $l, m \in \mathbb{N}_0$ s.t. $0 \leq m \leq l$, where

$$\tilde{A}_{l,m} := \frac{(l+m+2)(l+m+1)}{2(2l+1)(l+1)} \tag{34}$$

$$\tilde{B}_{l,m} := \begin{cases} -\frac{l}{2(2l+1)} & \text{if } l - m \geq 2 \\ 0 & \text{otherwise.} \end{cases} \tag{35}$$

$$\tilde{D}_{l,m} := -\frac{2(l-m+2)(l-m+1)}{(2l+1)(l+1)} \tag{36}$$

$$\tilde{E}_{l,m} := \frac{2l}{2l+1}. \tag{37}$$

We can now write down expressions for the multiplication of $Y_l^m(x,y,z)$ by x, y or z for some point (x,y,z) on the unit sphere for $l \in \mathbb{N}_0$, $m \in \mathbb{Z}$ s.t. $0 \leq |m| \leq l$ as follows:

$$\begin{aligned}
x\, Y_l^m(x,y,z) &= \alpha_l^m \cos\varphi e^{im\varphi} \sin\theta (1-z^2)^{|m|/2} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= \frac{1}{2}\alpha_l^m (e^{i(m+1)\varphi} + e^{i(m-1)\varphi})(1-z^2)^{\frac{|m|+1}{2}} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= \frac{1}{2}\alpha_l^m e^{i(m+1)\varphi}(1-z^2)^{\frac{|m|+1}{2}} \left[\tilde{A}_{l,m} P_{l-|m|}^{(|m|+1,|m|+1)}(z) + \tilde{B}_{l,m} P_{l-|m|-2}^{(|m|+1,|m|+1)}(z)\right] \\
&\quad + \frac{1}{2}\alpha_l^m e^{i(m-1)\varphi}(1-z^2)^{\frac{|m|-1}{2}} \left[\tilde{D}_{l,m} P_{l-|m|+2}^{(|m|-1,|m|-1)}(z) + \tilde{E}_{l,m} P_{l-|m|}^{(|m|-1,|m|-1)}(z)\right] \\
&= A_{l,m} Y_{l+1}^{m+1}(x,y,z) + B_{l,m} Y_{l-1}^{m+1}(x,y,z) \\
&\qquad + D_{l,m} Y_{l+1}^{m-1}(x,y,z) + E_{l,m} Y_{l-1}^{m-1}(x,y,z),
\end{aligned} \tag{38}$$

$$\begin{aligned}
y\, Y_l^m(x,y,z) &= \alpha_l^m \sin\varphi e^{im\varphi} \sin\theta (1-z^2)^{|m|/2} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= -\frac{1}{2} i \alpha_l^m (e^{i(m+1)\varphi} - e^{i(m-1)\varphi})(1-z^2)^{\frac{|m|+1}{2}} P_{l-|m|}^{(|m|,|m|)}(z) \\
&= -i \left[A_{l,m} Y_{l+1}^{m+1}(x,y,z) + B_{l,m} Y_{l-1}^{m+1}(x,y,z)\right] \\
&\qquad + i \left[D_{l,m} Y_{l+1}^{m-1}(x,y,z) + E_{l,m} Y_{l-1}^{m-1}(x,y,z)\right],
\end{aligned} \tag{39}$$

$$\begin{aligned}
z\, Y_l^m(x,y,z) &= \alpha_l^m e^{im\varphi} (1-z^2)^{|m|/2} z P_{l-|m|}^{(|m|,|m|)}(z) \\
&= \alpha_l^m e^{im\varphi} (1-z^2)^{|m|/2} \left[\tilde{F}_{l,m} P_{l-|m|+1}^{(|m|,|m|)}(z) + \tilde{G}_{l,m} P_{l-|m|-1}^{(|m|,|m|)}(z)\right] \\
&= F_{l,m} Y_{l+1}^m(x,y,z) + G_{l,m} Y_{l-1}^m(x,y,z),
\end{aligned} \tag{40}$$

where

$$A_{l,m} := \begin{cases} \frac{\alpha_l^m}{2\alpha_{l+1}^{m+1}} \tilde{A}_{l,m} & \text{if } m \geq 0 \\ \frac{\alpha_l^m}{2\alpha_{l+1}^{m+1}} \tilde{D}_{l,|m|} & \text{if } m < 0 \end{cases} \tag{41}$$

$$B_{l,m} := \begin{cases} \frac{\alpha_l^m}{2\alpha_{l-1}^{m+1}} \tilde{B}_{l,m} & \text{if } m \geq 0,\ l-|m| \geq 2 \\ \frac{\alpha_l^m}{2\alpha_{l-1}^{m+1}} \tilde{E}_{l,|m|} & \text{if } m < 0 \\ 0 & \text{otherwise.} \end{cases} \tag{42}$$

$$D_{l,m} := \begin{cases} \frac{\alpha_l^m}{2\alpha_{l+1}^{m-1}} \tilde{D}_{l,m} & \text{if } m > 0 \\ \frac{\alpha_l^m}{2\alpha_{l+1}^{m-1}} \tilde{A}_{l,|m|} & \text{if } m \leq 0 \end{cases} \tag{43}$$

$$E_{l,m} := \begin{cases} \frac{\alpha_l^m}{2\alpha_{l-1}^{m-1}} \tilde{E}_{l,m} & \text{if } m > 0 \\ \frac{\alpha_l^m}{2\alpha_{l-1}^{m-1}} \tilde{B}_{l,|m|} & \text{if } m \leq 0,\ l-|m| \geq 2 \\ 0 & \text{otherwise.} \end{cases} \tag{44}$$

$$F_{l,m} := \frac{\alpha_l^m}{\alpha_{l+1}^m} \tilde{F}_{l,m} \tag{45}$$

$$G_{l,m} := \frac{\alpha_l^m}{\alpha_{l-1}^m} \tilde{G}_{l,m}. \tag{46}$$

2.2 Jacobi matrices

Define, for $l \in \mathbb{N}_0$, $\mathbb{P}_l$ as the column vector of the degree l spherical harmonic polynomials, and $\mathbb{P}$ as the stacked block vector of the $\mathbb{P}_l$'s; that is

$$\mathbb{P}_l := \begin{bmatrix} Y_l^{-l} \\ \vdots \\ Y_l^l \end{bmatrix} \in \mathbb{C}^{2l+1}, \qquad \mathbb{P} := \begin{bmatrix} \mathbb{P}_0 \\ \hline \mathbb{P}_1 \\ \hline \mathbb{P}_2 \\ \hline \vdots \end{bmatrix}. \tag{47}$$

Define the (Jacobi) matrices J^x, J^y, J^z by

$$J^x \mathbb{P} = x\mathbb{P}, \quad J^y \mathbb{P} = y\mathbb{P}, \quad J^z \mathbb{P} = z\mathbb{P}. \tag{48}$$

Then, using equations (38–40), we have that the Jacobi matrices take the following block-tridiagonal form:

$$J^x = \begin{bmatrix} B_0^x & A_0^x & & & & \\ C_1^x & B_1^x & A_1^x & & & \\ & C_2^x & B_2^x & A_2^x & & \\ & & C_3^x & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{49}$$

$$J^y = \begin{bmatrix} B_0^y & A_0^y & & & & \\ C_1^y & B_1^y & A_1^y & & & \\ & C_2^y & B_2^y & A_2^y & & \\ & & C_3^y & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{50}$$

$$J^z = \begin{bmatrix} B_0^z & A_0^z & & & & \\ C_1^z & B_1^z & A_1^z & & & \\ & C_2^z & B_2^z & A_2^z & & \\ & & C_3^z & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{51}$$

where for $l \in \mathbb{N}_0$,

$$A_l^x := \begin{bmatrix} D_{l,-l} & 0 & A_{l,-l} & & \\ & \ddots & \ddots & \ddots & \\ & & D_{l,l} & 0 & A_{l,l} \end{bmatrix} \in \mathbb{R}^{(2l+1)\times(2l+3)}, \tag{52}$$

$$B_l^x := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)} \tag{53}$$

$$C_l^x := \begin{bmatrix} B_{l,-l} & & \\ 0 & \ddots & \\ E_{l,-l+2} & \ddots & B_{l,l-2} \\ & \ddots & 0 \\ & & E_{l,l} \end{bmatrix} \in \mathbb{R}^{(2l+1)\times(2l-1)} \quad (l \neq 0), \tag{54}$$

$$A_l^y := -i \begin{bmatrix} -D_{l,-l} & 0 & A_{l,-l} & & \\ & \ddots & \ddots & \ddots & \\ & & -D_{l,l} & 0 & A_{l,l} \end{bmatrix} \in \mathbb{C}^{(2l+1)\times(2l+3)}, \tag{55}$$

$$B_l^y := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)} \tag{56}$$

$$C_l^y := -i \begin{bmatrix} B_{l,-l} & & \\ 0 & \ddots & \\ -E_{l,-l+2} & \ddots & B_{l,l-2} \\ & \ddots & 0 \\ & & -E_{l,l} \end{bmatrix} \in \mathbb{C}^{(2l+1)\times(2l-1)} \quad (l \neq 0), \tag{57}$$

$$A_l^z := \begin{bmatrix} 0 & F_{l,-l} & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & F_{l,l} & 0 \end{bmatrix} \in \mathbb{R}^{(2l+1)\times(2l+3)}, \tag{58}$$

$$B_l^z := 0 \in \mathbb{R}^{(2l+1)\times(2l+1)} \tag{59}$$

$$C_l^z := \begin{bmatrix} 0 & & \\ G_{l,-l+1} & \ddots & \\ 0 & \ddots & 0 \\ & \ddots & G_{l,l-1} \\ & & 0 \end{bmatrix} \in \mathbb{R}^{(2l+1)\times(2l-1)} \quad (l \neq 0). \tag{60}$$

$$\tag{61}$$

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

Combining each system in (48) we can write the tridiagonal-block system

$$\left[\begin{array}{c|c|cc}
1 & & & \\
\hline
B_0^x - xI_1 & A_0^x & & \\
B_0^y - yI_1 & A_0^y & & \\
B_0^z - zI_1 & A_0^z & & \\
\hline
C_1^x & B_1^x - xI_3 & A_1^x & \\
C_1^y & B_1^y - yI_3 & A_1^y & \\
C_1^z & B_1^z - zI_3 & A_1^z & \\
\hline
 & C_2^x & \ddots & \ddots \\
 & C_2^y & & \\
 & C_2^z & & \\
\hline
 & & \ddots &
\end{array}\right] \mathbb{P} = \begin{bmatrix} \alpha_0^0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ \end{bmatrix}, \tag{62}$$

where I_{2l+1} is the $(2l+1) \times (2l+1)$ identity matrix.

Let us define the joint matrices that comprise each block. For each $l \in \mathbb{N}_0$:

$$A_l := \begin{bmatrix} A_l^x \\ A_l^y \\ A_l^z \end{bmatrix} \in \mathbb{R}^{3(2l+1)\times(2l+3)}, \quad C_l := \begin{bmatrix} C_l^x \\ C_l^y \\ C_l^z \end{bmatrix} \in \mathbb{R}^{3(2l+1)\times(2l-1)} \quad (l \neq 0), \tag{63}$$

$$B_l := \begin{bmatrix} B_l^x \\ B_l^y \\ B_l^z \end{bmatrix} \in \mathbb{R}^{3(2l+1)\times(2l+1)}, \quad G_l(x,y,z) := \begin{bmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{bmatrix} \in \mathbb{R}^{3(2l+1)\times(2l+1)}. \tag{64}$$

Then our system (62) simply becomes

$$\begin{bmatrix}
1 & & & \\
B_0 - G_0(x,y,z) & A_0 & & \\
C_1 & B_1 - G_1(x,y,z) & A_1 & \\
 & C_2 & \ddots & \ddots \\
 & & \ddots &
\end{bmatrix} \mathbb{P} = \begin{bmatrix} \alpha_0^0 \\ 0 \\ 0 \\ \vdots \\ \end{bmatrix}. \tag{65}$$

Cite Dunkl and Xu here.

For each $l \in \mathbb{N}_0$ let D_l^T be any matrix that is a left inverse of A_l, i.e. such that $D_l^T A_l = I_{2l+3}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the D_l^T's, we obtain the lower triangular system

$$\begin{bmatrix} 1 & & & & \\ D_0^T(B_0 - G_0) & I_1 & & & \\ D_1^T C_1 & D_1^T(B_1 - G_1) & I_3 & & \\ & D_2^T C_2 & \ddots & \ddots & \\ & & \ddots & & \end{bmatrix} \mathbb{P} = \begin{bmatrix} \alpha_0^0 \\ 0 \\ 0 \\ \vdots \\ \ \end{bmatrix}. \tag{66}$$

Expanding this we can solve the system (66) to find a three-term recurrence relation for each $\mathbb{P}_{l+1}$ in terms of the previous two sub-vectors $\mathbb{P}_l$ and $\mathbb{P}_{l-1}$:

$$\begin{cases} \mathbb{P}_{-1} := 0 \\ \mathbb{P}_0 := \alpha_0^0 \\ \mathbb{P}_{l+1} = -D_l^T(B_l - G_l)\mathbb{P}_l - D_l^T C_l \, \mathbb{P}_{l-1}, \quad l \in \mathbb{N}. \end{cases} \tag{67}$$

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

$$D_l^T = \begin{bmatrix} \hat{A}_l^{x,y} & 0_{(2l+3)\times(2l+1)} \end{bmatrix} \in \mathbb{R}^{(2l+3)\times 3(2l+1)} \tag{68}$$

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

$$\hat{A}_l^{x,y} = \begin{bmatrix} \frac{1}{2D_{l,-l}} & 0 & \dots & 0 & -\frac{i}{2D_{l,-l}} & 0 & \dots & 0 \\ & \ddots & & & & \ddots & & \\ & & \ddots & & & & \ddots & \\ & & & \frac{1}{2D_{l,l}} & 0 & \dots & 0 & -\frac{i}{2D_{l,l}} \\ 0 & \dots & \frac{1}{2A_{l,l-1}} & 0 & \dots & 0 & \frac{i}{2A_{l,l-1}} & 0 \\ 0 & \dots & 0 & \frac{1}{2A_{l,l}} & 0 & \dots & 0 & \frac{i}{2A_{l,l}} \end{bmatrix}. \tag{69}$$

For $l = 0$ we set

$$D_0^T = \begin{bmatrix} \frac{1}{2D_{0,0}} & -\frac{i}{2D_{0,0}} & 0 \\ 0 & 0 & \frac{1}{F_{0,0}} \\ \frac{1}{2A_{0,0}} & \frac{i}{2A_{0,0}} & 0 \end{bmatrix}. \tag{70}$$

2.4 Evaluation of a scalar function on the sphere

We can use the Clenshaw algorithm to evaluate a function at a given point (x, y, z) on the unit sphere provided we know the coefficients of the function when expanded in the spherical harmonic basis, i.e. suppose $f(x, y, z)$ is a function and we know the set $\{\mathbf{f}_l\}$ s.t.

$$f(x,y,z) \approx \sum_{l=0}^{N} \mathbf{f}_l^T \, \mathbb{P}_l(x,y,z), \quad \text{where } \mathbb{P}_l(x,y,z), \mathbf{f}_l \in \mathbb{R}^{2l+1} \text{ for each } l \in \{0, \ldots, N\}. \tag{71}$$

The Clenshaw algorithm is then as follows:

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

   set $\boldsymbol{\gamma}_n^T = \mathbf{f}_n^T - \boldsymbol{\gamma}_{n+1}^T D_n^T (B_n - G_n) - \boldsymbol{\gamma}_{n+2}^T D_{n+1}^T C_{n+1}$
3) Output: $f(x, y, z) \approx \mathbb{P}_0(x, y, z) f_0 + \boldsymbol{\gamma}_1^T \mathbb{P}_1(x, y, z) - \mathbb{P}_0(x, y, z) \boldsymbol{\gamma}_2^T D_1^T C_1$.

Mention $a(J^x, J^y, J^z)$ for variable coefficients here. Mention it is banded-block-banded.

3 Tangent space

Since the spherical harmonics are a basis for the surface of the sphere, and the tangent space of the sphere is spanned by the gradient and perpendicular gradient of a scalar function, we have that the gradients and perpendicular gradients of the spherical harmonics are a basis for the tangent space, namely ∇Y_l^m, $\nabla^{\perp} Y_l^m$. Note that the perpendicular gradient is related to the regular surface gradient by

$$\nabla^{\perp} Y_l^m(x,y,z) = \hat{\boldsymbol{k}} \times \nabla Y_l^m(x,y,z), \tag{72}$$

where $\hat{\boldsymbol{k}}$ is the unit vector normal to the surface of the sphere at the point (x, y, z), i.e. as we are looking at the unit sphere, $\hat{\boldsymbol{k}}$ is simply given by

$$\hat{\boldsymbol{k}} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}. \tag{73}$$

Importantly, ∇Y_l^m, $\nabla^{\perp} Y_l^m$ are in fact vector-valued orthogonal polynomials, that span all vector-valued polynomials modulo the vanishing ideal $\{\boldsymbol{p} \in (\Pi_3)^3 : \hat{\boldsymbol{k}} \cdot \boldsymbol{p} = 0\}$. A simple calculation shows that such orthogonal polynomials must still have block-tridiagonal Jacobi operators, as multiplication by x, y, or z remains inside the ideal. In the following, we determine the coefficients of these Jacobi operators, as well as other important operators needed.

3.1 Spin-1 tensor spherical harmonics

The gradient and perpendicular gradient of a spherical harmonic $Y_l^m(x, y, z)$ can be expressed in terms of spin-1 tensor spherical harmonics, which in turn can each be expressed as a vector-weighted sum of spherical harmonics.

I think the following should also be moved to appendix because it's technical details

We start by defining what we mean by a spin-1 tensor spherical harmonic. In general, the tensor spherical harmonic is given by, for $2l,\ j,\ 2s \in \mathbb{N}_0$,

$$\boldsymbol{\mathcal{Y}}_{l,m}^{j,s}(x, y, z) = \sum_{m_s=-s}^{s} \langle j \quad m - m_s\ ;\ s \quad m_s \mid l \quad m\rangle\, Y_j^{m-m_s}(x, y, z)\, \boldsymbol{\chi}_{s,m_s}, \tag{74}$$

where $\boldsymbol{\chi}_{s,m_s}$ are the simultaneous eigenstates of the spin operators $\mathbf{S}^2$ and S_z, and where $\langle j \quad m - m_s\ ;\ 1 \quad m_s \mid l \quad m\rangle$ is a Clebsch-Gordan coefficient. We note that a property of the Clebsch–Gordan coefficients means that they vanish unless $|j - s| \le l \le j + s$. We further note that there are simple calculable expressions for the Clebsch–Gordan coefficients when the spin $s = 1$.

This notation is hard to read.

Thus we have that the three spin-1 tensor spherical harmonics are given by

$$\boldsymbol{\mathcal{Y}}_{l,m}^{l\pm1,s}(x, y, z) = \sum_{m_s=-1}^{1} \langle l \pm 1 \quad m - m_s\ ;\ 1 \quad m_s \mid l \quad m\rangle\, Y_{l\pm1}^{m-m_s}(x, y, z)\, \boldsymbol{\chi}_{1,m_s}, \tag{75}$$

$$\boldsymbol{\mathcal{Y}}_{l,m}^{l,s}(x, y, z) = \sum_{m_s=-1}^{1} \langle l \quad m - m_s\ ;\ 1 \quad m_s \mid l \quad m\rangle\, Y_{l}^{m-m_s}(x, y, z)\, \boldsymbol{\chi}_{1,m_s}. \tag{76}$$

Here, the vectors $\boldsymbol{\chi}_{1,m_s}$ are the orthonormal eigenvectors of the spin-1spinmatrix

Fix

$$S_3 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{77}$$

and so are given as

$$\boldsymbol{\chi}_{1,\pm1} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mp1 \\ -i \\ 0 \end{bmatrix}, \quad \boldsymbol{\chi}_{1,0} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{78}$$

Then, for any $l \in \mathbb{N}_0$, $m \in \mathbb{Z}$ s.t. $0 \leq |m| \leq l$ we have that

$$\nabla Y_l^m = \beta_{l,-1}\, \boldsymbol{\mathcal{Y}}_{l,m}^{l-1,1} + \beta_{l,1} \boldsymbol{\mathcal{Y}}_{l,m}^{l+1,1}, \tag{79}$$

$$\nabla^{\perp} Y_l^m = \beta_{l,0}\, \boldsymbol{\mathcal{Y}}_{l,m}^{l,1}, \tag{80}$$

where

$$\beta_{l,-1} := (l+1) \left(\frac{l}{2l+1} \right)^{\frac{1}{2}}, \quad \beta_{l,0} := i \left(l(l+1) \right)^{\frac{1}{2}}, \quad \beta_{l,1} := l \left(\frac{l+1}{2l+1} \right)^{\frac{1}{2}}. \tag{81}$$

3.2 Deriving expressions for the multiplication by x, y, z of ∇Y_l^m, $\nabla^{\perp} Y_l^m$

We start by establishing some equations to be used to find $x\, \nabla Y_l^m(x,y,z)$, $x\, \nabla^{\perp} Y_l^m(x,y,z)$ etc. in terms of $\nabla Y_{l'}^{m'}(x,y,z)$, $\nabla^{\perp} Y_{l'}^{m'}(x,y,z)$. First, for compactness of notation, we define

$$\mathcal{C}_{l,m}^{L,m_s} := \langle L \quad m - m_s \; ; \; 1 \quad m_s \mid l \quad m \rangle. \tag{82}$$

Now, we have that

$$\begin{aligned} x\, \nabla Y_l^m &= x\, \beta_{l,-1}\, \boldsymbol{\mathcal{Y}}_{l,m}^{l-1,1} + x\, \beta_{l,1} \boldsymbol{\mathcal{Y}}_{l,m}^{l+1,1} \\ &= \sum_{m_s=-1}^{1} \boldsymbol{\chi}_{1,m_s} \Big[\beta_{l,-1}\, \mathcal{C}_{l,m}^{l-1,m_s} \big\{ A_{l-1,m-m_s}\, Y_l^{m-m_s+1} + B_{l-1,m-m_s}\, Y_{l-2}^{m-m_s+1} \\ &\qquad\qquad + D_{l-1,m-m_s}\, Y_l^{m-m_s-1} + E_{l-1,m-m_s}\, Y_{l-2}^{m-m_s-1} \big\} \\ &\qquad + \beta_{l,1}\, \mathcal{C}_{l,m}^{l+1,m_s} \big\{ A_{l+1,m-m_s}\, Y_{l+2}^{m-m_s+1} + B_{l+1,m-m_s}\, Y_l^{m-m_s+1} \\ &\qquad\qquad + D_{l+1,m-m_s}\, Y_{l+2}^{m-m_s-1} + E_{l+1,m-m_s}\, Y_l^{m-m_s-1} \big\} \Big] \end{aligned} \tag{83}$$

$$\begin{aligned} \implies x\, \nabla Y_l^m &= a_{l,m} \nabla Y_{l+1}^{m+1} + b_{l,m} \nabla Y_{l-1}^{m+1} + d_{l,m} \nabla Y_{l+1}^{m-1} + e_{l,m} \nabla Y_{l-1}^{m-1} \\ &\quad + h_{l,m} \nabla^{\perp} Y_l^{m+1} + j_{l,m} \nabla^{\perp} Y_l^{m-1}, \end{aligned} \tag{84}$$

where, for any valid m_s value,

$$a_{l,m} := \frac{\beta_{l,1}}{\beta_{l+1,1}} \frac{\mathcal{C}_{l,m}^{l+1,m_s}}{\mathcal{C}_{l+1,m+1}^{l+2,m_s}} A_{l+1,m-m_s}, \tag{85}$$

$$b_{l,m} := \frac{\beta_{l,-1}}{\beta_{l-1,-1}} \frac{\mathcal{C}_{l,m}^{l-1,m_s}}{\mathcal{C}_{l-1,m+1}^{l-2,m_s}} B_{l-1,m-m_s}, \tag{86}$$

$$d_{l,m} := \frac{\beta_{l,1}}{\beta_{l+1,1}} \frac{\mathcal{C}_{l,m}^{l+1,m_s}}{\mathcal{C}_{l+1,m-1}^{l+2,m_s}} D_{l+1,m-m_s}, \tag{87}$$

$$e_{l,m} := \frac{\beta_{l,-1}}{\beta_{l-1,-1}} \frac{\mathcal{C}_{l,m}^{l-1,m_s}}{\mathcal{C}_{l-1,m-1}^{l-2,m_s}} E_{l-1,m-m_s}, \tag{88}$$

$$\begin{aligned} h_{l,m} := \frac{1}{\beta_{l,0}\, \mathcal{C}_{l,m+1}^{l,m_s}} \Big[& \mathcal{C}_{l,m}^{l-1,m_s}\, \beta_{l,-1}\, A_{l-1,m-m_s} + \mathcal{C}_{l,m}^{l+1,m_s}\, \beta_{l,1}\, B_{l+1,m-m_s} \\ & - a_{l,m}\, \beta_{l+1,-1}\, \mathcal{C}_{l+1,m+1}^{l,m_s} - b_{l,m}\, \beta_{l-1,1}\, \mathcal{C}_{l-1,m+1}^{l,m_s} \Big], \end{aligned} \tag{89}$$

$$\begin{aligned} j_{l,m} := \frac{1}{\beta_{l,0}\, \mathcal{C}_{l,m-1}^{l,m_s}} \Big[& \mathcal{C}_{l,m}^{l-1,m_s}\, \beta_{l,-1}\, D_{l-1,m-m_s} + \mathcal{C}_{l,m}^{l+1,m_s}\, \beta_{l,1}\, E_{l+1,m-m_s} \\ & - d_{l,m}\, \beta_{l+1,-1}\, \mathcal{C}_{l+1,m-1}^{l,m_s} - e_{l,m}\, \beta_{l-1,1}\, \mathcal{C}_{l-1,m-1}^{l,m_s} \Big]. \end{aligned} \tag{90}$$

Note that (it can be shown) these are constants for each l, m pair despite appearing to depend on the value of m_s; we need only use any valid m_s value for each expression. By "valid", we mean the Clebsch–Gordan coefficients do not vanish for that m_s value when used.

Similarly, we have that

$$\begin{aligned} y\, \nabla Y_l^m = i \Big[& - a_{l,m} \nabla Y_{l+1}^{m+1} - b_{l,m} \nabla Y_{l-1}^{m+1} + d_{l,m} \nabla Y_{l+1}^{m-1} + e_{l,m} \nabla Y_{l-1}^{m-1} \\ & - h_{l,m} \nabla^{\perp} Y_l^{m+1} + j_{l,m} \nabla^{\perp} Y_l^{m-1} \Big]. \end{aligned} \tag{91}$$

Further, we also have that

$$\begin{aligned} z\, \nabla Y_l^m &= z\, \beta_{l,0}\, \boldsymbol{\mathcal{Y}}_{l,m}^{l,1} \\ &= \sum_{m_s=-1}^{1} \boldsymbol{\chi}_{1,m_s} \Big[\beta_{l,-1}\, \mathcal{C}_{l,m}^{l-1,m_s} \big\{ F_{l-1,m-m_s}\, Y_l^{m-m_s} + G_{l-1,m-m_s}\, Y_{l-2}^{m-m_s} \big\} \\ &\qquad + \beta_{l,1}\, \mathcal{C}_{l,m}^{l+1,m_s} \big\{ F_{l+1,m-m_s}\, Y_{l+2}^{m-m_s} + G_{l+1,m-m_s}\, Y_l^{m-m_s} \big\} \Big] \end{aligned} \tag{92}$$

$$\implies z\,\nabla Y_l^m = f_{l,m}\nabla Y_{l+1}^m + g_{l,m}\nabla Y_{l-1}^m + k_{l,m}\nabla^\perp Y_l^m, \tag{93}$$

where, for any valid m_s value,

$$f_{l,m} := \frac{\beta_{l,1}}{\beta_{l+1,1}}\frac{\mathcal{C}_{l,m}^{l+1,m_s}}{\mathcal{C}_{l+1,m+1}^{l+2,m_s}}F_{l+1,m-m_s}, \tag{94}$$

$$g_{l,m} := \frac{\beta_{l,-1}}{\beta_{l-1,-1}}\frac{\mathcal{C}_{l,m}^{l-1,m_s}}{\mathcal{C}_{l-1,m+1}^{l-2,m_s}}G_{l-1,m-m_s}, \tag{95}$$

$$\begin{aligned} k_{l,m} := \frac{1}{\beta_{l,0}\,\mathcal{C}_{l,m}^{l,m_s}}\Big[&\mathcal{C}_{l,m}^{l-1,m_s}\,\beta_{l,-1}\,F_{l-1,m-m_s} + \mathcal{C}_{l,m}^{l+1,m_s}\,\beta_{l,1}\,G_{l+1,m-m_s} \\ &- f_{l,m}\,\beta_{l+1,-1}\,\mathcal{C}_{l+1,m}^{l,m_s} - g_{l,m}\,\beta_{l-1,1}\,\mathcal{C}_{l-1,1}^{l,m_s}\Big]. \end{aligned} \tag{96}$$

We can similarly yield the relations for the perpendicular gradients:

$$\begin{aligned} x\,\nabla^\perp Y_l^m &= a_{l,m}^\perp\nabla^\perp Y_{l+1}^{m+1} + b_{l,m}^\perp\nabla^\perp Y_{l-1}^{m+1} + d_{l,m}^\perp\nabla^\perp Y_{l+1}^{m-1} + e_{l,m}^\perp\nabla^\perp Y_{l-1}^{m-1} \\ &\qquad + h_{l,m}^\perp\nabla Y_l^{m+1} + j_{l,m}^\perp\nabla Y_l^{m-1}, \qquad (97)\\ y\,\nabla^\perp Y_l^m &= i\Big[-a_{l,m}^\perp\nabla^\perp Y_{l+1}^{m+1} - b_{l,m}^\perp\nabla^\perp Y_{l-1}^{m+1} + d_{l,m}^\perp\nabla^\perp Y_{l+1}^{m-1} + e_{l,m}^\perp\nabla^\perp Y_{l-1}^{m-1} \\ &\qquad - h_{l,m}^\perp\nabla Y_l^{m+1} + j_{l,m}^\perp\nabla Y_l^{m-1}, \qquad (98)\\ z\,\nabla^\perp Y_l^m &= f_{l,m}^\perp\nabla^\perp Y_{l+1}^m + g_{l,m}^\perp\nabla^\perp Y_{l-1}^m + k_{l,m}^\perp\nabla Y_l^m, \qquad (99) \end{aligned}$$

where it can be shown that

$$\begin{gathered} a_{l,m}^\perp = a_{l,m}^*, \quad b_{l,m}^\perp = b_{l,m}^*, \quad d_{l,m}^\perp = d_{l,m}^*, \quad e_{l,m}^\perp = e_{l,m}^*, \\ f_{l,m}^\perp = f_{l,m}^*, \quad g_{l,m}^\perp = g_{l,m}^*, \quad h_{l,m}^\perp = h_{l,m}^*, \quad j_{l,m}^\perp = j_{l,m}^*, \quad k_{l,m}^\perp = k_{l,m}^*, \end{gathered} \tag{100}$$

where * denotes the complex conjugate.

3.3 Jacobi matrices

Define $\nabla\mathbb{P}$ as the column vector

$$\nabla\mathbb{P} = \begin{bmatrix}\nabla\mathbb{P}_0\\ \nabla\mathbb{P}_1\\ \vdots\end{bmatrix}, \quad \text{where} \quad \nabla\mathbb{P}_l = \begin{bmatrix}\nabla Y_l^{-l}\\ \nabla^\perp Y_l^{-l}\\ \vdots\\ \nabla Y_l^l\\ \nabla^\perp Y_l^l\end{bmatrix} \quad \forall\, l\in\mathbb{N}_0. \tag{101}$$

This notation could be confusing. I'd say use either $T\mathbb{P}$ or $\mathbb{P}^T$

Then we can define the Jacobi operators $J^x_\nabla, J^y_\nabla, J^z_\nabla$ by

$$J^x_\nabla \nabla\mathbb{P} = x\nabla\mathbb{P}, \quad J^y_\nabla \nabla\mathbb{P} = y\nabla\mathbb{P}, \quad J^z_\nabla \nabla\mathbb{P} = z\nabla\mathbb{P}, \tag{102}$$

where each entry ∇Y_l^m, $\nabla^\perp Y_l^m$ is pseudo-treatedas a single element of the vector $\nabla\mathbb{P}$.

I don't know what this means

The Jacobi matrices have the following form:

$$J^x_\nabla = \begin{bmatrix} B^x_0 & A^x_0 & & & & \\ C^x_1 & B^x_1 & A^x_1 & & & \\ & C^x_2 & B^x_2 & A^x_2 & & \\ & & C^x_3 & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{103}$$

$$J^y_\nabla = \begin{bmatrix} B^y_0 & A^y_0 & & & & \\ C^y_1 & B^y_1 & A^y_1 & & & \\ & C^y_2 & B^y_2 & A^y_2 & & \\ & & C^y_3 & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{104}$$

$$J^z_\nabla = \begin{bmatrix} B^z_0 & A^z_0 & & & & \\ C^z_1 & B^z_1 & A^z_1 & & & \\ & C^z_2 & B^z_2 & A^z_2 & & \\ & & C^z_3 & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{105}$$

where for $l \in \mathbb{N}_0$,

$$A^x_l := \begin{bmatrix} d_{l,-l} & 0 & 0 & 0 & a_{l,-l} & & & & \\ & d^\perp_{l,-l} & 0 & 0 & 0 & a_{l,-l} & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & d_{l,l} & 0 & 0 & 0 & a_{l,l} & \\ & & & & d^\perp_{l,l} & 0 & 0 & 0 & a^\perp_{l,-l} \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)}, \tag{106}$$

$$
B_l^x := \begin{bmatrix}
0 & 0 & 0 & h_{l,-l} & & & & \\
0 & 0 & h_{l,-l}^{\perp} & 0 & & & & \\
0 & j_{l,-l+1} & 0 & 0 & 0 & h_{l,-l+1} & & \\
j_{l,-l+1}^{\perp} & 0 & 0 & 0 & h_{l,-l+1}^{\perp} & 0 & & \\
 & \ddots & & \ddots & & \ddots & & \\
 & & \ddots & & \ddots & & \ddots & \\
 & & 0 & j_{l,l-1} & 0 & 0 & 0 & h_{l,l-1} \\
 & & j_{l,l-1}^{\perp} & 0 & 0 & 0 & h_{l,l-1}^{\perp} & 0 \\
 & & & & 0 & j_{l,l} & 0 & 0 \\
 & & & & j_{l,l}^{\perp} & 0 & 0 & 0
\end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)}, \tag{107}
$$

$$
C_l^x := \begin{bmatrix}
b_{l,-l} & & & & & \\
0 & b_{l,-l}^{\perp} & & & & \\
0 & 0 & \ddots & & & \\
0 & 0 & \ddots & \ddots & & \\
e_{l,-l+2} & 0 & \ddots & \ddots & b_{l,l-2} & \\
 & e_{l,-l+2}^{\perp} & \ddots & \ddots & 0 & b_{l,l-2}^{\perp} \\
 & & \ddots & \ddots & 0 & 0 \\
 & & & \ddots & 0 & 0 \\
 & & & & e_{l,l} & 0 \\
 & & & & & e_{l,l}^{\perp}
\end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l-1)} \quad (l \neq 0), \tag{108}
$$

$$
A_l^y := \begin{bmatrix}
-d_{l,-l} & 0 & 0 & 0 & a_{l,-l} & & & & \\
 & -d_{l,-l}^{\perp} & 0 & 0 & 0 & a_{l,-l} & & & \\
 & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & -d_{l,l} & 0 & 0 & 0 & a_{l,l} & \\
 & & & & -d_{l,l}^{\perp} & 0 & 0 & 0 & a_{l,-l}^{\perp}
\end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)}, \tag{109}
$$

$$B_l^y := \begin{bmatrix} 0 & 0 & 0 & h_{l,-l} & & & & \\ 0 & 0 & h_{l,-l}^{\perp} & 0 & & & & \\ 0 & -j_{l,-l+1} & 0 & 0 & 0 & h_{l,-l+1} & & \\ -j_{l,-l+1}^{\perp} & 0 & 0 & 0 & h_{l,-l+1}^{\perp} & 0 & & \\ & \ddots & & \ddots & & \ddots & & \\ & & \ddots & & \ddots & & \ddots & \\ & & 0 & -j_{l,l-1} & 0 & 0 & 0 & h_{l,l-1} \\ & & -j_{l,l-1}^{\perp} & 0 & 0 & 0 & h_{l,l-1}^{\perp} & 0 \\ & & & & 0 & -j_{l,l} & 0 & 0 \\ & & & & -j_{l,l}^{\perp} & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)}, \tag{110}$$

$$C_l^y := \begin{bmatrix} b_{l,-l} & & & & & \\ 0 & b_{l,-l}^{\perp} & & & & \\ 0 & 0 & \ddots & & & \\ 0 & 0 & \ddots & \ddots & & \\ -e_{l,-l+2} & 0 & \ddots & \ddots & b_{l,l-2} & \\ & -e_{l,-l+2}^{\perp} & \ddots & \ddots & 0 & b_{l,l-2}^{\perp} \\ & & \ddots & \ddots & 0 & 0 \\ & & & \ddots & 0 & 0 \\ & & & & -e_{l,l} & 0 \\ & & & & & -e_{l,l}^{\perp} \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l-1)} \quad (l \neq 0), \tag{111}$$

$$A_l^z := \begin{bmatrix} 0 & 0 & f_{l,-l} & & & & & & \\ & & & f_{l,-l}^{\perp} & & & & & \\ & & & & \ddots & & & & \\ & & & & & f_{l,l} & & & \\ & & & & & & f_{l,l}^{\perp} & 0 & 0 \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+3)}, \tag{112}$$

$$\tag{113}$$

$$B_l^z := \begin{bmatrix} 0 & k_{l,-l} & & & \\ k_{l,-l}^{\perp} & 0 & & & \\ & & \ddots & & \\ & & & 0 & k_{l,l} \\ & & & k_{l,l}^{\perp} & 0 \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l+1)}, \tag{114}$$

$$C_l^z := \begin{bmatrix} 0 & & & & \\ 0 & & & & \\ g_{l,-l+1} & & & & \\ & g_{l,-l+1}^{\perp} & & & \\ & & \ddots & & \\ & & & g_{l,l-1} & \\ & & & & g_{l,l-1}^{\perp} \\ & & & & 0 \\ & & & & 0 \end{bmatrix} \in \mathbb{R}^{2(2l+1)\times 2(2l-1)} \quad (l \neq 0). \tag{115}$$

$$\tag{116}$$

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

Combining each system in (102) we can write, for (x, y, z) on the unit sphere, the tridiagonal-block system

Is 0_3 wrong below?

$$\left[\begin{array}{c|c|c|c} I_2 & & & \\ \hline & I_6 & & \\ \hline & B_1^x - xI_6 & A_1^x & \\ & B_1^y - yI_6 & A_1^y & \\ & B_1^z - zI_6 & A_1^z & \\ \hline & C_2^x & B_2^x - xI_{10} & A_2^x \\ & C_2^y & B_2^y - yI_{10} & A_2^y \\ & C_2^z & B_2^z - zI_{10} & A_2^z \\ \hline & & C_3^x & \ddots \quad \ddots \\ & & C_3^y & \\ & & C_3^z & \\ \hline & & & \ddots \end{array}\right] \nabla\mathbb{P} = \begin{bmatrix} \underline{0}_3 \\ \underline{0}_3 \\ \nabla\mathbb{P}_1 \\ \underline{0}_3 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}, \tag{117}$$

where I_{2l+1} is the $(2l+1) \times (2l+1)$ identity matrix. For clarity we again treat each sub-vector $\nabla Y_l^m, \nabla^{\perp} Y_l^m$ of $\nabla\mathbb{P}$ in the matrix-vector multiplication as a single element.

Let us define the joint matrices that comprise each block. For each $l \in \mathbb{N}$:

$$A_l := \begin{bmatrix} A_l^x \\ A_l^y \\ A_l^z \end{bmatrix} \in \mathbb{R}^{6(2l+1)\times 2(2l+3)}, \quad C_l := \begin{bmatrix} C_l^x \\ C_l^y \\ C_l^z \end{bmatrix} \in \mathbb{R}^{6(2l+1)\times 2(2l-1)} \quad (l \neq 1), \tag{118}$$

$$B_l := \begin{bmatrix} B_l^x \\ B_l^y \\ B_l^z \end{bmatrix} \in \mathbb{R}^{6(2l+1)\times 2(2l+1)}, \quad G_l(x,y,z) := \begin{bmatrix} xI_{2l+1} \\ yI_{2l+1} \\ zI_{2l+1} \end{bmatrix} \in \mathbb{R}^{6(2l+1)\times 2(2l+1)}. \tag{119}$$

Then our system simply becomes

$$\begin{bmatrix} I_2 & & & & \\ 0 & I_6 & & & \\ D_1^T C_1 & D_1^1(B_1 - G_1) & A_1 & & \\ & D_2^T C_2 & \ddots & \ddots & \\ & & \ddots & & \end{bmatrix} \mathbb{P} = \begin{bmatrix} \underline{0}_3 \\ \underline{0}_3 \\ \nabla \mathbb{P}_1 \\ \underline{0}_3 \\ \\ \vdots \end{bmatrix}. \tag{120}$$

For each $l \in \mathbb{N}$ let D_l^T be any matrix that is a left inverse of A_l, i.e. such that $D_l^T A_l = I_{2(2l+3)}$. Multiplying our system by the preconditioner matrix that is given by the block diagonal matrix of the D_l^T's, we obtain the lower triangular system

$$\begin{bmatrix} I_2 & & & & \\ 0 & I_6 & & & \\ D_1^T C_1 & D_1^T(B_1 - G_1) & I_{10} & & \\ & D_2^T C_2 & \ddots & \ddots & \\ & & \ddots & & \end{bmatrix} \mathbb{P} = \begin{bmatrix} \underline{0}_3 \\ \underline{0}_3 \\ \nabla \mathbb{P}_1 \\ \underline{0}_3 \\ \\ \vdots \end{bmatrix}. \tag{121}$$

Expanding this we can find a three-term recurrence relation for each $\nabla \mathbb{P}_{l+1}$ in terms of the previous two sub-vectors $\nabla\mathbb{P}_l$ and $\nabla\mathbb{P}_{l-1}$:

$$
\begin{cases}
\nabla\mathbb{P}_0(x,y,z) := \underline{0}_6 \\[2ex]
\nabla\mathbb{P}_1(x,y,z) := \begin{bmatrix} \nabla Y_1^{-1}(x,y,z) \\ \nabla^\perp Y_1^{-1}(x,y,z) \\ \nabla Y_1^{0}(x,y,z) \\ \nabla^\perp Y_1^{0}(x,y,z) \\ \nabla Y_1^{1}(x,y,z) \\ \nabla^\perp Y_1^{1}(x,y,z) \end{bmatrix} \\[2ex]
\nabla\mathbb{P}_{l+1}(x,y,z) = -D_l^T[B_l - G_l(x,y,z)]\nabla\mathbb{P}_l(x,y,z) - D_l^T C_l\,\nabla\mathbb{P}_{l-1}(x,y,z), \quad l \in \mathbb{N}.
\end{cases}
\tag{122}
$$

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

$$
D_l^T = \begin{bmatrix} \hat{A}_l^{x,y} & 0_{2(2l+3)\times 2(2l+1)} \end{bmatrix} \in \mathbb{R}^{2(2l+3)\times 6(2l+1)} \tag{123}
$$

where $0_{2(2l+3)\times 2(2l+1)}$ the zero matrix in $\mathbb{R}^{2(2l+3)\times 2(2l+1)}$, and $\hat{A}_l^{x,y} \in \mathbb{R}^{2(2l+3)\times 4(2l+1)}$ is the left inverse of the matrix $\begin{bmatrix} A_l^x \\ A_l^y \end{bmatrix}$, given by

$$
\hat{A}_l^{x,y} = \begin{bmatrix}
\frac{1}{2d_{l,-l}} & 0 & \dots & 0 & -\frac{i}{2d_{l,-l}} & 0 & \dots & & & \\
0 & \frac{1}{2d^\perp_{l,-l}} & 0 & \dots & 0 & -\frac{i}{2d^\perp_{l,-l}} & 0 & \dots & & \\
 & & \ddots & & & & \ddots & & & \\
\vdots & & & \ddots & & & & \ddots & & \\
 & & & & \frac{1}{2d_{l,l}} & 0 & \dots & 0 & -\frac{i}{2d_{l,l}} & \\
 & & & & & \frac{1}{2d^\perp_{l,l}} & 0 & \dots & 0 & -\frac{i}{2d^\perp_{l,l}} \\
0 & \dots & \frac{1}{2a_{l,l-1}} & 0 & \dots & 0 & \frac{i}{2a_{l,l-1}} & 0 & 0 & 0 \\
0 & \dots & 0 & \frac{1}{2a^\perp_{l,l-1}} & 0 & \dots & 0 & \frac{i}{2a^\perp_{l,l-1}} & 0 & 0 \\
0 & \dots & \dots & 0 & \frac{1}{2a_{l,l}} & 0 & \dots & 0 & \frac{i}{2a_{l,l}} & 0 \\
0 & \dots & \dots & & 0 & \frac{1}{2a^\perp_{l,l}} & 0 & \dots & 0 & \frac{i}{2a^\perp_{l,l}}
\end{bmatrix}.
\tag{124}
$$

3.5 Deriving matrices and calculations for certain operations

Define $\hat{\boldsymbol{k}}$ as the unit outward normal vector at the point on the sphere (x, y, z), so that

$$\hat{\boldsymbol{k}} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}. \tag{125}$$

Let $S := \{\mathbf{x} := (x, y, z) \quad | \quad ||\mathbf{x}|| = 1\}$ be the unit sphere in $\mathbb{R}^3$ and let T_x^S denote the tangent space at the point $\mathbf{x} \in S$. Further, let $\mathbf{u}(x, y, z)$, $\mathbf{v}(x, y, z)$ be two vector valued functions for (x, y, z) on the unit sphere with values in the tangent space (representing the tangential velocity of a flow for example) and let $h(x, y, z)$ be a scalar function on the sphere.

Then,

$$\mathbf{u} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m], \tag{126}$$

$$\mathbf{v} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [v_{l,m} \nabla Y_l^m + v_{l,m}^{\perp} \nabla^{\perp} Y_l^m], \tag{127}$$

$$h = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} h_{l,m} Y_l^m, \tag{128}$$

for some real coefficients $u_{l,m}, u_{l,m}^{\perp}, v_{l,m}, v_{l,m}^{\perp}, h_{l,m}$. Define the vectors of these coefficients as

$$\mathbf{u}^c = \begin{bmatrix} \mathbf{u}_0^c \\ \mathbf{u}_1^c \\ \vdots \end{bmatrix}, \quad \mathbf{v}^c = \begin{bmatrix} \mathbf{v}_0^c \\ \mathbf{v}_1^c \\ \vdots \end{bmatrix}, \quad \mathbf{h}^c = \begin{bmatrix} \mathbf{h}_0^c \\ \mathbf{h}_1^c \\ \vdots \end{bmatrix}, \tag{129}$$

where

$$\mathbf{u}_l^c = \begin{bmatrix} u_{l,-l} \\ u_{l,-l}^{\perp} \\ \vdots \\ u_{l,l} \\ u_{l,l}^{\perp} \end{bmatrix}, \quad \mathbf{v}_l^c = \begin{bmatrix} v_{l,-l} \\ v_{l,-l}^{\perp} \\ \vdots \\ v_{l,l} \\ v_{l,l}^{\perp} \end{bmatrix}, \quad \mathbf{h}_l^c = \begin{bmatrix} h_{l,-l} \\ \vdots \\ h_{l,l} \end{bmatrix}, \quad \forall l \in \mathbb{N}_0 \tag{130}$$

.

Then, for large enough $N \in \mathbb{N}$ we have that

$$\mathbf{u} \approx \sum_{l=0}^{N} \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m], \tag{131}$$

$$\mathbf{v} \approx \sum_{l=0}^{N} \sum_{m=-l}^{l} [v_{l,m} \nabla Y_l^m + v_{l,m}^{\perp} \nabla^{\perp} Y_l^m], \tag{132}$$

$$h \approx \sum_{l=0}^{N} \sum_{m=-l}^{l} h_{l,m} Y_l^m, \tag{133}$$

and so we define the truncated coefficient vectors for some $N \in \mathbb{N}$ as

$$\mathbf{u}^c = \begin{bmatrix} \mathbf{u}_0^c \\ \mathbf{u}_1^c \\ \vdots \\ \mathbf{u}_N^c \end{bmatrix}, \quad \mathbf{v}^c = \begin{bmatrix} \mathbf{v}_0^c \\ \mathbf{v}_1^c \\ \vdots \\ \mathbf{v}_N^c \end{bmatrix}, \quad \mathbf{h}^c = \begin{bmatrix} \mathbf{h}_0^c \\ \mathbf{h}_1^c \\ \vdots \\ \mathbf{h}_N^c \end{bmatrix}. \tag{134}$$

We note that

$$\nabla^{\perp} Y_l^m = \hat{\boldsymbol{k}} \times \nabla Y_l^m, \quad \forall\, l \in \mathbb{N}_0,\ m \in \mathbb{Z} \text{ s.t. } |m| \leq l. \tag{135}$$

Isn't there a name for this Operator? Maybe "Unit Curl Operator"?

3.5.1 Operator for "$\hat{\boldsymbol{k}}\times$ "

$$\hat{\boldsymbol{k}} \times \mathbf{u} = \hat{\boldsymbol{k}} \times \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m] \tag{136}$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \hat{\boldsymbol{k}} \times \nabla Y_l^m + u_{l,m}^{\perp} \hat{\boldsymbol{k}} \times \nabla^{\perp} Y_l^m] \tag{137}$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \hat{\boldsymbol{k}} \times \nabla Y_l^m + u_{l,m}^{\perp} \hat{\boldsymbol{k}} \times (\hat{\boldsymbol{k}} \times \nabla Y_l^m)] \tag{138}$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \nabla^{\perp} Y_l^m + u_{l,m}^{\perp} ((\hat{\boldsymbol{k}} \cdot \nabla^{\perp} Y_l^m) \hat{\boldsymbol{k}} - (\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}) \nabla Y_l^m)] \tag{139}$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [u_{l,m} \nabla^{\perp} Y_l^m - u_{l,m}^{\perp} \nabla Y_l^m)]. \tag{140}$$

$$\tag{141}$$

Thus the operator matrix for the cross product from the left by the normal unit vector at the point (x, y, z) is given by

$$K = \begin{bmatrix} 0 & -1 & & & & \\ 1 & 0 & & & & \\ & & 0 & -1 & & \\ & & 1 & 0 & & \\ & & & & \ddots & \\ & & & & & \ddots \end{bmatrix} \quad \in \quad \mathbb{R}^{2(N+1)^2 \times 2(N+1)^2}. \tag{142}$$

so that $K\mathbf{u}^c$ gives the vector of coefficients for for expansion of $\hat{\boldsymbol{k}} \times \mathbf{u}$ in the vector spherical harmonic basis (up to degree N).

3.5.2 Operator for Div

$$\begin{aligned} \nabla \cdot \mathbf{u} &= \nabla \cdot \Big(\sum_l \sum_{m=-l}^{l} [u_{l,m} \nabla Y_l^m + u_{l,m}^{\perp} \nabla^{\perp} Y_l^m] \Big) && (143) \\ &= \sum_l \sum_{m=-l}^{l} [u_{l,m}\, \Delta Y_l^m + u_{l,m}^{\perp} \nabla \cdot (\hat{\boldsymbol{k}} \times \nabla Y_l^m)] && (144) \\ &= \sum_l \sum_{m=-l}^{l} u_{l,m}\, \Delta Y_l^m && (145) \\ &= \sum_l \sum_{m=-l}^{l} -u_{l,m}\, l(l+1) Y_l^m, && (146) \\ & && (147) \end{aligned}$$

using the fact that

$$\Delta Y_l^m(x, y, z) = -l(l+1) Y_l^m(x, y, z), \quad \forall\, l \in \mathbb{N}_0,\ m \in \mathbb{Z} \text{ s.t. } |m| \leq l. \tag{148}$$

Thus, the operator matrix for the divergence of a vector in the tangent space is

$$D = \begin{bmatrix} -l(l+1)|_{l=0} & 0 & & & & & & & \\ & & -l(l+1)|_{l=1} & 0 & & & & & \\ & & & & -l(l+1)|_{l=1} & 0 & & & \\ & & & & & & -l(l+1)|_{l=1} & 0 & \\ & & & & & & & & \ddots \end{bmatrix} \tag{149}$$

$$= \begin{bmatrix} 0 & 0 & & & & & & & \\ & & -2 & 0 & & & & & \\ & & & & -2 & 0 & & & \\ & & & & & & -2 & 0 & \\ & & & & & & & & \ddots \end{bmatrix} \quad \in \quad \mathbb{R}^{(N+1)^2 \times 2(N+1)^2}, \tag{150}$$

so that $D\mathbf{u}^c$ gives the vector of coefficients of the expansion for $\nabla \cdot u$ in the spherical harmonic basis.

3.5.3 Operator for Grad

$$\nabla h = \nabla \Big(\sum_l \sum_{m=-l}^{l} h_{l,m} Y_l^m \Big) \tag{151}$$

$$= \sum_l \sum_{m=-l}^{l} h_{l,m} \nabla Y_l^m \tag{152}$$

Thus, the operator matrix for the gradient of a scalar function on the sphere is

$$G = \begin{bmatrix} \tilde{G}_0 & & & \\ & \tilde{G}_1 & & \\ & & \tilde{G}_2 & \\ & & & \ddots \end{bmatrix} \quad \in \quad \mathbb{R}^{2(N+1)^2 \times (N+1)^2}, \tag{153}$$

where

$$\tilde{G}_l = \begin{bmatrix} 1 & & & \\ 0 & & & \\ & 1 & & \\ & 0 & & \\ & & 1 & \\ & & 0 & \\ & & & \ddots \end{bmatrix} \quad \in \quad \mathbb{R}^{2(2l+1) \times (2l+1)}, \tag{154}$$

so that $G\mathbf{h}^c$ gives the vector of coefficients of the expansion for ∇h in the tangent space (vector spherical harmonic) basis.

3.5.4 Dot products

We consider the general case that $\mathbf{u}$ is expanded up to order $N_1 \in \mathbb{N}$ and $\mathbf{v}$ is expanded up to order $N_2 \in \mathbb{N}$, i.e.

$$\mathbf{u}^c = \begin{bmatrix} \mathbf{u}_0^c \\ \mathbf{u}_1^c \\ \vdots \\ \mathbf{u}_{N_1}^c \end{bmatrix}, \quad \mathbf{v}^c = \begin{bmatrix} \mathbf{v}_0^c \\ \mathbf{v}_1^c \\ \vdots \\ \mathbf{v}_{N_2}^c \end{bmatrix}. \tag{155}$$

Let (x, y, z) lie on the unit sphere and let $l = 1$, $m \in -1, 0, 1$ and define $\tilde{N} := N_1 + N_2$. Then

$$\nabla Y_l^m(x, y, z) \cdot \mathbf{v}(x, y, z) = (\mathbf{b}^c)^T\, \mathbb{P}(x, y, z) \tag{156}$$

where

$$\mathbb{P} := \begin{bmatrix} \mathbb{P}_0 \\ \mathbb{P}_1 \\ \mathbb{P}_2 \\ \vdots \\ \mathbb{P}_{N_2} \end{bmatrix}, \quad \mathbb{P}_l := \begin{bmatrix} Y_l^{-l} \\ \vdots \\ Y_l^l \end{bmatrix}, \tag{157}$$

for some coefficient vector $\mathbf{b}^c \in \mathbb{R}^{(N_2+1)^2}$. In other words, the dot product of one of the $l = 1$ tangent space's orthogonal polynomials with a vector valued function on the unit sphere can naturally be written as an expansion in the scalar spherical harmonic OP basis. Similarly,

$$\nabla^\perp Y_l^m(x, y, z) \cdot \mathbf{v}(x, y, z) = (\mathbf{b}^{\perp c})^T\, \mathbb{P}(x, y, z) \tag{158}$$

for some coefficient vector $\mathbf{b}^{\perp c} \in \mathbb{R}^{(N_2+2)^2}$.

Then,

$$\mathbf{b}^c = J_{l,m}\, \mathbf{v}^c, \quad \mathbf{b}^{\perp c} = J_{l,m}^\perp\, \mathbf{v}^c \tag{159}$$

where $J_{l,m}$, $J^{\perp}_{l,m}$ are (operator) matrices for the dot product with $\nabla Y_l^m(x,y,z)$ and $\nabla^{\perp} Y_l^m(x,y,z)$ respectively. Each $J_{l,m}$, $J^{\perp}_{l,m}$ will have the $(\tilde{N} \times N_2)$ block structure:

$$
\begin{array}{c|c|c|c}
1\times 6 & 1\times 10 & & \\
\hline
3\times 6 & 3\times 10 & 3\times 14 & \\
\hline
5\times 6 & 5\times 10 & 5\times 14 & \ddots \\
\hline
 & 7\times 10 & 7\times 14 & \ddots \\
\hline
 & & \ddots & \ddots
\end{array}
\tag{160}
$$

i.e. a `BandedBlockBandedMatrix(J, (rows, cols), (2,1), (?,?))` [note: I am not sure what the sub-block bands should be] where

```
rows = 1:2:2N+1
cols = 6:4:2(2N_2+1).
```

Define

$$
T_0^{\mathbb{P}} := 0, \quad T_1^{\mathbb{P}} := \begin{bmatrix} J_{1,-1} \\ J^{\perp}_{1,-1} \\ J_{1,0} \\ J^{\perp}_{1,0} \\ J_{1,1} \\ J^{\perp}_{1,1} \end{bmatrix}. \tag{161}
$$

Then by linearity of the dot product, we can use the recurrence relation (122) for $\nabla \mathbb{P}_l$ to gain a recurrence for $T_l^{\mathbb{P}}$:

$$
T_{l+1}^{\mathbb{P}} = -D_l^T [B_l - G_l(J^x, J^y, J^z)]\, T_l^{\mathbb{P}} - D_l^T C_l\, T_{l-1}^{\mathbb{P}}, \quad l \in \{1, \dots, N_1 - 1\}, \tag{162}
$$

where J^x, J^y, J^z are the $\tilde{N} \times \tilde{N}$ Jacobi operator matrices for multiplication of the scalar spherical harmonic basis by x, y, z respectively. We then have that for each $l \in 1, \dots, N_1$,

$$
T_l^{\mathbb{P}} := \begin{bmatrix} J_{l,-l} \\ J^{\perp}_{l,-l} \\ \vdots \\ J_{l,l} \\ J^{\perp}_{l,l} \end{bmatrix}. \tag{163}
$$

Then,

$$
\mathbf{u}(x,y,z) \cdot \mathbf{v}(x,y,z) = (\mathbf{b}^c)^T\, \mathbb{P}(x,y,z) \tag{164}
$$

where $\mathbf{b}^c \in \mathbb{R}^{(\tilde{N}+1)^2}$ and is given by

$$\mathbf{b}^c = \Big(\sum_{l=0}^{N_1} \sum_{m=-l}^{l} [u_{l,m} J_{l,m} + u_{l,m}^{\perp} J_{l,m}^{\perp}] \Big) \mathbf{v}^c. \tag{165}$$