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A Fortran Module For Vector Spherical Harmonics Computations

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ABSTRACT

The *Tensor Spherical Harmonics* (TSH) are crucial ingredients to robust representation of curvilinear coordinates and reference frames in mathematical physics. A special limit of the TSH called the *Vector Spherical Harmonics* (VSH) are the focus of this manuscript. Fast and efficient calculation of the VSH is required for many high-performance computing applications, including for magneto-hydrodynamics (MHD), quantum mechanical systems, and other spectral codes.

Contents

1. BACKGROUND

The tensor spherical harmonics (TSH) are irreducible tensor products of scalar spherical harmonics $Y_L^M(\Omega)$ and spin functions χ_S (Edmonds 1960). Throughout this text we adopt the normalization for Y_l^m as follows:

$$Y_l^m = \sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi} \tag{1}$$

An arbitrary TSH may be written as a sum over non-zero eigenstates and projections as

$$\mathbf{Y}_{JM}^{LS} = \sum_{m,\sigma} C_{LmS\sigma}^{JM} Y_L^M \chi_{S_\sigma}, \tag{2}$$

where the non-negative integer or half-integer S indicates the tensor rank, and $C_{a\alpha b\beta}^{c\gamma}$ is a Clebsch-Gordan coefficient. Applications in physics commonly require the evaluation of integrals of products of scalar (*i.e.*, $S = 0$) spherical harmonics, and their angular spatial derivatives, on the 3D unit sphere (Rädler 1973; Winch 1974; Barrera et al. 1985). Such a problem may be cast in terms of the $S = 1$ vector spherical harmonics with the generalised form

$$S(\vec{n},\vec{m};\vec{\lambda}) = \int_{4\pi} \mathrm{d}\Omega\, \left[\left(\mathbf{Y}_{n_1m_1}^{(\lambda_1)} \times \mathbf{Y}_{n_2m_2}^{(\lambda_2)}\right) \times \mathbf{Y}_{n_3m_3}^{(\lambda_3)} \times ... \times \mathbf{Y}_{n_Nm_N}^{(\lambda_N)}\right] \cdot \mathbf{Y}_{n'm'}^{(\lambda')*}. \tag{3}$$

In Eq. (3) components of the vector spherical harmonics (VSH) of order n and azimuthal degree m, written as $\mathbf{Y}_{nm}^L$, are encoded into the polar-VSH (pVSH) via the orientation index λ. These pVSH are denoted by $\mathbf{Y}_{nm}^{(\lambda)}$, following the notation of Akheizer & Berestetskii (1965) and Varshalovich et al. (1988) which will be used henceforth. Here the VSH are constructed in the spherical

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basis, such that the unit vectors $\chi_{1\mu} = \hat{e}_\mu$ correspond to the longitudinal direction ($\mu = \lambda = -1$) and the transverse directions ($\mu = 0, +1$; $\lambda = 0, +1$) relative to the radial unit normal $\hat{r} = \vec{r}/r$. These conventions are chosen for situations where it is beneficial to decompose the system into poloidal and toroidal components (Krause & Rädler 1980), . The VSH and pVSH components are related to the scalar spherical harmonics Y_n^m and their spatial derivatives (in polar coordinates) by

$$\hat{r} Y_n^m = \mathbf{Y}_{nm}^{(-1)} = \frac{1}{\sqrt{2n+1}} \left[\sqrt{n} \mathbf{Y}_{nm}^{n-1} - \sqrt{n+1} \mathbf{Y}_{nm}^{n+1} \right] \tag{4}$$

$$\frac{1}{\sqrt{\Lambda_n}} \widehat{\mathbf{L}} Y_n^m = -\frac{i}{\sqrt{\Lambda_n}} \hat{r} \times \vec{\nabla}_\omega Y_n^m = \mathbf{Y}_{nm}^{(0)} = \mathbf{Y}_{nm}^n \tag{5}$$

$$\frac{1}{\sqrt{\Lambda_n}} \vec{\nabla}_\omega Y_n^m = \mathbf{Y}_{nm}^{(+1)} = \frac{1}{\sqrt{2n+1}} \left[\sqrt{n+1} \mathbf{Y}_{nm}^{n-1} + \sqrt{n} \mathbf{Y}_{nm}^{n+1} \right]. \tag{6}$$

The VSH and pVSH independently constitute complete orthonormal bases, and are therefore candidates for describing vector fields in poloidal-toroidal decomposition. Here $\sqrt{\Lambda_n} = \sqrt{n(n+1)}$ is the eigenvalue for the angular momentum operator $\widehat{\mathbf{L}}$.

2. IDENTITIES INVOLING VECTOR SPHERICAL HARMONICS

$$\vec{\nabla} \times \left(f(r) \mathbf{Y}_{nm}^{(-1)} \right) = -\frac{i}{R_n} f(r) \mathbf{Y}_{nm}^{(0)} \tag{7}$$

$$\vec{\nabla} \times \left(f(r) \mathbf{Y}_{nm}^{(+1)} \right) = \frac{i}{r} \frac{d}{dr} \left(r f(r) \right) \mathbf{Y}_{nm}^{(0)} \tag{8}$$

$$\vec{\nabla} \times \left(f(r) \mathbf{Y}_{nm}^{(0)} \right) = \frac{i}{R_n} \left[f(r) \mathbf{Y}_{nm}^{(-1)} + \frac{d}{dr} \left(R_n f(r) \right) \mathbf{Y}_{nm}^{(+1)} \right] \tag{9}$$

$$\begin{aligned}
\mathbf{Y}_{kl}^{(+1)} \cdot \mathbf{Y}_{nm}^{(+1)} &= \frac{1}{\sqrt{\Lambda_k \Lambda_n}} \vec{\nabla}_\omega Y_k^l \cdot \vec{\nabla}_\omega Y_n^m \\
&= \sum_L (-1)^{k+n+L-1} \frac{(2k+1)(2n+1)}{\sqrt{4\pi(2L+1)}} \begin{Bmatrix} k & n & L \\ n & k & 1 \end{Bmatrix} C_{k0n0}^{L0} C_{klnm}^{Ll+m} Y_L^{l+m} \\
&= \sum_L \frac{2(2k+1)(2n+1)}{\sqrt{4\pi(2L+1)}} \sqrt{\frac{(2k-1)!(2n-1)!}{(2k+2)!(2n+2)!}} (\Lambda_k + \Lambda_n - \Lambda_L) C_{k0n0}^{L0} C_{klnm}^{Ll+m} Y_L^{l+m} \\
&= \sum_L \frac{\Lambda_k + \Lambda_n - \Lambda_L}{2\sqrt{\Lambda_k \Lambda_n}} I_{klnm}^{Ll+m} Y_L^{l+m}
\end{aligned} \tag{10}$$

$$\begin{aligned}
\mathbf{Y}_{kl}^{(0)} \cdot \mathbf{Y}_{nm}^{(0)} &= \frac{-1}{\sqrt{\Lambda_k \Lambda_n}} \vec{\nabla}_\omega Y_k^l \cdot \vec{\nabla}_\omega Y_n^m \\
&= -\sum_L \frac{\Lambda_k + \Lambda_n - \Lambda_L}{2\sqrt{\Lambda_k \Lambda_n}} I_{klnm}^{Ll+m} Y_L^{l+m}
\end{aligned} \tag{11}$$

$$\begin{aligned}
\mathbf{Y}_{kl}^{(+1)} \cdot \mathbf{Y}_{nm}^{(0)} &= \frac{-i}{\sqrt{\Lambda_k \Lambda_n}} \vec{\nabla}_\omega Y_k^l \cdot \left(\hat{r} \times \vec{\nabla}_\omega Y_n^m \right) \\
&= (2n+1)(-1)^{n+k+L+1} \sum_L C_{klnm}^{LM} Y_L^M \times \\
&\quad \times \left[\sqrt{\frac{(k+1)(2k-1)}{4\pi(2L+1)}} \begin{Bmatrix} k-1 & n & L \\ n & k & 1 \end{Bmatrix} C_{k-10n0}^{L0} + \sqrt{\frac{k(2k+3)}{4\pi(2L+1)}} \begin{Bmatrix} k+1 & n & L \\ n & k & 1 \end{Bmatrix} C_{k+10n0}^{L0} \right] \\
&= \sum_L \sqrt{(k+n+L+2)(k-n+L+1)(k+n-L+1)(-k+n+L)} C_{k+10n0}^{L0} C_{klnm}^{LM} Y_L^M \times \\
&\quad \times \frac{1}{2} \sqrt{\frac{2n+1}{4\pi(2L+1)n(n+1)}} \left[\sqrt{\frac{k+1}{k(2k+1)}} + \sqrt{\frac{k}{(2k+1)(k+1)}} \right]
\end{aligned}$$

$$=\frac{-i}{\sqrt{\Lambda_k\Lambda_n}}\sum_L J^{LM}_{nmkl}Y^M_L \tag{12}$$

$$\begin{aligned}\mathbf{Y}^{(-1)}_{kl}\cdot\mathbf{Y}^{(-1)}_{nm} =& Y^l_kY^m_n\\ =&\frac{1}{\sqrt{(2k+1)(2n+1)}}\sum_L(-1)^{n+k+L+1}\sqrt{\frac{(2k+1)(2n+1)}{4\pi(2L+1)}}C^{LM}_{klnm}Y^M_L\times\\ &\times\sum_{\nu,\sigma=\pm1}\sqrt{(2k+\sigma+1)\,(2n+\nu+1)\left(k+\sigma+\frac{1}{2}\right)\left(n+\nu+\frac{1}{2}\right)}\begin{Bmatrix}k+\sigma & n+\nu & L\\ n & k & 1\end{Bmatrix}C^{L0}_{k+\sigma 0 n+\nu 0}\\ =&\sum_L I^{LM}_{klnm}Y^M_L\end{aligned} \tag{13}$$

In many cases the above relations must be modifed when a VSH component is conjugated, *e.g.* for $\vec{\nabla}_\omega Y^l_k\cdot\vec{\nabla}_\omega Y^{m*}_n$. The complex conjugates of the VSH and pVSH are well-known:

$$\mathbf{Y}^{L*}_{JM}=(-1)^{J+L+M+1}\mathbf{Y}^L_{J-M} \tag{14}$$

$$\mathbf{Y}^{(\lambda)*}_{JM}=(-1)^{\lambda+M+1}\mathbf{Y}^{(\lambda)}_{J-M}. \tag{15}$$

In combination with the VSH scalar products in Eqs. (11–13), it may be directly shown that

$$\begin{aligned}\mathbf{Y}^{(+1)}_{kl}\cdot\mathbf{Y}^{(+1)*}_{nm} =&\frac{1}{\sqrt{\Lambda_k\Lambda_n}}\vec{\nabla}_\omega Y^l_k\cdot\vec{\nabla}_\omega Y^{m*}_n\\ =&\sum_L\frac{\Lambda_k+\Lambda_n-\Lambda_L}{2\sqrt{\Lambda_k\Lambda_n}}I^{nm}_{klLm-l}Y^{m-l*}_L\end{aligned} \tag{16}$$

$$\begin{aligned}\mathbf{Y}^{(0)}_{kl}\cdot\mathbf{Y}^{(0)*}_{nm} =&\frac{1}{\sqrt{\Lambda_k\Lambda_n}}\vec{\nabla}_\omega Y^l_k\cdot\vec{\nabla}_\omega Y^{m*}_n\\ =&\sum_L\frac{\Lambda_k+\Lambda_n-\Lambda_L}{2\sqrt{\Lambda_k\Lambda_n}}I^{nm}_{klLm-l}Y^{m-l*}_L\end{aligned} \tag{17}$$

$$\begin{aligned}\mathbf{Y}^{(+1)}_{kl}\cdot\mathbf{Y}^{(0)*}_{nm} =&\frac{i}{\sqrt{\Lambda_k\Lambda_n}}\vec{\nabla}_\omega Y^l_k\cdot\left(\hat{r}\times\vec{\nabla}_\omega Y^{m*}_n\right)\\ =&\frac{i}{\sqrt{\Lambda_k\Lambda_n}}\sum_L J^{nm}_{klLm-l}Y^{m-l*}_L\end{aligned} \tag{18}$$

$$\begin{aligned}\mathbf{Y}^{(0)}_{nm}\cdot\mathbf{Y}^{(+1)*}_{kl} =&\frac{-i}{\sqrt{\Lambda_k\Lambda_n}}\left(\hat{r}\times\vec{\nabla}_\omega Y^m_n\right)\cdot\vec{\nabla}_\omega Y^{l*}_k\\ =&\frac{i}{\sqrt{\Lambda_k\Lambda_n}}\sum_L J^{kl}_{nmLl-m}Y^{l-m*}_L\end{aligned} \tag{19}$$

$$\begin{aligned}\mathbf{Y}^{(-1)}_{kl}\cdot\mathbf{Y}^{(-1)*}_{nm} =&Y^l_kY^{m*}_n\\ =&\sum_L I^{nm}_{klLm-l}Y^{m-l*}_L\end{aligned} \tag{20}$$

Considering these results, it becomes trivial to verify the quadratic angular couplings presented in Geppert & Wiebicke (1991), which were presented in the context of the magnetic Hall drift in the neutron star crust.

3. NOTATION AND IDENTITIES INVOLVING CLEBSCH-GORDAN, 3-J, AND 6-J COEFFICIENTS

$$I^{n\,m}_{k'\,l'\,k\,l} = \sqrt{\frac{(2k'+1)(2k+1)}{4\pi(2n+1)}}C^{n\,0}_{k'\,0\,k\,0}C^{nm}_{k'\,l'\,k\,l} \tag{21}$$

$$J^{nm}_{k'l'kl} = -\frac{i}{2}\sqrt{\frac{(2k'+1)(2k+1)}{4\pi(2n+1)}}\sqrt{(k'+k+n+2)(k+n-k')(k'+k-n+1)(k'-k+n+1)} \times C^{n0}_{k'+10k0}C^{nm}_{k'l'kl} \tag{22}$$

$$\begin{Bmatrix} a & b & a+b \\ d & e & f \end{Bmatrix} = (-1)^{a+b+d+e}\sqrt{\frac{(2a)!(2b)!(a+b+d+e+1)!(a+b-d+e)!(a+b+d-e)!}{(2a+2b+1)!(-a-b+d+e)!(a+e-f)!(a-e+f)!(a+e+f+1)!}} \times \sqrt{\frac{(-a+e+f)!(-b+d+f)!}{(b+d-f)!(b-d+f)!(b+d+f+1)!}} \tag{23}$$

$$\begin{Bmatrix} a & a & 1 \\ b & b & f \end{Bmatrix} = 2(-1)^{a+b+f+1}\sqrt{\frac{(2a-1)!(2b-1)!}{(2a+2)!(2b+2)!}}(a(a+1)+b(b+1)-f(f+1)) \tag{24}$$

$$C^{n0}_{k0p-10} = -C^{n0}_{k0p+10}\sqrt{\frac{(k+n+p+2)(k+p-n+1)(k+n-p)(-k+n+p+1)}{(k+n+p+1)(k+p-n)(k+n-p+1)(-k+p+n)}} \tag{25}$$

$$C^{L0}_{k+10n0} = C^{L0}_{k0n+10}\sqrt{\frac{(k-n+L)(-k+n+L+1)}{(k-n+L+1)(-k+n+L)}} \tag{26}$$

4. NUMERICAL MODULE

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