Spherical Lighting with Spherical Harmonics Hessian Supplemental Document

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This supplemental document explains the details of derivations in Sec. 3.2 of the main paper and the first/second derivatives of spherical harmonics (SH) using solid spherical harmonics (SSH).

1 Gradient of ZH coefficient $\nabla\tilde{L}_l$

The ZH coefficient $\tilde{L}_l$ is represented with:

$$\tilde{L}_l(\mathbf{x}) = \sqrt{\frac{\pi}{2l+1}}(P_{l-1}(\alpha) - P_{l+1}(\alpha)), \tag{1}$$

$$\alpha = \cos(a(\mathbf{x})), \tag{2}$$

$$a(\mathbf{x}) = \arcsin\left(r/\|\mathbf{y}-\mathbf{x}\|\right), \tag{3}$$

The gradient of $\tilde{L}_l(\mathbf{x})$ is calculated as:

$$\nabla\tilde{L}_l(\mathbf{x}) = \sqrt{\frac{\pi}{2l+1}}(\nabla P_{l-1}(\alpha) - \nabla P_{l+1}(\alpha)) \tag{4}$$

The gradient of Legendre polynomial $\nabla P_l(\alpha)$ is calculated as:

$$\nabla P_l(\alpha) = P_l'(\alpha)\nabla\alpha = P_l'(\alpha)(-\sin(a(\mathbf{x}))\nabla a(\mathbf{x})) \tag{5}$$

By substituting Eq. (5) into Eq. (4), $\nabla\tilde{L}_l(\mathbf{x})$ is calculated as:

$$\nabla P_l(\alpha) = \sqrt{\frac{\pi}{2l+1}}\sin(a(\mathbf{x}))\nabla a(\mathbf{x})(P_{l+1}'(\alpha) - P_{l-1}'(\alpha)). \tag{6}$$

By using the following identity $(2l+1)P_l(x) = P_{l+1}'(x) - P_{l-1}'(x)$, $\nabla P_l(\alpha)$ is calculated as:

$$\nabla P_l(\alpha) = \sqrt{\frac{\pi}{2l+1}}\sin(a(\mathbf{x}))\nabla a(\mathbf{x})(2l+1)P_l(\alpha) \tag{7}$$

$$= \sqrt{(2l+1)\pi}\sin(a(\mathbf{x}))\nabla a(\mathbf{x})P_l(\alpha). \tag{8}$$

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2 SH gradient using SSH gradient

The derivative of solid spherical harmonics (SSH) $\tilde{Y}_l^m = r^l Y_l^m$ with respect to x is calculated as:

$$\partial_x\tilde{Y}_l^m = lr^{l-1}(x/r)Y_l^m + r^l\partial_x Y_l^m = lxr^{l-2}Y_l^m + r^l\partial_x Y_l^m.$$

Since we are interested in the derivative $\nabla\tilde{Y}_l^m$ for unit directions, we substitute $r=1$ and the gradient $\nabla\tilde{Y}_l^m$ is simplified as:

$$\nabla\tilde{Y}_l^m(\omega) = lY_l^m(\omega)\omega + \nabla Y_l^m(\omega). \tag{9}$$

Cartesian derivatives of Q_l^m, s_m, and c_m are simply represented as the following equations [Bigi et al. 2023]:

$$\begin{aligned}
\partial_x Q_l^m &= xQ_{l-1}^{m+1},\\
\partial_y Q_l^m &= yQ_{l-1}^{m+1},\\
\partial_z Q_l^m &= (l+m)Q_{l-1}^m,\\
\partial_x s_m &= ms_{m-1},\\
\partial_y s_m &= mc_{m-1},\\
\partial_x c_m &= mc_{m-1},\\
\partial_y c_m &= -ms_{m-1}.
\end{aligned} \tag{10}$$

To simplify the notation, we define $s_m' = ms_{m-1}$ and $c_m' = mc_{m-1}$. Then the partial derivatives of s_m and c_m with respect to x and y are expressed as:

$$\begin{aligned}
\partial_x s_m &= ms_{m-1} = s_m',\\
\partial_y s_m &= mc_{m-1} = c_m',\\
\partial_x c_m &= mc_{m-1} = c_m',\\
\partial_y c_m &= -ms_{m-1} = -s_m'.
\end{aligned} \tag{11}$$

We also define the second derivatives $s_m'' = m(m-1)s_{m-2}$ and $c_m'' = m(m-1)c_{m-2}$ as:

$$\begin{aligned}
\partial_{xx} s_m &= m\partial_x s_{m-1} = m(m-1)s_{m-2} = s_m'',\\
\partial_{xy} s_m &= m\partial_x c_{m-1} = m(m-1)c_{m-2} = c_m'',\\
\partial_{yy} s_m &= m\partial_y c_{m-1} = -m(m-1)s_{m-2} = -s_m'',\\
\partial_{xx} c_m &= m\partial_x c_{m-1} = m(m-1)c_{m-2} = c_m'',\\
\partial_{xy} c_m &= -m\partial_x s_{m-1} = -m(m-1)s_{m-2} = -s_m'',\\
\partial_{yy} c_m &= -m\partial_y s_{m-1} = -m(m-1)c_{m-2} = -c_m''.
\end{aligned} \tag{12}$$

To unify the constant terms $\sqrt{2}K_l^m$ for $m \neq 0$ and K_l^0 for $m=0$, we define k_l^m as:

$$k_l^m = \begin{cases} \sqrt{2}K_l^m & m \neq 0 \\ K_l^0 & m = 0 \end{cases} \tag{13}$$

3 Derivative of SSH

By using the Cartesian derivatives in Eq. (10), the derivatives of SSH $\tilde{Y}_l^m(x,y,z)$ are simply calculated from the following recurrence formulae. For $m>0$, the derivatives of SSH are:

$$\begin{aligned}\partial_x \tilde{Y}_l^m &= k_l^m(xQ_{l-1}^{m+1}c_m + Q_l^m c_m'),\\ \partial_y \tilde{Y}_l^m &= k_l^m(yQ_{l-1}^{m+1}c_m - Q_l^m s_m'),\\ \partial_z \tilde{Y}_l^m &= k_l^m(l+m)Q_{l-1}^m c_m.\end{aligned} \tag{14}$$

For $m=0$, the derivatives of SSH are:

$$\begin{aligned}\partial_x \tilde{Y}_l^0 &= k_l^0 xQ_{l-1}^1,\\ \partial_y \tilde{Y}_l^0 &= k_l^0 yQ_{l-1}^1,\\ \partial_z \tilde{Y}_l^0 &= k_l^0 lQ_{l-1}^0.\end{aligned} \tag{15}$$

The derivatives of SSH Y_l^{-m} are:

$$\begin{aligned}\partial_x \tilde{Y}_l^{-m} &= k_l^m(xQ_{l-1}^{m+1}s_m + Q_l^m s_m'),\\ \partial_y \tilde{Y}_l^{-m} &= k_l^m(yQ_{l-1}^{m+1}s_m + Q_l^m c_m'),\\ \partial_z \tilde{Y}_l^{-m} &= k_l^m(l+m)Q_{l-1}^m s_m.\end{aligned} \tag{16}$$

4 Second Derivative of SSH

The second derivatives of SSH $\tilde{Y}_l^m(x,y,z)$ are represented with the following equations.

$$\begin{aligned}\partial_{xx}\tilde{Y}_l^m &= k_l^m(x^2Q_{l-2}^{m+2}c_m + Q_{l-1}^{m+1}(2xc_m' + c_m) + Q_l^m c_m''),\\ \partial_{xy}\tilde{Y}_l^m &= k_l^m(xyQ_{l-2}^{m+2}c_m + Q_{l-1}^{m+1}(yc_m' - xs_m') - Q_l^m s_m''),\\ \partial_{xz}\tilde{Y}_l^m &= k_l^m(l+m)(xQ_{l-2}^{m+1}c_m + Q_{l-1}^m c_m'),\\ \partial_{yy}\tilde{Y}_l^m &= k_l^m(y^2Q_{l-2}^{m+2}c_m - Q_{l-1}^{m+1}(2ys_m' - c_m) - Q_l^m c_m''),\\ \partial_{yz}\tilde{Y}_l^m &= k_l^m(l+m)(yQ_{l-2}^{m+1}c_m - Q_{l-1}^m s_m'),\\ \partial_{zz}\tilde{Y}_l^m &= k_l^m(l+m)(l+m-1)Q_{l-2}^m c_m.\end{aligned} \tag{17}$$

For $m=0$, the second derivatives of $\tilde{Y}_l^0$ are represented as:

$$\begin{aligned}\partial_{xx}\tilde{Y}_l^0 &= k_l^0(x^2Q_{l-2}^2 + Q_{l-1}^1),\\ \partial_{xy}\tilde{Y}_l^0 &= k_l^0 xyQ_{l-2}^2,\\ \partial_{xz}\tilde{Y}_l^0 &= k_l^0 lxQ_{l-2}^1,\\ \partial_{yy}\tilde{Y}_l^0 &= k_l^0(y^2Q_{l-2}^2 + Q_{l-1}^1),\\ \partial_{yz}\tilde{Y}_l^0 &= k_l^0 lyQ_{l-2}^1,\\ \partial_{zz}\tilde{Y}_l^0 &= k_l^0 l(l-1)Q_{l-2}^0.\end{aligned} \tag{18}$$

The second derivative of $\tilde{Y}_l^{-m}$ are calculated as:

$$\begin{aligned}\partial_{xx}\tilde{Y}_l^{-m} &= k_l^m(x^2Q_{l-2}^{m+2}s_m + Q_{l-1}^{m+1}(2xs_m' + s_m) + Q_l^m s_m''),\\ \partial_{xy}\tilde{Y}_l^{-m} &= k_l^m(xyQ_{l-2}^{m+2}s_m + Q_{l-1}^{m+1}(xc_m' + ys_m') + Q_l^m c_m''),\\ \partial_{xz}\tilde{Y}_l^{-m} &= k_l^m(l+m)(xQ_{l-2}^{m+1}s_m + Q_{l-1}^m s_m'),\\ \partial_{yy}\tilde{Y}_l^{-m} &= k_l^m(y^2Q_{l-2}^{m+2}s_m + Q_{l-1}^{m+1}(2yc_m' + s_m) - Q_l^m s_m''),\\ \partial_{yz}\tilde{Y}_l^{-m} &= k_l^m(l+m)(yQ_{l-2}^{m+1}s_m + Q_{l-1}^m c_m'),\\ \partial_{zz}\tilde{Y}_l^{-m} &= k_l^m(l+m)(l+m-1)Q_{l-2}^m s_m.\end{aligned} \tag{19}$$

5 Explicit Formulae for Second Derivatives of SH

The second derivatives of SH Y_l^m for positive m are calculated as:

$$\begin{aligned}\partial_{xx}Y_l^m &= (k_l^mQ_{l-2}^{m+2}c_m - l(l-2)Y_l^m)x^2 + (2k_l^mQ_{l-1}^{m+1}c_m')x\\ &\quad - 2l(\partial_x Y_l^m)x + (k_l^mQ_{l-1}^{m+1}c_m - lY_l^m) + k_l^mQ_l^m c_m'',\\ \partial_{yy}Y_l^m &= (k_l^mQ_{l-2}^{m+2}c_m - l(l-2)Y_l^m)y^2 - (2k_l^mQ_{l-1}^{m+1}s_m')y\\ &\quad - 2l(\partial_y Y_l^m)y + (k_l^mQ_{l-1}^{m+1}c_m - lY_l^m) - k_l^mQ_l^m c_m'',\\ \partial_{xy}Y_l^m &= (k_l^mQ_{l-2}^{m+2}c_m - l(l-2)Y_l^m)xy - (k_l^mQ_{l-1}^{m+1}s_m')x\\ &\quad + (k_l^mQ_{l-1}^{m+1}c_m')y - lx(\partial_y Y_l^m) - ly(\partial_x Y_l^m) - k_l^mQ_l^m s_m'',\\ \partial_{xz}Y_l^m &= ((l+m)k_l^mQ_{l-2}^{m+1}c_m - l(l-2)Y_l^m z)x + (l+m)k_l^mQ_{l-1}^m c_m'\\ &\quad - lx(\partial_z Y_l^m) - lz(\partial_x Y_l^m),\\ \partial_{yz}Y_l^m &= ((l+m)k_l^mQ_{l-2}^{m+1}c_m - l(l-2)Y_l^m z)y - (l+m)k_l^mQ_{l-1}^m s_m',\\ \partial_{zz}Y_l^m &= -l(l-2)Y_l^m z^2 - 2l(\partial_x Y_l^m)z + (l+m)(l+m-1)k_l^mQ_{l-2}^m\\ &\quad - lY_l^m.\end{aligned} \tag{20}$$

The second derivatives of SH Y_l^{-m} are calculated as:

$$\begin{aligned}\partial_{xx}Y_l^{-m} &= (k_l^mQ_{l-2}^{m+2}s_m - l(l-2)Y_l^{-m})x^2 + (2k_l^mQ_{l-1}^{m+1}s_m')x\\ &\quad - 2l(\partial_x Y_l^{-m})x + (k_l^mQ_{l-1}^{m+1}s_m - lY_l^{-m}) + k_l^mQ_l^m s_m'',\\ \partial_{yy}Y_l^{-m} &= (k_l^mQ_{l-2}^{m+2}s_m - l(l-2)Y_l^{-m})y^2 + (2k_l^mQ_{l-1}^{m+1}c_m')y\\ &\quad - 2l(\partial_y Y_l^{-m})y + (k_l^mQ_{l-1}^{m+1}s_m - lY_l^{-m}) - k_l^mQ_l^m s_m'',\\ \partial_{xy}Y_l^{-m} &= (k_l^mQ_{l-2}^{m+2}s_m - l(l-2)Y_l^{-m})xy - (k_l^mQ_{l-1}^{m+1}c_m')x\\ &\quad + (k_l^mQ_{l-1}^{m+1}s_m')y - lx(\partial_y Y_l^{-m}) - ly(\partial_x Y_l^{-m}) + k_l^mQ_l^m c_m'',\\ \partial_{xz}Y_l^{-m} &= ((l+m)k_l^mQ_{l-2}^{m+1}s_m - l(l-2)Y_l^{-m} z)x + (l+m)k_l^mQ_{l-1}^m s_m'\\ &\quad - lx(\partial_z Y_l^{-m}) - lz(\partial_x Y_l^{-m}),\\ \partial_{yz}Y_l^{-m} &= ((l+m)k_l^mQ_{l-2}^{m+1}s_m - l(l-2)Y_l^{-m} z)y + (l+m)k_l^mQ_{l-1}^m c_m',\\ \partial_{zz}Y_l^{-m} &= -l(l-2)Y_l^{-m} z^2 - 2l(\partial_x Y_l^{-m})z + (l+m)(l+m-1)k_l^mQ_{l-2}^m\\ &\quad - lY_l^{-m}.\end{aligned} \tag{21}$$

As shown in Eqs. (20) and (21), $\partial_{xx}Y_l^m$, $\partial_{xy}Y_l^m$, $\partial_{yy}Y_l^m$, $\partial_{xx}Y_l^{-m}$, $\partial_{xy}Y_l^{-m}$, and $\partial_{yy}Y_l^{-m}$ have common components that can be reused. By defining the following terms, these second derivatives can be computed as:

$$\begin{aligned}a_l^m &= k_l^mQ_{l-2}^{m+2}c_m - l(l-2)Y_l^m,\\ b_l^m &= k_l^mQ_{l-1}^{m+1}c_m',\\ c_l^m &= k_l^mQ_{l-1}^{m+1}s_m',\\ d_l^m &= k_l^mQ_l^m c_m'',\\ e_l^m &= k_l^mQ_l^m s_m'',\\ f_l^m &= k_l^mQ_{l-1}^{m+1}c_m - lY_l^m,\\ g_l^m &= k_l^mQ_{l-2}^{m+2}s_m - l(l-2)Y_l^{-m},\\ h_l^m &= k_l^mQ_{l-1}^{m+1}s_m - lY_l^{-m}.\end{aligned} \tag{22}$$

$$\begin{aligned}
\partial_{xx} Y_l^m &= a_l^m x^2 + 2(b_l^m - l\partial_x Y_l^m)x + d_l^m + f_l^m \\
\partial_{yy} Y_l^m &= a_l^m y^2 - 2(c_l^m + l\partial_y Y_l^m)y - d_l^m + f_l^m \\
\partial_{xy} Y_l^m &= a_l^m xy - (c_l^m + l\partial_y Y_l^m)x + (b_l^m - l\partial_x Y_l^m)y - e_l^m \\
\partial_{xx} Y_l^{-m} &= g_l^m x^2 + 2(c_l^m - l\partial_x Y_l^{-m})x + e_l^m + h_l^m \\
\partial_{yy} Y_l^{-m} &= g_l^m y^2 + 2(b_l^m - l\partial_y Y_l^{-m})y - e_l^m + h_l^m \\
\partial_{xy} Y_l^{-m} &= g_l^m xy + (b_l^m - l\partial_y Y_l^{-m})x + (c_l^m - l\partial_x Y_l^{-m})y + d_l^m
\end{aligned} \tag{23}$$

6 Spherical Harmonics Hessian using Spherical Coordinate Derivative Method

This section explains a derivation of SH Hessian based on spherical coordinate derivative (SCD) method. We first review the derivation of SH gradient $\partial_\theta Y_l^m$ and $\partial_\phi Y_l^m$ proposed by [Mézières et al. 2022]. The derivative $\partial_\phi Y_l^m$ with respect to the azimuthal angle ϕ is calculated as:

$$\partial_\phi Y_l^m = \begin{cases} -mY_l^{-m}(\theta,\phi) & m<0 \\ 0 & m=0 \\ -mY_l^{-m}(\theta,\phi) & m>0 \end{cases}, \tag{24}$$

The derivative $\partial_\theta Y_l^m$ with respect to θ is represented as:

$$\partial_\theta Y_l^m = \begin{cases} \sqrt{2}K_l^{-m}\partial_\theta P_l^{-m}\sin(-m\theta) & m<0 \\ K_l^0\partial_\theta P_l(\cos\theta) & m=0 \\ \sqrt{2}K_l^m\partial_\theta P_l^m\cos(m\theta) & m>0 \end{cases}, \tag{25}$$

To evaluate the derivative $\partial_\theta Y_l^m$, the derivative of associate Legendre polynomial $\partial_\theta P_l^m$ is required. To compute $\partial_\theta P_l^m$, Mezieres et al. derived the following equation:

$$\frac{\partial_\theta P_l^m(\cos\theta)}{\sin^m\theta} = \frac{P_l^m(\cos\theta)}{\sin^m\theta}\frac{m\cos\theta}{\sin\theta} + \partial_\theta\left(\frac{P_l^m(\cos\theta)}{\sin^m\theta}\right) \tag{26}$$

By defining $q_l^m = P_l^m(\cos\theta)/\sin^m\theta$ and $t_l^m = \partial_\theta(P_l^m(\cos\theta)/\sin^m\theta)$, Eq. (26) is rewritten as:

$$\frac{\partial_\theta P_l^m(\cos\theta)}{\sin^m\theta} = q_l^m\frac{m\cos\theta}{\sin\theta} + t_l^m. \tag{27}$$

As described in our paper and shown in the following equations, SCD method, by definition, suffers from the division by $\sin\theta$ shown in q_l^m itself and $m\cos\theta/\sin\theta$. q_l^m and t_l^m are calculated via the recurrence formulae (please refer to [Mézières et al. 2022]).

6.1 Second derivative of SH with respect to spherical coordinate (θ,ϕ)

We derive the second derivatives of SH $\partial_{\theta\theta} Y_l^m$, $\partial_{\theta\phi} Y_l^m$, and $\partial_{\phi\phi} Y_l^m$ by differentiating Eqs. (24) and (25). $\partial_{\theta\phi} Y_l^m$ and $\partial_{\phi\phi} Y_l^m$ can be computed easily by using the first derivative of SH $\partial_\theta Y_l^m$ as:

$$\partial_{\theta\phi} Y_l^m = \begin{cases} -m\partial_\theta Y_l^{-m}(\theta,\phi) & m<0 \\ 0 & m=0 \\ -m\partial_\theta Y_l^{-m}(\theta,\phi) & m>0 \end{cases}, \tag{28}$$

$$\partial_{\phi\phi} Y_l^m = \begin{cases} -m^2\partial_\theta Y_l^m(\theta,\phi) & m\neq 0 \\ 0 & m=0 \end{cases}, \tag{29}$$

On the other hand, $\partial_{\theta\theta} Y_l^m$ requires the second derivative of associated Legendre polynomial $\partial_{\theta\theta} P_l^m$ as:

$$\partial_{\theta\theta} Y_l^m = \begin{cases} \sqrt{2}K_l^{-m}\partial_{\theta\theta} P_l^{-m}\sin(-m\theta) & m<0 \\ K_l^0\partial_{\theta\theta} P_l(\cos\theta) & m=0 \\ \sqrt{2}K_l^m\partial_{\theta\theta} P_l^m\cos(m\theta) & m>0 \end{cases}. \tag{30}$$

By differentiating $\partial_\theta P_l^m(\cos\theta)$ and dividing $\sin^m\theta$ in the same way as the previous methods [Mézières et al. 2022; Sloan 2013], the second derivative $\partial_{\theta\theta} Y_l^m$ is calculated as:

$$\frac{\partial_{\theta\theta} P_l^m(\cos\theta)}{\sin^m\theta} = m(m-1)\frac{\cos^2\theta}{\sin^2\theta}q_l^m - mq_l^m + 2m\frac{\cos\theta}{\sin\theta}t_l^m + s_l^m, \tag{31}$$

where s_l^m is defined as:

$$s_l^m = \partial_\theta t_l^m = \partial_{\theta\theta}\left(\frac{P_l^m(\cos\theta)}{\sin^m\theta}\right). \tag{32}$$

s_l^m is calculated by the following recurrence formulae:

$$\begin{aligned}
s_m^m &= 0, \\
s_{m+1}^m &= -(2m+1)(\cos\theta q_l^m), \\
s_l^m &= \frac{(2l-1)(\cos\theta(s_{l-1}^m - q_l^m) - 2\sin\theta t_{l-1}^m) - (l+m-1)s_{l-2}^m}{l-m}.
\end{aligned} \tag{33}$$

The second derivatives with respect to Cartesian coordinates are represented with those with spherical coordinates as:

$$\begin{aligned}
\partial_{xx} Y_l^m &= \partial_{xx}\theta\partial_\theta Y_l^m + (\partial_x\theta)^2\partial_{\theta\theta} Y_l^m \\
&\quad + 2\partial_x\theta\partial_x\phi\partial_{\theta\phi} Y_l^m + \partial_{xx}\phi\partial_\phi Y_l^m + (\partial_x\phi)^2\partial_{\phi\phi} Y_l^m. \\
\partial_{xy} Y_l^m &= \partial_{xy}\theta\partial_\theta Y_l^m + \partial_x\theta\partial_y\theta\partial_{\theta\theta} Y_l^m + \partial_x\theta\partial_y\phi\partial_{\theta\phi} Y_l^m \\
&\quad + \partial_x\phi\partial_y\theta\partial_{\theta\phi} Y_l^m + \partial_x\phi\partial_y\phi\partial_{\phi\phi} Y_l^m + \partial_{xy}\phi\partial_\phi Y_l^m. \\
\partial_{xz} Y_l^m &= \partial_{xy}\theta\partial_\theta Y_l^m + \partial_x\theta\partial_z\theta\partial_{\theta\theta} Y_l^m + \partial_x\phi\partial_z\theta\partial_{\theta\phi} Y_l^m
\end{aligned} \tag{34}$$

$$\begin{aligned}
\partial_{yy} Y_l^m &= \partial_{yy}\theta\partial_\theta Y_l^m + (\partial_y\theta)^2\partial_{\theta\theta} Y_l^m \\
&\quad + 2\partial_y\theta\partial_y\phi\partial_{\theta\phi} Y_l^m + \partial_{yy}\phi\partial_\phi Y_l^m + (\partial_y\phi)^2\partial_{\phi\phi} Y_l^m. \\
\partial_{yz} Y_l^m &= \partial_{yz}\theta\partial_\theta Y_l^m + \partial_\theta\partial_y\theta\partial_{\theta\theta} Y_l^m + \partial_z\theta\partial_y\phi\partial_{\theta\phi} Y_l^m \\
\partial_{zz} Y_l^m &= \partial_{zz}\theta\partial_\theta Y_l^m + \partial_z\theta\partial_z\theta\partial_{\theta\theta} Y_l^m
\end{aligned} \tag{35}$$

The second derivatives of spherical coordinates (θ,ϕ) with respect to Cartesian coordinates (x,y,z) are calculated as:

$$\begin{aligned}
\partial_{xx}\theta &= \frac{z(-2x^4 - x^2y^2 + y^4 + y^2z^2)}{(x^2+y^2)^{3/2}(x^2+y^2+z^2)^2} \\
\partial_{xy}\theta &= -\frac{xyz(3x^2+3y^2+z^2)}{(x^2+y^2)^{3/2}(x^2+y^2+z^2)^2} \\
\partial_{xz}\theta &= \frac{x(x^2+y^2-z^2)}{\sqrt{x^2+y^2}(x^2+y^2+z^2)^2} \\
\partial_{yy}\theta &= \frac{z(x^4+x^2(z^2-y^2)-2y^4)}{(x^2+y^2)^{3/2}(x^2+y^2+z^2)^2} \\
\partial_{yz}\theta &= \frac{y(x^2+y^2-z^2)}{\sqrt{x^2+y^2}(x^2+y^2+z^2)^2} \\
\partial_{zz}\theta &= \frac{2z(x^2+y^2)}{\sqrt{x^2+y^2}(x^2+y^2+z^2)^2}
\end{aligned} \tag{36}$$

$$\begin{aligned}
\partial_{xx}\phi &= \frac{2xy}{(x^2+y^2)^2} \\
\partial_{xy}\phi &= \frac{y^2-x^2}{(x^2+y^2)^2} \\
\partial_{xz}\phi &= 0 \\
\partial_{yy}\phi &= -\frac{2xy}{(x^2+y^2)^2} \\
\partial_{yz}\phi &= 0
\end{aligned} \tag{37}$$

The above derivatives are the elements of the conversion matrix from spherical coordinates to Cartesian coordinates for the Hessian matrix calculation.

7 Generated C++ codes to compute SH, SH gradient, and SH Hessian

We have implemented a code generator for C++ to compute SH Y_l^m, SH gradient ∇Y_l^m, and SH Hessian $\mathcal{H}Y_l^m$ using the recurrence formulae described in the submitted paper. Here, we show a part of the generated code for fourth-order SH. The codes for higher orders are included in the supplemental material. As shown in the code, SH gradient ∇Y_l^m and SH Hessian $\mathcal{H}Y_l^m$ are calculated by reusing Q_l^m (variable qlm in the code).

Figs. 2 compare the numbers of (a) multiplication operations and (b) addition/subtraction operations that are counted in the generated codes with different SH orders. As shown in Fig. 2(a), the number of multiplication operations in the SCD method is 1.5× compared with that of our method, since the SCD method requires the matrix multiplication of the gradient from the spherical coordinate to the Cartesian coordinate.

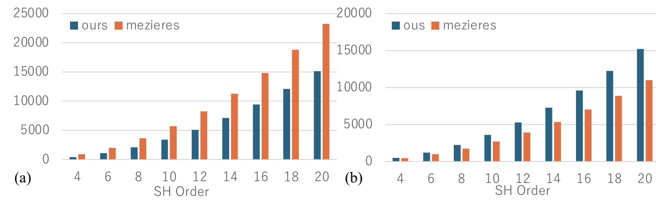

Fig. 2. The numbers of (a) multiplication operations and (b) addition/subtraction operations between our method and SCD method.

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```cpp
 // x, y, z are normalized coordinates of the evaluation direction
#pragma once
template< size_t L > void shhessian( const float x, const float y, const float z, float *ylm, std::array< glm::vec3, L * L > &glm, std::array< glm::mat3, L * L > &hlm );
template<> void shhessian<  4 >( const float x, const float y, const float z, float *ylm, std::array< glm::vec3,  16 > &glm, std::array< glm::mat3,  16 > &hlm )
{
    float c0, c1, cm, cs, s0, s1, sm, ss, tmp, tmp0, tmp1, tmp2, tmp3, tmp4, tmp5, tmp6, tmp7, lx, ly, lz;
    const float x2 = x * x;
    const float y2 = y * y;
    const float z2 = z * z;
    const float xy = x * y;
    const float xz = x * z;
    const float yz = y * z;
    std::array< float,  16 > qlm {};
    //zonal harmonics(m=0)
    ylm[   0 ] = qlm[   0 ] = 0.2820947917738781f;
    ylm[   2 ] = qlm[   4 ] = 0.4886025119029199f * z;
    ylm[   6 ] = qlm[   8 ] = 0.9461746957575601f * z2 - 0.3153915652525200f;
    ylm[  12 ] = qlm[  12 ] = 1.9720265943665387f * z * ylm[   6 ] - 1.0183501544346309f * ylm[   2 ];
    c0 = x; s0 = y; c1 = 1; s1 = 0;
    //m = 001
    qlm[   5 ] = -0.4886025119029200f;
    ylm[   3 ] = qlm[   5 ] * c0;
    ylm[   1 ] = qlm[   5 ] * s0;
    qlm[   9 ] = -1.0925484305920792f * z;
    ylm[   7 ] = qlm[   9 ] * c0;
    ylm[   5 ] = qlm[   9 ] * s0;
    qlm[  13 ] = -2.2852289973223292f * z2 + 0.4570457994644658f;
    ylm[  13 ] = qlm[  13 ] * c0;
    ylm[  11 ] = qlm[  13 ] * s0;
    s1 = s0; c1 = c0; c0 = x * c1 - y * s1; s0 = y * c1 + x * s1;
    //m = 002
    qlm[  10 ] = 0.5462742152960396f;
    ylm[   8 ] = qlm[  10 ] * c0;
    ylm[   4 ] = qlm[  10 ] * s0;
    qlm[  14 ] = 1.4453057213202773f * z;
    ylm[  14 ] = qlm[  14 ] * c0;
    ylm[  10 ] = qlm[  14 ] * s0;
    s1 = s0; c1 = c0; c0 = x * c1 - y * s1; s0 = y * c1 + x * s1;
    //m = 003
    qlm[  15 ] = -0.5900435899266435f;
    ylm[  15 ] = qlm[  15 ] * c0;
    ylm[   9 ] = qlm[  15 ] * s0;
    //calculate gradient and hessian
    glm[   0 ] = {};
    hlm[   0 ] = glm::mat3( 0.f );
    lx = x; ly = y; lz = z;
    glm[   2 ].x = - x * ylm[   2 ];
    glm[   2 ].y = - y * ylm[   2 ];
    glm[   2 ].z = - z * ylm[   2 ] + 0.4886025119029199f;
    hlm[   2 ][ 0 ][ 0 ] = - ( ( 1 - x2 ) * ylm[   2 ] + 2 * x * glm[   2 ].x );
    hlm[   2 ][ 0 ][ 1 ] = - ( - xy * ylm[   2 ] + y * glm[   2 ].x + x * glm[   2 ].y );
    hlm[   2 ][ 0 ][ 2 ] = - ( - xz * ylm[   2 ] + z * glm[   2 ].x + x * glm[   2 ].z );
    hlm[   2 ][ 1 ][ 0 ] = hlm[   2 ][ 0 ][ 1 ];
    hlm[   2 ][ 1 ][ 1 ] = - ( ( 1 - y2 ) * ylm[   2 ] + 2 * y * glm[   2 ].y );
    hlm[   2 ][ 1 ][ 2 ] = - ( - yz * ylm[   2 ] + z * glm[   2 ].y + y * glm[   2 ].z );
    hlm[   2 ][ 2 ][ 0 ] = hlm[   2 ][ 0 ][ 2 ];
    hlm[   2 ][ 2 ][ 1 ] = hlm[   2 ][ 1 ][ 2 ];
    hlm[   2 ][ 2 ][ 2 ] = - ( ( 1 - z2 ) * ylm[   2 ] + 2 * z * glm[   2 ].z );
```

Fig. 1. A part of generated C++ code to evaluate SH Y_l^m (float *ylm), SH gradient ∇Y_l^m (std::array<glm::vec3,16> glm), and SH Hessian $\mathcal{H}Y_l^m$ (std::array<glm::mat3,16> hlm).