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APM 502 Master's Portfolio Project
Spherical Harmonics

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Introduction

Spherical harmonics are the angular portion of the solution to Laplace's differential equation $\triangle u = 0$, or, equivalently, the solutions to Laplace's differential equation on the unit sphere. They form a complete orthonormal basis for functions defined on the surface of a sphere; that is, any function on the surface of a sphere can be written as a sum of spherical harmonics.

The complex spherical harmonics of degree ℓ and order m are:

$$\boldsymbol{Y_\ell^m(\theta,\phi) := \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}e^{im\phi}P_\ell^m(\cos\theta)}$$

with $\boldsymbol{P_\ell^m}$ denoting the associated Legendre functions:

$$\boldsymbol{P_\ell^m(x) = (-1)^m(1-x^2)^{m/2}\frac{1}{2^\ell \ell!}\frac{d^{(\ell+m)}}{dx^{(\ell+m)}}(x^2-1)^\ell}$$

Spherical harmonics are widely used in physics, most notably for the solution of the atomic orbitals of the hydrogen atom, from which the indicies ℓ and m are well known as the azimuthal, angular, or orbital $(\ell)$and magnetic (m) quantum numbers for atomic orbitals.

Spherical harmonics are also used to efficiently represent directional lightning, shadows, and matte reflections in computer graphics.

In this project, I will briefly review the derivation, properties, and applications of the spherical harmonics, with emphasis on their use in physics.

Notation and Preliminaries

I will generally follow the notation used by Evans 2010. In this notation, partial derivatives are denoted with either $\frac{\partial}{\partial c}$ or a coordinate subscript:

$$u_x = \frac{\partial}{\partial x}u \qquad u_{zz} = \frac{\partial^2}{\partial z^2}$$

the Laplace operator or Laplacian (the divergence of the gradient) is denoted with the symbol $\triangle$, for example the Laplacian in three dimensional Cartesian coordinates is:

$$\triangle u = u_{xx} + u_{yy} + u_{zz}$$

and functions are generally written without arguments, when doing so isn't unclear, for example, I will write $\triangle u$ instead of $\triangle u(r, \theta, \phi)$.

Because spherical harmonics originated in and often appear in physics, I will use the notation for spherical coordinates that is common in physics, as shown in Figure 1, in which:

r is the distance from the origin,
ϕ is the angle from the x-axis, and
θ is the angle from the z-axis.

and therefore:

$$\begin{aligned} x &= r\sin\theta\cos\phi & r &= \sqrt{x^2+y^2+z^2} \\ y &= r\sin\theta\sin\phi & \theta &= \arccos\left(\frac{z}{r}\right) \\ z &= r\cos\theta & \phi &= \arctan\left(\frac{y}{z}\right) \end{aligned}$$

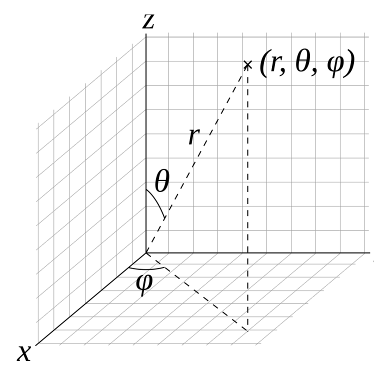

Figure 1: Spherical Coordinates (Wikipedia 2020)

With this notation, the Laplacian in spherical coordinates can be written in the following forms (among others):

$$\begin{aligned} \triangle &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\ &= \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\ &= \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \end{aligned}$$

a full derivation of which can be found in David 2007.

Solving Laplace's Equation in Spherical Coordinates

If we consider the ansatz $u = R(r)T(\theta)F(\phi)$ then the Laplacian of u is:

$$\triangle u = R_{rr}TF + \frac{2}{r}R_rTF + \frac{1}{r^2}T_{\theta\theta}RF + \frac{\cos\theta}{r^2\sin\theta}T_\theta RF + \frac{1}{r^2\sin^2\theta}F_{\phi\phi}RT = 0$$

We can isolate terms in r by multiplying by $r^2/(RTF)$:

$$r^2\frac{R_{rr}}{R} + \frac{2rR_r}{R} + \frac{T_{\theta\theta}}{T} + \frac{\cos\theta}{\sin\theta}\frac{T_\theta}{T} + \frac{1}{\sin^2\theta}\frac{F_{\phi\phi}}{F} = 0$$

and by separation of variables, with a bit of simple algebra, we obtain the system:

$$\begin{align} r^2R'' + 2rR' &= \lambda R \tag{1} \\ \frac{T_{\theta\theta}}{T} + \frac{\cos\theta}{\sin\theta}\frac{T_\theta}{T} + \frac{1}{\sin^2\theta}\frac{F_{\phi\phi}}{F} &= -\lambda \end{align}$$

Equation (1) is a Cauchy-Euler differential equation with solutions of the form $R = r^\ell$, with $\ell \geq 0$ (or else the solution is undefined at the origin). Thus $\ell(\ell-1)r^\ell + 2\ell r^\ell = \lambda r^\ell$, and therefore $\lambda = \ell(\ell-1) + 2\ell = \ell^2 + \ell = \ell(\ell+1)$, giving the updated system:

$$\begin{align} r^2R'' + 2rR' &= \ell(\ell+1)R \\ \frac{T_{\theta\theta}}{T} + \frac{\cos\theta}{\sin\theta}\frac{T_\theta}{T} + \frac{1}{\sin^2\theta}\frac{F_{\phi\phi}}{F} &= -\ell(\ell+1) \tag{2} \end{align}$$

Now we multiply equation (2) by $\sin^2\theta$ and separate again to obtain the system:

$$\begin{align} r^2R'' + 2rR' &= \ell(\ell+1)R \tag{3} \\ (\sin^2\theta)T'' + (\sin\theta\cos\theta)T' + \ell(\ell+1)(\sin^2\theta)T &= m^2T \tag{4} \\ F'' &= -m^2F \tag{5} \end{align}$$

where the separation constant m^2 was chosen, with a bit of foreknowledge, to fit the associated Legendre functions, as we shall soon see.

The third equation of this system, (5), has the well known solution $F(\phi) = Ce^{im\phi}$, and because ϕ is a periodic variable, we must have $F(\phi) = F(\phi + k2\pi)$ for any $k \in \mathbb{Z}$, so $e^{imk2\pi} = 1$ for all $k \in \mathbb{Z}$ and therefore we must also have $m \in \mathbb{Z}$, yielding the solution to the third equation:

$$F(\phi) = Ce^{im\phi}, \quad m \in \mathbb{Z}.$$

And we divide the second equation of this system, (4), by $\sin^2\theta$ and rearrange to obtain:

$$0 = T'' + \frac{\cos\theta}{\sin\theta}T' + \left[\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]T \tag{6}$$

which is the associated Legendre differential equation whose canonical solutions are the associated Legendre functions, which I will now briefly digress to introduce properly.

Legendre polynomials and associated Legendre functions

In 1785, Adrien-Marie Legendre investigated the differential equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + \ell(\ell+1)y = 0$$

and found an infinite set of solutions $y = P_n$, the Legendre polynomials (Legendre 1785), the first few of which are:

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= (3x^2 - 1)/2 \\
P_3(x) &= (5x^3 - 3x)/2
\end{aligned}$$

In 1816, Olinde Rodrigues discovered what is now called Rodrigues' formula for the Legendre polynomials:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$

A similar differential equation:

$$\frac{d}{dx}\left[(1 - x^2)\frac{dy}{dx}\right] + \left[\ell(\ell+1) - \frac{m^2}{1 - x^2}\right] y = 0 \tag{7}$$

called the *associated Legendre differential equation* was later found to have solutions related to the Legendre polynomials, named *associated Legendre functions*, and denoted:

$$P_\ell^m(x) := (-1)^m (1 - x^2)^{m/2} \frac{d^m}{dx^m}(P_\ell(x)) = y \tag{8}$$

If we expand P_ℓ in this formula using Rodrigues' formula, we obtain:

$$P_\ell^m(x) = (-1)^m (1 - x^2)^{m/2} \frac{1}{2^\ell \ell!} \frac{d^m}{dx^m} \left(\frac{d^\ell}{dx^\ell} (x^2 - 1)^\ell \right) \tag{9}$$

$$= (-1)^m (1 - x^2)^{m/2} \frac{1}{2^\ell \ell!} \frac{d^{(\ell+m)}}{dx^{(\ell+m)}} (x^2 - 1)^\ell \tag{10}$$

for $\ell \in \mathbb{Z}$ and $m \in \mathbb{Z}, -\ell \leq m \leq \ell$.

Now (6) is an instance of (7) with $x = \cos\theta$ and $y = T$, so we finally obtain:

$$T = P_\ell^m(\cos\theta)$$

and thus we arrive at the traditional formula for the spherical harmonics:

$$\boldsymbol{Y_\ell^m(\theta, \phi) := T(\theta)F(\phi) = N e^{im\phi} P_\ell^m(\cos\theta)}$$

in which the normalizing constant C has been renamed N as is traditional.

Note: Condon–Shortley phase

The factor $(-1)^m$ in (8), (9), and (10), called the Condon-Shortley phase, is not always included in the formula for the associated Legendre functions. Sometimes it is instead found in the definition of the spherical harmonics, and sometimes it is omitted entirely.

Properties

Relation between solutions for positive and negative m

The associated Legendre functions have the following property:

$$P_\ell^{-m} = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m$$

for which Westra 2020 provides a proof. From this it's easy to see that:

$$Y_\ell^{-m}(\theta,\phi) = Ne^{-im\phi}(-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\cos\theta) = e^{-2im\phi}(-1)^m \frac{(\ell-m)!}{(\ell+m)!} Y_\ell^m$$

Orthogonality and Normalization

Westra 2020 also provides a proof that the associated Legendre functions are orthogonal:

$$\int_{-1}^{1} P_k^m P_\ell^m dx = \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!}\delta_{k,\ell}$$

from which orthogonality of the spherical harmonics follows naturally, with the weighting function $\sin\theta$:

$$\begin{aligned}
\int_0^{2\pi} d\phi \int_0^{\pi} Y_k^m (Y_\ell^m)^* \sin\theta d\theta &= \int_0^{2\pi} d\phi \int_0^{\pi} (Ne^{im\phi} P_k^m(\cos\theta))(Ne^{-im\phi} P_\ell^m(\cos\theta)) \sin\theta d\theta \\
&= N^2 \int_0^{2\pi} e^{i(m-n)\phi} d\phi \int_0^{\pi} P_k^m(\cos\theta) P_\ell^m(\cos\theta) \sin\theta d\theta \\
&= 2\pi N^2 \delta_{m,n} \int_0^{\pi} P_k^m(\cos\theta) P_\ell^m(\cos\theta) \sin\theta d\theta \\
&= 2\pi N^2 \delta_{m,n} \int_{-1}^{1} P_k^m(s) P_\ell^m(s) ds \\
&= 2\pi N^2 \delta_{m,n} \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!}\delta_{k,\ell}
\end{aligned}$$

and therefore, to make the spherical harmonics orthonormal, we define

$$N = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}$$

Real spherical harmonics

Equation (5) can also be solved in the reals:

$$\begin{aligned} F(\phi) &= C && (m = 0) \\ F(\phi) &= C_1 \cos(m\phi) + C_2 \sin(m\phi) && (m > 0) \end{aligned}$$

which leads to the definition of the real spherical harmonics:

$$Y_{m\ell}(\theta,\phi) := \begin{cases} (-1)^m \sqrt{\frac{2\ell+1}{2\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} P_\ell^{|m|}(\cos\theta) \sin(|m|\phi) & (m < 0) \\ \sqrt{\frac{2\ell+1}{4\pi}} P_\ell^{|m|}(\cos\theta) & (m = 0) \\ (-1)^m \sqrt{\frac{2\ell+1}{2\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} P_\ell^{|m|}(\cos\theta) \cos(|m|\phi) & (m > 0) \end{cases}$$

which are orthonormal because of the orthogonality of sine and cosine:

$$\int_0^{2\pi} \sin(mt)\sin(nt)dt = \pi\ \delta_{m,n}$$

$$\int_0^{2\pi} \cos(mt)\cos(nt)dt = \pi\ \delta_{m,n}$$

$$\int_0^{2\pi} \sin(mt)\cos(nt)dt = 0$$

The real spherical harmonics are equivalent to:

$$Y_{m\ell}(\theta,\phi) := \begin{cases} ((-1)^m \sqrt{2}) \Im(Y_\ell^{|m|}) & (m < 0) \\ Y_\ell^{|m|} & (m = 0) \\ ((-1)^m \sqrt{2}) \Re(Y_\ell^{|m|}) & (m > 0) \end{cases}$$

Basis for functions on the unit sphere

Both the real and complex spherical harmonics provide a complete frequency-space basis for functions on the sphere. Jarosz 2008 provides an excellent review of this in Appendix B, which I summarize briefly here:

Any real valued spherical function f can be written as a linear combination of the real spherical harmonics:

$$f = \sum_\ell \sum_m c_{\ell,m} Y_{\ell,m}$$

with the coefficients determined by projection onto each real spherical harmonic:

$$c_{\ell,m} = \iint_{S^2} Y_{\ell,m} f \, dS$$

This representation is exact if ℓ is allowed to go to infinity, but this requires infinitely many coefficients. A low-frequency approximation can be obtained by limiting ℓ to a finite maximum m, using $(m+1)^2$ coefficients.

Because of the orthonormality of the spherical harmonics, we can calculate integrated products in this representation as a simple dot product of the coefficients:

$$\begin{aligned}\iint_{S^2} fg dS &= \iint_{S^2} \left[\sum_\ell \sum_m c_{\ell,m} Y_{\ell,m}\right] \left[\sum_\ell \sum_m d_{\ell,m} Y_{\ell,m}\right] dS \\ &= \iint_{S^2} \sum_\ell \sum_m c_{\ell,m} d_{\ell,m} Y_{\ell,m} dS\end{aligned}$$

And because rotations do not alter frequencies, these low-frequency approximations can be efficiently rotated with simple matrix multiplications. Maintz, Esser, and Dronskowski 2016 and Romanowski, Krukowski, and Jalbout 2008 provide algorithms for these rotations given only a rotation axis and rotation angle.

Values

The first few positive associated Legendre polynomials

$$\begin{aligned}P_0^0 &= 1 \\ P_1^0 &= x \\ P_1^1 &= -(1-x^2)^{1/2} \\ P_2^0 &= (3x^2-1)/2 \\ P_2^1 &= -3x(1-x^2)^{1/2} \\ P_2^2 &= 3(1-x^2) \\ P_3^0 &= x(5x^2-3)/2 \\ P_3^1 &= \frac{3}{2}(1-5x^2)(1-x^2)^{1/2} \\ P_3^2 &= 15x(1-x^2) \\ P_3^3 &= -15(1-x^2)^{3/2}\end{aligned}$$

Values for negative m can be obtained with the relation discussed above.

The first few complex spherical harmonics

$$Y_0^0 = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

$$
\begin{aligned}
Y_1^{-1} &= \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\phi} \\
Y_1^{0} &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \\
Y_1^{1} &= -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi} \\
Y_2^{-2} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{-2i\phi} \\
Y_2^{-1} &= \frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta e^{-i\phi} \\
Y_2^{0} &= \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) \\
Y_2^{1} &= -\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta e^{i\phi} \\
Y_2^{2} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi}
\end{aligned}
$$

The first few real spherical harmonics

$$
\begin{aligned}
Y_{0,0} &= \frac{1}{2}\sqrt{\frac{1}{\pi}} \\
Y_{1,-1} &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin\theta\sin\phi \\
Y_{1,0} &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta \\
Y_{1,1} &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin\theta\cos\phi \\
Y_{2,-2} &= \frac{1}{4}\sqrt{\frac{15}{\pi}}\sin^2\theta\sin(2\phi) \\
Y_{2,-1} &= \frac{1}{2}\sqrt{\frac{15}{\pi}}\sin\theta\cos\theta\sin\phi \\
Y_{2,0} &= \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) \\
Y_{2,1} &= \frac{1}{2}\sqrt{\frac{15}{\pi}}\sin\theta\cos\theta\cos\phi \\
Y_{2,2} &= \frac{1}{4}\sqrt{\frac{15}{\pi}}\sin^2\theta\cos(2\phi)
\end{aligned}
$$

Visualization

Figures 2 and 3 show two common visualizations of the spherical harmonics with $\ell \leq 3$. I'd like to emphasize that the first visualization, in which the sphere is stretched and distorted, is merely meant to make it easier to see the value of the spherical harmonics at particular angles, and the domain of the spherical harmonics is still the surface of the sphere, as in Figure 3.

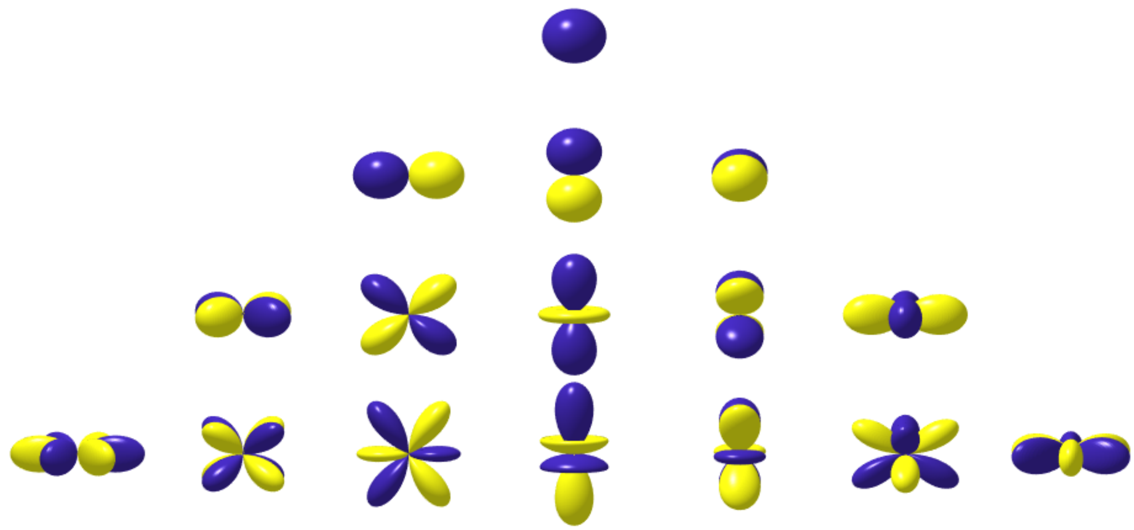

Figure 2: Spherical harmonics drawn by stretching the unit sphere. Regions where Y_ℓ^m is positive are purple, and regions where it is negative are yellow. The distance of the surface from the origin indicates the absolute value of Y_ℓ^m.

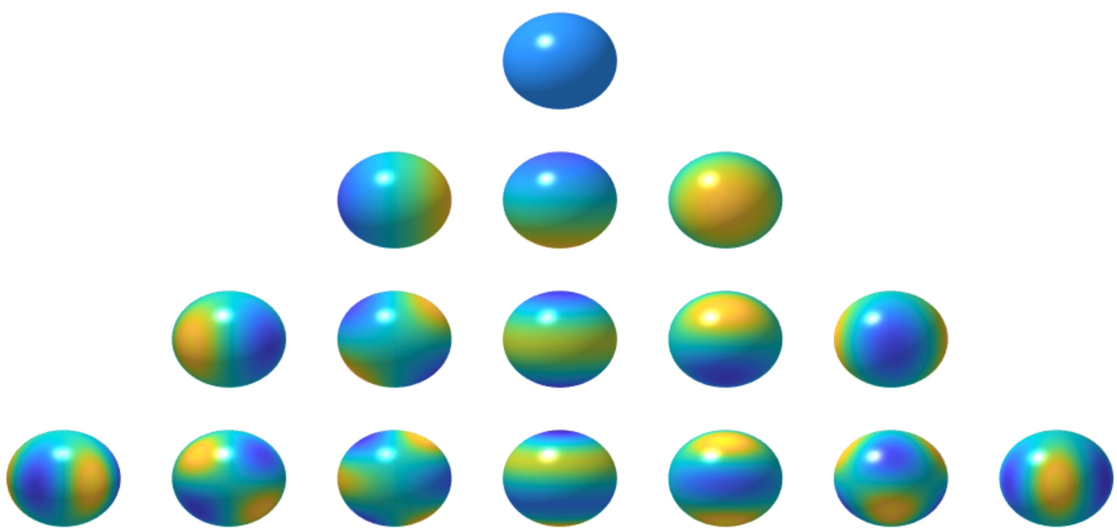

Figure 3: Spherical harmonics drawn by shading the unit sphere. Colors represent the value of Y_ℓ^m, blue for positive, green near zero, and yellow for negative.

The MATLAB code I wrote to create these visualizations is included in the appendix.

Further study

Applications in science

Spherical harmonics have been called the "Swiss army knife of mathematical physics", and that appellation appears to be well-deserved. A Google Scholar search for "'spherical harmonics' in physics" returns 144,000 matches, including applications ranging from semiconductor physics (Rupp, Jüngel, and Grasser 2010) and the cosmic microwave background (White and Srednicki 1994) to light propagation in biological tissue (Klose and Larsen 2006; Chu et al. 2009; Domínguez and Bérubé-Lauzière 2011) and protein shape analysis (Venkatraman, Sael, and Kihara 2009).

Applications in computer graphics

Low-order spherical harmonics can also efficiently represent directional lightning, shadows, and reflections in computer graphics, a technique explained well by Green 2003 (who credits Sloan, Kautz, and Snyder 2002 for introducing the technique).

For example, Weta Digital (the digital effects studio founded by Peter Jackson whose credits include Avatar and the Lord of the Rings trilogy) uses the first nine spherical harmonics Y_0^0, Y_1^m, Y_2^m as a basis to quickly calculate directional ambient lightning. (Seymour 2013)

Spherical harmonics are well suited to this use because common graphical operations reduce to matrix operations that can be quickly computed on a GPU. (see Schönefeld 2005)

In pure mathematics

There is much more to study in pure math as well. The scalar spherical harmonics in 3D discussed herein have been extended to include the radius (the solid harmonics), into higher-dimensional Euclidean space (see Axler, Bourdon, and Wade 2001), and to create vector (Hill 1954; Blatt and Weisskopf 1979; Barrera, Estevez, and Giraldo 1985) and tensor (James 1976; Sandberg 1978) forms.

Clearly the study of spherical harmonics could fill a lifetime, but alas, I must stop here.

Appendix: MATLAB code

The code to make the plots in the Visualizations section:

```
% Draw a stretch sphere if extend=1,
% or a shaded sphere if extend=0
extend = 0;

% Calculate the first few real spherical harmonics Y_lm
for l = 0:3
        for m = -l:l % lowercase L, not one
        % Set up a grid
                phis = linspace(0, 2 * pi, 200);
                thetas = linspace(0, 1 * pi, 200);
                [phi, theta] = ndgrid(phis, thetas);

                % First calculate the associated Legendre function of
                % cos(theta) with degree l and order abs(m)
                P = legendre(l,cos(theta));
                if(l > 0)
                        % If l == 0, legendre returns an order 3 tensor
                        % containing results for m=0, m=1, ...
                        Plm = reshape(P(abs(m)+1,:,:), size(phi));
                else
                        % If l == 0, legendre returns just
                        % the matrix for m=0
                        Plm = P;
                end

                % Calculate the normalization constant N
                a = (2*l+1)*factorial(l-abs(m));
                b = 4*pi*factorial(l+abs(m));
                N = sqrt(a/b);

                % Finally, calculate the real spherical harmonic
                if(m == 0)
                        H = N .* Plm;
                elseif(m < 0)
                        H = sqrt(2) * N * Plm .* sin(abs(m)*phi);
                elseif(m > 0)
                        H = sqrt(2) * N * Plm .* cos(m*phi);
                end
```

```
                if(extend) % Draw by stretching the sphere
                        C = sign(H); % Color value
                        S = abs(2 * H); % stretch factor
                        Xm = cos(phi) .* sin(theta) .* S;
                        Ym = sin(phi) .* sin(theta) .* S;
                        Zm = cos(theta) .* S;

                else % Draw as a shaded sphere
                        C = H; % Color value
                        Xm = cos(phi) .* sin(theta);
                        Ym = sin(phi) .* sin(theta);
                        Zm = cos(theta);
                end

                % Translate to position in larger grid
                X = Xm;
                Y = Ym + m * 2.9;
                Z = Zm + 3 - l * 2.9;

                % Draw it
                colormap default;
                oldcmap = colormap;
                colormap( flipud(oldcmap) );
                h = surf(X, Y, Z, C);
                h.AmbientStrength = 0.6;
                h.DiffuseStrength = 0.6;
                h.SpecularStrength = 0.8;
                h.SpecularExponent = 25;
                shading flat;
                hold on;
        end
end
axis ([-10, 10, -10, 10, -10, 10])
view(90, 7);
grid off;
xlabel("X");
ylabel("Y");
zlabel("Z");
light('Position',[10 -10 20],'Style','local');
colorbar

% Reverse the X axis (MATLAB usually draws x going into the page)
gca.XDir = 'reverse';

hold off
```

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