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6.8 Spherical Harmonics

Spherical harmonics occur in a large variety of physical problems, for example, whenever a wave equation, or Laplace's equation, is solved by separation of variables in spherical coordinates. The spherical harmonic $Y_{lm}(\theta, \phi)$, $-l \leq m \leq l$, is a function of the two coordinates θ, ϕ on the surface of a sphere.

The spherical harmonics are orthogonal for different l and m, and they are normalized so that their integrated square over the sphere is unity:

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) Y_{l'm'}{}^*(\theta, \phi) Y_{lm}(\theta, \phi) = \delta_{l'l}\delta_{m'm} \qquad (6.8.1)$$

Here asterisk denotes complex conjugation.

Mathematically, the spherical harmonics are related to *associated Legendre polynomials* by the equation

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi} \qquad (6.8.2)$$

By using the relation

$$Y_{l,-m}(\theta, \phi) = (-1)^m Y_{lm}{}^*(\theta, \phi) \qquad (6.8.3)$$

we can always relate a spherical harmonic to an associated Legendre polynomial with $m \geq 0$. With $x \equiv \cos\theta$, these are defined in terms of the ordinary Legendre polynomials (cf. §4.5 and §5.5) by

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \qquad (6.8.4)$$

The first few associated Legendre polynomials, and their corresponding normalized spherical harmonics, are

$P_0^0(x) = 1$	$Y_{00} = \sqrt{\frac{1}{4\pi}}$
$P_1^1(x) = -(1-x^2)^{1/2}$	$Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}$
$P_1^0(x) = x$	$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$
$P_2^2(x) = 3\,(1-x^2)$	$Y_{22} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2i\phi}$
$P_2^1(x) = -3\,(1-x^2)^{1/2}x$	$Y_{21} = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}$
$P_2^0(x) = \frac{1}{2}\,(3x^2-1)$	$Y_{20} = \sqrt{\frac{5}{4\pi}}(\frac{3}{2}\cos^2\theta - \frac{1}{2})$

(6.8.5)

There are many bad ways to evaluate associated Legendre polynomials numerically. For example, there are explicit expressions, such as

$$P_l^m(x) = \frac{(-1)^m(l+m)!}{2^m m!(l-m)!}(1-x^2)^{m/2}\left[1 - \frac{(l-m)(m+l+1)}{1!(m+1)}\left(\frac{1-x}{2}\right)\right.$$
$$\left. + \frac{(l-m)(l-m-1)(m+l+1)(m+l+2)}{2!(m+1)(m+2)}\left(\frac{1-x}{2}\right)^2 - \cdots\right] \tag{6.8.6}$$

where the polynomial continues up through the term in $(1-x)^{l-m}$. (See [1] for this and related formulas.) This is not a satisfactory method because evaluation of the polynomial involves delicate cancellations between successive terms, which alternate in sign. For large l, the individual terms in the polynomial become very much larger than their sum, and all accuracy is lost.

In practice, (6.8.6) can be used only in single precision (32-bit) for l up to 6 or 8, and in double precision (64-bit) for l up to 15 or 18, depending on the precision required for the answer. A more robust computational procedure is therefore desirable, as follows:

The associated Legendre functions satisfy numerous recurrence relations, tabulated in [1-2]. These are recurrences on l alone, on m alone, and on both l and m simultaneously. Most of the recurrences involving m are unstable, and so dangerous for numerical work. The following recurrence on l is, however, stable (compare 5.5.1):

$$(l-m)P_l^m = x(2l-1)P_{l-1}^m - (l+m-1)P_{l-2}^m \tag{6.8.7}$$

It is useful because there is a closed-form expression for the starting value,

$$P_m^m = (-1)^m(2m-1)!!(1-x^2)^{m/2} \tag{6.8.8}$$

(The notation $n!!$ denotes the product of all *odd* integers less than or equal to n.) Using (6.8.7) with $l = m+1$, and setting $P_{m-1}^m = 0$, we find

$$P_{m+1}^m = x(2m+1)P_m^m \tag{6.8.9}$$

Equations (6.8.8) and (6.8.9) provide the two starting values required for (6.8.7) for general l.

The function that implements this is

```
#include <math.h>

float plgndr(int l, int m, float x)
```
Computes the associated Legendre polynomial $P_l^m(x)$. Here m and l are integers satisfying $0 \le m \le l$, while x lies in the range $-1 \le x \le 1$.
```
{
    void nrerror(char error_text[]);
    float fact,pll,pmm,pmmp1,somx2;
    int i,ll;

    if (m < 0 || m > l || fabs(x) > 1.0)
        nrerror("Bad arguments in routine plgndr");
    pmm=1.0;                        Compute P_m^m.
    if (m > 0) {
        somx2=sqrt((1.0-x)*(1.0+x));
        fact=1.0;
        for (i=1;i<=m;i++) {
            pmm *= -fact*somx2;
            fact += 2.0;
        }
    }
    if (l == m)
        return pmm;
    else {                          Compute P_{m+1}^m.
        pmmp1=x*(2*m+1)*pmm;
        if (l == (m+1))
            return pmmp1;
        else {                      Compute P_l^m, l > m + 1.
            for (ll=m+2;ll<=l;ll++) {
                pll=(x*(2*ll-1)*pmmp1-(ll+m-1)*pmm)/(ll-m);
                pmm=pmmp1;
                pmmp1=pll;
            }
            return pll;
        }
    }
}
```

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6.9 Fresnel Integrals, Cosine and Sine Integrals

Fresnel Integrals

The two Fresnel integrals are defined by

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right) dt, \qquad S(x) = \int_0^x \sin\left(\frac{\pi}{2}t^2\right) dt \tag{6.9.1}$$

The most convenient way of evaluating these functions to arbitrary precision is to use power series for small x and a continued fraction for large x. The series are

$$\begin{aligned} C(x) &= x - \left(\frac{\pi}{2}\right)^2 \frac{x^5}{5 \cdot 2!} + \left(\frac{\pi}{2}\right)^4 \frac{x^9}{9 \cdot 4!} - \cdots \\ S(x) &= \left(\frac{\pi}{2}\right) \frac{x^3}{3 \cdot 1!} - \left(\frac{\pi}{2}\right)^3 \frac{x^7}{7 \cdot 3!} + \left(\frac{\pi}{2}\right)^5 \frac{x^{11}}{11 \cdot 5!} - \cdots \end{aligned} \tag{6.9.2}$$

There is a complex continued fraction that yields both $S(x)$ and $C(x)$ simultaneously:

$$C(x) + iS(x) = \frac{1+i}{2} \operatorname{erf} z, \qquad z = \frac{\sqrt{\pi}}{2}(1-i)x \tag{6.9.3}$$

where

$$\begin{aligned} e^{z^2} \operatorname{erfc} z &= \frac{1}{\sqrt{\pi}} \left(\frac{1}{z+}\ \frac{1/2}{z+}\ \frac{1}{z+}\ \frac{3/2}{z+}\ \frac{2}{z+} \cdots \right) \\ &= \frac{2z}{\sqrt{\pi}} \left(\frac{1}{2z^2+1-}\ \frac{1 \cdot 2}{2z^2+5-}\ \frac{3 \cdot 4}{2z^2+9-} \cdots \right) \end{aligned} \tag{6.9.4}$$

In the last line we have converted the "standard" form of the continued fraction to its "even" form (see §5.2), which converges twice as fast. We must be careful not to evaluate the alternating series (6.9.2) at too large a value of x; inspection of the terms shows that $x = 1.5$ is a good point to switch over to the continued fraction.

Note that for large x

$$C(x) \sim \frac{1}{2} + \frac{1}{\pi x} \sin\left(\frac{\pi}{2}x^2\right), \qquad S(x) \sim \frac{1}{2} - \frac{1}{\pi x} \cos\left(\frac{\pi}{2}x^2\right) \tag{6.9.5}$$

Thus the precision of the routine `frenel` may be limited by the precision of the library routines for sine and cosine for large x.