Record of Things I Know - Spherical Laplace

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March 4, 2014

1 Standard Presentation

From Beatson-Greengard summary, the standard formulation of spherical harmonic expansions appears as follows.

Given the Laplace Green's function

$$K(t,s) = \frac{1}{|s-t|}$$

the spherical harmonics expansion is given by

$$K(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(L_n^m r^n + \frac{M_n^m}{r^{n+1}} \right) Y_n^m(\theta,\phi)$$

where

$$Y_n^m(\theta,\phi) = \sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\, P_n^{|m|}(\cos\theta)\, e^{\imath m\phi}$$

are the semi-normalized spherical harmonics and P_n^m are the associated Legendre functions. Note the symmetry

$$Y_n^m(\pi-\theta, \pi+\phi) = (-1)^n Y_n^m(\theta,\phi)$$

Additionally, note that with this definition,

$$Y_n^{-m} = (Y_n^m)^*$$

where $\cdot^*$ denotes complex conjugation.

1.1 P2M

With k charges of strength c_i, $i = 1,\dots,k$ and position $s_i = (\rho_i, \theta_i, \phi_i)$ with $\rho_i < a$. Then, for any $\mathbf{r} = (r,\theta,\phi) \in \mathbb{R}^3$ with $r > a$, the kernel value (potential) is given by

$$K(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}}\, Y_n^m(\theta,\phi)$$

where

$$M_n^m = \sum_{i=1}^{k} \rho_i^n \, Y_n^{-m}(\theta_i,\phi_i)\, c_i$$

Furthermore, for any $p \geq 1$,

$$\left| K(\mathbf{r}) - \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}}\, Y_n^m(\theta,\phi) \right| \leq \frac{1}{r-a} \left(\frac{a}{r}\right)^{p+1} \sum_{i=1}^{k} |c_i|$$

Thus, we compute and store the M_n^m for all $n = 0,\dots,p$, $-n \leq m \leq n$ from the source locations and charges.

Note: The "translation vector" is backwards to the typical definition. The vector $(\rho_i, \theta_i, \phi_i)$ points from the origin to s_i. Traditionally the translation vectors point from the source to the new center.

1.2 M2M

Suppose that charges are located inside a sphere D of radius a with center at $\mathbf{c} = (\rho, \alpha, \beta)$ and that for points $\mathbf{r} = (r, \theta, \phi)$ outside of D, the potential is given by the multipole expansion

$$K(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{M_n^m}{r'^{n+1}} Y_n^m(\theta', \phi')$$

where $\mathbf{r} - \mathbf{c} = (r', \theta', \phi')$. Then for any point outside the sphere D_1 of radius $(a + \rho)$,

$$K(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{\widetilde{M}_n^m}{r^{n+1}} Y_n^m(\theta, \phi)$$

where

$$\widetilde{M}_n^m = \sum_{j=0}^{n} \sum_{k=-j}^{j} M_{n-j}^{m-k} \frac{\imath^{|m|}}{\imath^{|k|} \imath^{|m-k|}} \frac{A_j^k A_{n-j}^{m-k}}{A_n^m} \rho^j Y_j^{-k}(\alpha, \beta)$$

with A_n^m defined by

$$A_n^m = \frac{(-1)^n}{\sqrt{(n-m)!(n+m)!}}$$

Note: The "translation vector" is backwards to the typical definition. This translation if going **from c** to the origin while traditionally the translation vectors point from the old center to the new center.

1.3 M2L

Suppose that charges are located inside the sphere D of radius a with center at $\mathbf{c} = (\rho, \alpha, \beta)$ and that $\rho > (c + 1)a$ with $c > 1$. Then the corresponding multipole expansion converges inside the sphere D' of radius a centered at the origin. For $\mathbf{r} = (r, \theta, \phi)$ inside D', the potential is

$$K(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_n^m r^n Y_n^m(\theta, \phi)$$

where

$$L_n^m = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} (-1)^j M_j^k \frac{\imath^{|m-k|}}{\imath^{|k|} \imath^{|m|}} \frac{A_j^k A_n^m}{A_{j+n}^{k-m}} \frac{Y_{j+n}^{k-m}(\alpha, \beta)}{\rho^{j+n+1}}$$

This incurs an error due to the truncation of the expansion. For any $p \geq 1$,

$$\left| K(\mathbf{r}) - \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_n^m r^n Y_n^m(\theta, \phi) \right| \leq \frac{1}{a(c-1)} \left(\frac{1}{c} \right)^{p+1} \sum_{i=1}^{k} |c_i|$$

Note: Again, this is a backwards "transfer vector".

1.4 L2L

Let $\mathbf{c} = (\rho, \alpha, \beta)$ be the origin of the local expansion so that

$$K(\mathbf{r}) = \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m r'^n Y_n^m(\theta', \phi')$$

where $\mathbf{r} = (r, \theta, \phi)$ and $\mathbf{r} - \mathbf{c} = (r', \theta', \phi')$. Then,

$$K(\mathbf{r}) = \sum_{n=0}^{p} \sum_{m=-n}^{n} \widetilde{L}_n^m r^n Y_n^m(\theta, \phi)$$

where

$$\widetilde{L}_n^m = \sum_{j=n}^{p} \sum_{k=-j}^{j} \frac{L_j^k}{(-1)^{j+n}} \frac{\imath^{|k|}}{\imath^{|k-m|}\imath^{|m|}} \frac{A_{j-n}^{k-m} A_n^m}{A_j^k} \rho^{j-n} Y_{j-n}^{k-m}(\alpha, \beta)$$

Note: Again, the "translation vector" is backwards.

1.5 L2P

Finally, the local expansion may be evaluated at $\mathbf{r} = (\rho, \theta, \phi)$,

$$K(\mathbf{r}) = \sum_{n=0}^{p} \sum_{m=-n}^{n} L_n^m \rho^n Y_n^m(\theta, \phi)$$

2 Alternate Presentation

In this section, we revise the standard formulation to be more computationally elegant. First, define

$$\begin{aligned} Z_n^m(\rho, \theta, \phi) &= \frac{A_n^m}{\imath^{|m|}} (-\rho)^n Y_n^m(\theta, \phi) \\ &= \frac{(-1)^n}{\imath^{|m|}\sqrt{(n-m)!(n+m)!}} (-\rho)^n Y_n^m(\theta, \phi) \\ &= \frac{\rho^n \imath^{-|m|}}{(n+|m|)!} P_n^{|m|}(\cos\theta) e^{\imath m \phi} \end{aligned}$$

Note the symmetry

$$Z_n^{-m} = (-1)^m (Z_n^m)^*$$

Then, we modify the representations of the multipole and local expansions:

$$\begin{aligned} \mathcal{M}_n^m &= \frac{A_n^m}{\imath^{|m|}} M_n^m \\ \mathcal{L}_n^m &= \frac{\imath^{|m|}}{A_n^m} (-1)^n L_n^m \end{aligned}$$

This allows a significant simplification of the FMM operators, detailed below.

In the following sections, the "translation" or "transfer vector" is denoted (ρ, θ, ϕ) and is always from the source location to the target location (i.e. new center minus old center).

2.1 P2M

Note: We flip the translation vector by multiplying by $(-1)^n$. Thus, the original becomes

$$M_n^m = \sum_{i=1}^{k} (-1)^n \rho_i^n \, Y_n^{-m}(\theta_i, \phi_i) \, c_i$$

Using the Z_n^m operator, we have

$$\begin{aligned}
\mathcal{M}_n^m &= \frac{A_n^m}{\imath^{|m|}} M_n^m \\
&= \sum_{i=1}^{k} \frac{A_n^m}{\imath^{|m|}} (-1)^n \rho_i^n Y_n^{-m}(\theta_i, \phi_i)\, c_i \\
&= \sum_{i=1}^{k} Z_n^{-m}(\rho_i, \theta_i, \phi_i)\, c_i
\end{aligned}$$

2.2 M2M

Note: We flip the translation vector by multiplying by $(-1)^j$. Thus, the original becomes

$$\widetilde{M}_n^m = \sum_{j=0}^{n} \sum_{k=-j}^{j} M_{n-j}^{m-k} \frac{\imath^{|m|}}{\imath^{|k|}\imath^{|m-k|}} \frac{A_j^k A_{n-j}^{m-k}}{A_n^m} (-1)^j \rho^j Y_j^{-k}(\alpha, \beta)$$

Then,

$$\begin{aligned}
\widetilde{\mathcal{M}}_n^m &= \frac{A_n^m}{\imath^{|m|}} \widetilde{M}_n^m \\
&= \sum_{j=0}^{n} \sum_{k=-j}^{j} M_{n-j}^{m-k} \frac{A_j^k A_{n-j}^{m-k}}{\imath^{|k|}\imath^{|m-k|}} (-1)^j \rho^j Y_j^{-k}(\theta, \phi) \\
&= \sum_{j=0}^{n} \sum_{k=-j}^{j} \mathcal{M}_{n-j}^{m-k} Z_j^{-k}(\rho, \theta, \phi) \\
&= \sum_{j=0}^{n} \sum_{k=-j}^{j} \mathcal{M}_{n-j}^{m-k} Z_j^{-k}(\rho, \theta, \phi)
\end{aligned}$$

2.3 M2L

Note: We flip the transfer vector by multiplying by $(-1)^{j+n}$. Thus, the original becomes

$$L_n^m = \sum_{j=0}^{\infty} \sum_{k=-j}^{j} (-1)^j M_j^k \frac{\imath^{|m-k|}}{\imath^{|k|}\imath^{|m|}} \frac{A_j^k A_n^m}{A_{j+n}^{k-m}} (-1)^{j+n} \frac{Y_{j+n}^{k-m}(\alpha, \beta)}{\rho^{j+n+1}}$$

Then,

$$\begin{aligned}
\mathcal{L}_n^m &= \frac{\imath^{|m|}}{A_n^m} (-1)^n L_n^m \\
&= \sum_{j=0}^{p} \sum_{k=-j}^{j} M_j^k \frac{\imath^{|m-k|}}{\imath^{|k|}} \frac{A_j^k}{A_{j+n}^{k-m}} \frac{Y_{j+n}^{k-m}(\theta, \phi)}{\rho^{j+n+1}} \\
&= \sum_{j=0}^{p} \sum_{k=-j}^{j} \mathcal{M}_j^k\, W_{j+n}^{k-m}(\rho, \theta, \phi)
\end{aligned}$$

where

$$
\begin{aligned}
W_n^m(\rho,\theta,\phi) &= \frac{\imath^{|m|}}{A_n^m}\rho^{-n-1}Y_n^m(\theta,\phi) \\
&= \imath^{|m|}(-1)^n\sqrt{(n-m)!(n+m)!}\rho^{-n-1}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}P_n^{|m|}(\cos\theta)e^{\imath m\phi} \\
&= \imath^{|m|}(-1)^n(n-|m|)!\rho^{-n-1}P_n^{|m|}(\cos\theta)e^{\imath m\phi}
\end{aligned}
$$

2.4 L2L

Note: We flip the transfer vector by multiplying by $(-1)^{j-n}$. Thus, the original becomes

$$
\widetilde{L}_n^m = \sum_{j=n}^{p}\sum_{k=-j}^{j}\frac{L_j^k}{(-1)^{j+n}}\frac{\imath^{|k|}}{\imath^{|k-m|}\imath^{|m|}}\frac{A_{j-n}^{k-m}A_n^m}{A_j^k}(-1)^{j-n}\rho^{j-n}Y_{j-n}^{k-m}(\alpha,\beta)
$$

Then,

$$
\begin{aligned}
\widetilde{\mathcal{L}}_n^m &= \frac{\imath^{|m|}}{A_n^m}(-1)^n\widetilde{L}_n^m \\
&= \sum_{j=n}^{p}\sum_{k=-j}^{j}L_j^k(-1)^j\frac{\imath^{|k|}}{\imath^{|k-m|}}\frac{A_{j-n}^{k-m}}{A_j^k}(-1)^{j-n}\rho^{j-n}Y_{j-n}^{k-m}(\theta,\phi) \\
&= \sum_{j=n}^{p}\sum_{k=-j}^{j}\mathcal{L}_j^k Z_{j-n}^{k-m}(\rho,\theta,\phi)
\end{aligned}
$$

2.5 L2P

$$
\begin{aligned}
K(\mathbf{r}) &= \sum_{n=0}^{p}\sum_{m=-n}^{n}L_n^m\rho^nY_n^m(\theta,\phi) \\
&= \sum_{n=0}^{p}\sum_{m=-n}^{n}\mathcal{L}_n^m Z_n^m(\rho,\theta,\phi)
\end{aligned}
$$