FMM Implementation Details

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November 30, 2020

1 General

In this implementation, following [1], we use the this definition of *surface spherical harmonics* that has non-standard normalization:

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

Again, following [1], we use this non-standard normalization for the *regular* and *irregular solid harmonics* as the base for multipole and local expansions:

$$\begin{aligned} R_l^m &= \frac{1}{\sqrt{(l-m)!(l+m)!}} r^l Y_l^m \\ &= (-1)^m \frac{1}{(l+m)!} r^l P_l^m e^{im\phi} \end{aligned} \tag{2}$$

and

$$\begin{aligned} I_l^m &= \sqrt{(l-m)!(l+m)!} \frac{1}{r^{l+1}} Y_l^m \\ &= (-1)^m (l-m)! \frac{1}{r^{l+1}} P_l^m e^{im\phi} \end{aligned} \tag{3}$$

In all these P_l^m are the associated Legendre polynomials, for which the following apply [2]:

$$P_0^0 = 1 \tag{4}$$

$$\begin{aligned} P_{m+1}^{m+1}(\cos\theta) &= -(2m+1)\sqrt{1-\cos^2\theta} P_m^m \\ &= -(2m+1)\sin\theta P_m^m \end{aligned} \tag{5}$$

$$P_{m+1}^m(\cos\theta) = (2m+1)\cos\theta P_m^m \tag{6}$$

$$P_{l+1}^m(\cos\theta) = \frac{(2l+1)\cos\theta P_l^m - (l+m)P_{l-1}^m}{l-m+1} \tag{7}$$

The last equation can be re-written as:

$$P_{l+2}^m(\cos\theta) = \frac{(2l+3)\cos\theta P_{l+1}^m - (l+m+1)P_l^m}{l-m+2} \tag{8}$$

2 Iterative computation of R_l^m

From (2):

$$R_m^m = (-1)^m \frac{1}{(2m)!} r^m P_m^m e^{im\phi} \tag{9}$$

and

$$R_{m+1}^{m+1} = (-1)^{m+1} \frac{1}{(2m+2)!} r^{m+1} P_{m+1}^{m+1} e^{i(m+1)\phi} \tag{10}$$

Using (5) we have:

$$\begin{aligned} R_{m+1}^{m+1} &= (-1)^{m+1} \frac{1}{(2m+2)!} r^{m+1} [-(2m+1)P_m^m \sin\theta] e^{i(m+1)\phi} \\ &= (-1)^m \frac{(2m+1)}{(2m+2)(2m+1)(2m)!} r^m P_m^m e^{im\phi} r \sin\theta e^{i\phi} \\ &= R_m^m \frac{1}{2m+2} r \sin\theta e^{i\phi} \end{aligned} \tag{11}$$

For standard spherical coordinates we have:

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned} \tag{12}$$

so

$$\begin{aligned} r\sin\theta e^{i\phi} &= r\sin\theta(\cos\phi + i\sin\phi) \\ &= r\sin\theta(\frac{x}{r\sin\theta} + i\frac{y}{r\sin\theta}) \\ &= x + iy \end{aligned} \tag{13}$$

and finally

$$\boxed{R_{m+1}^{m+1} = \frac{x+iy}{2(m+1)} R_m^m} \tag{14}$$

Additionally, from (2) and (4) it trivially follows that:

$$\boxed{R_0^0 = 1} \tag{15}$$

Together these allow us to calculate iteratively all R_m^m.
For R_{m+1}^m similary we have:

$$\begin{aligned} R_{m+1}^m &= (-1)^m \frac{1}{(2m+1)!} r^{m+1} [(2m+1) P_m^m \cos\theta] e^{im\phi} \\ &= (-1)^m \frac{(2m+1)}{(2m+1)(2m)!} r^m P_m^m e^{im\phi} r \cos\theta \\ &= R_m^m r \cos\theta \end{aligned} \tag{16}$$

The last part is just $z = r\cos\theta$, so:

$$\boxed{R_{m+1}^m = z R_m^m} \tag{17}$$

Next, we have from (2):

$$R_{l+2}^m = (-1)^m \frac{1}{(l+m+2)!} r^{l+2} P_{l+2}^m e^{im\phi} \tag{18}$$

Pluggin in (8):

$$\begin{aligned} R_{l+2}^m &= (-1)^m \frac{1}{(l+m+2)!} r^{l+2} \left[\frac{(2l+3)\cos\theta P_{l+1}^m - (l+m+1) P_l^m}{l-m+2} \right] e^{im\phi} \\ R_{l+2}^m &= \left[(-1)^m \frac{1}{(l+m+2)!} r^{l+2} \frac{(2l+3)\cos\theta P_{l+1}^m}{l-m+2} e^{im\phi} \right] - \\ &- \left[(-1)^m \frac{1}{(l+m+2)!} r^{l+2} \frac{(l+m+1) P_l^m}{l-m+2} e^{im\phi} \right] \end{aligned} \tag{19}$$

The first term in (19) is:

$$\begin{aligned} A &= (-1)^m \frac{1}{(l+m+2)!} r^{l+2} \frac{(2l+3)\cos\theta P_{l+1}^m}{l-m+2} e^{im\phi} \\ &= \frac{(2l+3)}{((l+2)+m)\,((l+2)-m)} (-1)^m \frac{1}{(l+m+1)!} r^{l+1} P_{l+1}^m e^{im\phi} z \\ &= \frac{(2l+3) z R_{l+1}^m}{(l+2)^2 - m^2} \end{aligned} \tag{20}$$

The second term in (19) is:

$$
\begin{aligned}
B &= (-1)^m \frac{1}{(l+m+2)!} r^{l+2} \frac{(l+m+1)P_l^m}{l-m+2} e^{im\phi} \\
&= \frac{1}{((l+2)+m)\,((l+2)-m)} (-1)^m \frac{1}{(l+m)!} r^l P_l^m e^{im\phi} r^2 \\
&= \frac{r^2 R_l^m}{(l+2)^2 - m^2}
\end{aligned} \tag{21}
$$

Finally, we have:

$$
R_{l+2}^m = \frac{1}{(l+2)^2 - m^2} \left[(2l+3) z R_{l+1}^m - r^2 R_l^m \right] \tag{22}
$$

We can also rewrite this as

$$
\boxed{R_l^m = \frac{1}{l^2 - m^2} \left[(2l-1) z R_{l-1}^m - r^2 R_{l-2}^m \right]} \tag{23}
$$

which is the form used in the implementation.

Together the four equations (14), (15), (17) and (23) allow us to calculate all needed R_m^m iteratively and efficiently.

3 Iterative computation of I_l^m

From (3):

$$
I_m^m = (-1)^m \frac{1}{r^{m+1}} P_m^m e^{im\phi} \tag{24}
$$

and

$$
I_{m+1}^{m+1} = (-1)^{m+1} \frac{1}{r^{m+2}} P_{m+1}^{m+1} e^{i(m+1)\phi} \tag{25}
$$

Using (5) we have:

$$
\begin{aligned}
I_{m+1}^{m+1} &= (-1)^{m+1} \frac{1}{r^{m+2}} \left[-(2m+1) \sin\theta P_m^m \right] e^{i(m+1)\phi} \\
&= (-1)^m \frac{1}{r^{m+1}} P_m^m e^{im\phi} (2m+1) \frac{1}{r} \sin\theta e^{i\phi} \\
&= I_m^m (2m+1) \frac{x+iy}{r^2}
\end{aligned} \tag{26}
$$

So

$$
\boxed{I_{m+1}^{m+1} = (2m+1) \frac{x+iy}{r^2} I_m^m} \tag{27}
$$

Additionally, from (3) and (4) it trivially follows that:

$$\boxed{I_0^0 = \frac{1}{r}} \tag{28}$$

Together these allow us to calculate iteratively all I_m^m.
For I_{m+1}^m similary we have:

$$\begin{aligned} I_{m+1}^m &= (-1)^m \frac{1}{r^{m+2}} P_{m+1}^m e^{im\phi} \\ &= (-1)^m \frac{1}{r^{m+2}} \left[(2m+1)\cos\theta P_m^m\right] e^{im\phi} \\ &= (-1)^m \frac{1}{r^{m+1}} P_m^m e^{im\phi} (2m+1)\cos\theta \frac{1}{r} \end{aligned} \tag{29}$$

So:

$$\boxed{I_{m+1}^m = (2m+1)\frac{z}{r^2} I_m^m} \tag{30}$$

Next, we have from (3):

$$I_{l+2}^m = (-1)^m (l+2-m)! \frac{1}{r^{l+3}} P_{l+2}^m e^{im\phi} \tag{31}$$

Pluggin in (8):

$$\begin{aligned} I_{l+2}^m &= (-1)^m (l+2-m)! \frac{1}{r^{l+3}} \left[\frac{(2l+3)\cos\theta P_{l+1}^m - (l+m+1)P_l^m}{l-m+2}\right] e^{im\phi} \\ I_{l+2}^m &= \left[(-1)^m (l+2-m)! \frac{1}{r^{l+3}} \frac{(2l+3)\cos\theta P_{l+1}^m}{l-m+2} e^{im\phi}\right] - \\ &- \left[(-1)^m (l+2-m)! \frac{1}{r^{l+3}} \frac{(l+m+1)P_l^m}{l-m+2} e^{im\phi}\right] \end{aligned} \tag{32}$$

The first term in (32) is:

$$\begin{aligned} C &= (-1)^m (l+2-m)! \frac{1}{r^{l+3}} \frac{(2l+3)\cos\theta P_{l+1}^m}{l-m+2} e^{im\phi} \\ &= (-1)^m (l+1-m)! \frac{1}{r^{l+2}} P_{l+1}^m e^{im\phi} (2l+3) \frac{1}{r} \cos\theta \\ &= (2l+3)\frac{z}{r^2} I_{l+1}^m \end{aligned} \tag{33}$$

The second term in (32) is:

$$
\begin{aligned}
D &= (-1)^m (l+2-m)! \frac{1}{r^{l+3}} \frac{(l+1+m) P_l^m}{l+2-m} e^{im\phi} \\
&= (-1)^m (l-m)! \frac{1}{r^{l+1}} P_l^m e^{im\phi} \left[(l+1)^2 - m^2 \right] \frac{1}{r^2} \\
&= \left[(l+1)^2 - m^2 \right] \frac{1}{r^2} I_l^m
\end{aligned}
\tag{34}
$$

Finally, we have:

$$
I_{l+2}^m = \frac{1}{r^2} \left[(2l+3) z I_{l+1}^m - \left[(l+1)^2 - m^2 \right] I_l^m \right] \tag{35}
$$

We can also rewrite this as

$$
\boxed{I_l^m = \frac{1}{r^2} \left[(2l-1) z I_{l-1}^m - \left[(l-1)^2 - m^2 \right] I_{l-2}^m \right]} \tag{36}
$$

which is the form used in the implementation.

Together the four equations (27), (28), (30) and (36) allow us to calculate all needed I_m^m iteratively and efficiently.

References

[1] Dehnen, W. *A fast multipole method for stellar dynamics.* Comput. Astrophys. 1, 1 (2014). `https://doi.org/10.1186/s40668-014-0001-7`

[2] `https://en.wikipedia.org/wiki/Associated_Legendre_polynomials`