Derivation of Fast Multipole Methods

1 Cartesian Taylor Expansions

We will use the following abbreviated expressions for multinomial factorials

$$\mathbf{n}! = n_x! n_y! n_z!,$$

multinomial powers

$$x^{\mathbf{n}} = x^{n_x} x^{n_y} x^{n_z},$$

multinomial summations

$$\sum_{\mathbf{n}=0}^{p} = \sum_{n_x=n_y=n_z=0}^{n_x+n_y+n_z=p},$$

multinomial gradients

$$\nabla^{(\mathbf{n})} = \frac{\partial}{\partial x}^{n_x} \frac{\partial}{\partial y}^{n_y} \frac{\partial}{\partial z}^{n_z}.$$

First, let us decompose the distance vector $\mathbf{x}_{ij} = (x_{ij}, y_{ij}, z_{ij})$ into three parts as shown in Figure 1.

$$\begin{aligned}
\mathbf{x}_{ij} &= \mathbf{x}_i - \mathbf{x}_j \\
&= (\mathbf{x}_i - \mathbf{x}_{ii'}) + (\mathbf{x}_{i'} - \mathbf{x}_{j'}) + (\mathbf{x}_{j'} - \mathbf{x}_j) \\
&= \mathbf{x}_{ii'} + \mathbf{x}_{i'j'} + \mathbf{x}_{j'j}
\end{aligned}$$

where $\mathbf{x}_{i'j'} \gg \mathbf{x}_{ii'} + \mathbf{x}_{j'j}$. Then, the Taylor expansion of a function $G(\mathbf{x}_{ij})$ in the neighborhood of $\mathbf{x}_{i'j'}$ can be written as

$$G(\mathbf{x}_{ij}) = \sum_{\mathbf{n}=0}^{p} \frac{1}{\mathbf{n}!} (\mathbf{x}_{ii'} + \mathbf{x}_{j'j})^{\mathbf{n}} \nabla^{(\mathbf{n})} G(\mathbf{x}_{i'j'}). \tag{1}$$

Using the binomial theorem on $(\mathbf{x}_{ii'} + \mathbf{x}_{j'j})^{\mathbf{n}}$ we have

$$= \sum_{\mathbf{n}=0}^{p} \frac{1}{\mathbf{n}!} \sum_{\mathbf{k}=0}^{\mathbf{n}} \frac{\mathbf{n}!}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \mathbf{x}_{j'j}^{\mathbf{n}-\mathbf{k}} \nabla^{(\mathbf{n})} G(\mathbf{x}_{i'j'}). \tag{2}$$

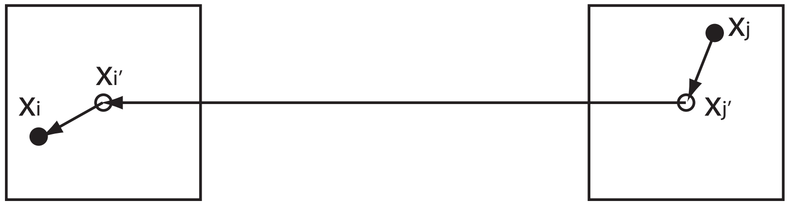

Figure 1: Decomposition of distance vectors into three parts

Cancel **n**!

$$= \sum_{\mathbf{n}=0}^{p} \sum_{\mathbf{k}=0}^{\mathbf{n}} \frac{1}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \mathbf{x}_{j'j}^{\mathbf{n}-\mathbf{k}} \nabla^{(\mathbf{n})} G(\mathbf{x}_{i'j'}). \tag{3}$$

Swap loop order between **n** and **k**

$$= \sum_{\mathbf{k}=0}^{p} \sum_{\mathbf{n}=\mathbf{k}}^{p} \frac{1}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \mathbf{x}_{j'j}^{\mathbf{n}-\mathbf{k}} \nabla^{(\mathbf{n})} G(\mathbf{x}_{i'j'}). \tag{4}$$

Redefine $\mathbf{n}-\mathbf{k}$ to $\mathbf{n}$

$$= \sum_{\mathbf{k}=0}^{p} \sum_{\mathbf{n}=0}^{p-\mathbf{k}} \frac{1}{\mathbf{n}!\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \mathbf{x}_{j'j}^{\mathbf{n}} \nabla^{(\mathbf{n}+\mathbf{k})} G(\mathbf{x}_{i'j'}). \tag{5}$$

Rearrange

$$= \sum_{\mathbf{k}=0}^{p} \frac{1}{\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \underbrace{\sum_{\mathbf{n}=0}^{p-\mathbf{k}} \nabla^{(\mathbf{n}+\mathbf{k})} G(\mathbf{x}_{i'j'}) \underbrace{\frac{1}{\mathbf{n}!} \mathbf{x}_{j'j}^{\mathbf{n}}}_{\mathbf{M}}}_{\mathbf{L}}. \tag{6}$$

M is the multipole expansion and **L** is the local expansion. Therefore, a potential u at point $\mathbf{x}_i$ induced by a charge q at point $\mathbf{x}_j$

$$u(\mathbf{x}_i) = G(\mathbf{x}_{ij}) q(\mathbf{x}_j) \tag{7}$$

can be factored into the following three expressions

$$u(\mathbf{x}_i) = \sum_{\mathbf{k}=0}^{p} \frac{1}{\mathbf{k}!} \mathbf{x}_{ii'}^{\mathbf{k}} \mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i'}) \quad (\mathbf{L2P}) \tag{8}$$

$$\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i'}) = \sum_{\mathbf{n}=0}^{p-\mathbf{k}} \nabla^{(\mathbf{n}+\mathbf{k})} G(\mathbf{x}_{i'j'}) \mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j'}) \quad (\mathbf{M2L}) \tag{9}$$

$$\mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j'}) = \frac{1}{\mathbf{n}!} \mathbf{x}_{j'j}^{\mathbf{n}} q(\mathbf{x}_j) \quad (\mathbf{P2M}) \tag{10}$$

Figure 2: Decomposition of distance vectors into five parts

We now perform a 5 vector decomposition shown in Figure 2, where the vectors $\mathbf{x}_{j''j}$ and $\mathbf{x}_{ii''}$ can be decomposed into

$$\begin{aligned}
\mathbf{x}_{j''j} &= \mathbf{x}_{j''j'} + \mathbf{x}_{j'j} \\
\mathbf{x}_{ii''} &= \mathbf{x}_{ii'} + \mathbf{x}_{i'i''}
\end{aligned}$$

The binomial theorem can be applied to Eq. (10) to yield

$$\begin{aligned}
\mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j''}) &= \frac{1}{\mathbf{n}!}(\mathbf{x}_{j''j'} + \mathbf{x}_{j'j})^{\mathbf{n}} q(\mathbf{x}_j) \\
&= \frac{1}{\mathbf{n}!}\sum_{\mathbf{k}=0}^{\mathbf{n}} \frac{\mathbf{n}!}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!}\mathbf{x}_{j''j'}^{\mathbf{n}-\mathbf{k}}\mathbf{x}_{j'j}^{\mathbf{k}} q(\mathbf{x}_j) \\
&= \sum_{\mathbf{k}=0}^{\mathbf{n}} \frac{1}{(\mathbf{n}-\mathbf{k})!}\mathbf{x}_{j''j'}^{\mathbf{n}-\mathbf{k}}\mathbf{M}^{\mathbf{k}}(\mathbf{x}_{j'}) \quad (\mathbf{M2M}) \qquad (11)
\end{aligned}$$

Similarly, Eq. (8) becomes

$$\begin{aligned}
u(\mathbf{x}_i) &= \sum_{\mathbf{k}=0}^{p} \frac{1}{\mathbf{k}!}(\mathbf{x}_{i\lambda} + \mathbf{x}_{i'i''})^{\mathbf{k}} \mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) \\
&= \sum_{\mathbf{k}=0}^{p} \sum_{\mathbf{n}=0}^{\mathbf{k}} \frac{1}{(\mathbf{k}-\mathbf{n})!\mathbf{n}!}\mathbf{x}_{ii'}^{\mathbf{n}}\mathbf{x}_{i'i''}^{\mathbf{k}-\mathbf{n}}\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) \\
&= \sum_{\mathbf{n}=0}^{p} \sum_{\mathbf{k}=\mathbf{n}}^{p} \frac{1}{(\mathbf{k}-\mathbf{n})!\mathbf{n}!}\mathbf{x}_{ii'}^{\mathbf{n}}\mathbf{x}_{i'i''}^{\mathbf{k}-\mathbf{n}}\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) \\
&= \sum_{\mathbf{n}=0}^{p} \frac{1}{\mathbf{n}!}\mathbf{x}_{ii'}^{\mathbf{n}}\mathbf{L}^{\mathbf{n}}(\mathbf{x}_{i'}) \\
\mathbf{L}^{\mathbf{n}}(\mathbf{x}_{i'}) &= \sum_{\mathbf{k}=\mathbf{n}}^{p} \frac{1}{(\mathbf{k}-\mathbf{n})!}\mathbf{x}_{i'i''}^{\mathbf{k}-\mathbf{n}}\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) \quad (\mathbf{L2L}) \qquad (12)
\end{aligned}$$

To summarize the 6 stages,

$$u(\mathbf{x}_i) = G(\mathbf{x}_{ij})q(\mathbf{x}_j) \tag{\textbf{P2P}}$$

$$\mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j'}) = \frac{1}{\mathbf{n}!}\mathbf{x}_{j'j}^{\mathbf{n}}q(\mathbf{x}_j) \tag{\textbf{P2M}}$$

$$\mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j''}) = \sum_{\mathbf{k}=0}^{\mathbf{n}} \frac{1}{(\mathbf{n}-\mathbf{k})!}\mathbf{x}_{j''j'}^{\mathbf{n}-\mathbf{k}}\mathbf{M}^{\mathbf{k}}(\mathbf{x}_{j'}) \tag{\textbf{M2M}}$$

$$\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) = \sum_{\mathbf{n}=0}^{p-\mathbf{k}} \nabla^{(\mathbf{n}+\mathbf{k})}G(\mathbf{x}_{i''j''})\mathbf{M}^{\mathbf{n}}(\mathbf{x}_{j''}) \tag{\textbf{M2L}}$$

$$\mathbf{L}^{\mathbf{n}}(\mathbf{x}_{i'}) = \sum_{\mathbf{k}=\mathbf{n}}^{p} \frac{1}{(\mathbf{k}-\mathbf{n})!}\mathbf{x}_{i'i''}^{\mathbf{k}-\mathbf{n}}\mathbf{L}^{\mathbf{k}}(\mathbf{x}_{i''}) \tag{\textbf{L2L}}$$

$$u(\mathbf{x}_i) \approx \sum_{\mathbf{k}=0}^{p} \frac{1}{\mathbf{k}!}\mathbf{x}_{ii'}^{\mathbf{k}}\mathbf{L}^{\mathbf{k}}(\mathbf{x}_i') \tag{\textbf{L2P}}$$

By defining the function

$$T_{\mathbf{n}} = \frac{1}{\mathbf{n}!}\nabla^{(\mathbf{n})}G(\mathbf{x}_{i''j''}) \tag{13}$$

the following recursive relation can be used to determine the derivative terms for the M2L translation

$$||\mathbf{n}||\ ||\mathbf{x}||T_{\mathbf{n}} = -(2||\mathbf{n}||-1)\sum_{i=1}^{3} x_i T_{\mathbf{n}-e_i} - (||\mathbf{n}||-1)\sum_{i=1}^{3} T_{\mathbf{n}-2e_i} \tag{14}$$

where

$$\begin{aligned}
||\mathbf{n}|| &= n_x + n_y + n_z \\
||\mathbf{x}|| &= x^2 + y^2 + z^2 \\
\mathbf{n} - e_1 &= \{n_x - 1, n_y, n_z\} \\
\mathbf{n} - e_2 &= \{n_x, n_y - 1, n_z\} \\
\mathbf{n} - e_3 &= \{n_x, n_y, n_z - 1\}
\end{aligned}$$

2 Spherical Harmonics Expansions

Spherical harmonics are the angular portion of the solution to Laplace's equation in spherical coordinates. Laplace's equation

$$\nabla^2 u = 0, \tag{15}$$

in spherical coordinates becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2} = 0. \tag{16}$$

Factoring $u(r,\theta,\phi) = R(r)Y(\theta,\phi)$ gives

$$\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = 0. \tag{17}$$

Multiplying by $r^2/(RY)$ gives

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = 0. \tag{18}$$

Separation of variables

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = \lambda, \tag{19}$$

$$\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = -\lambda. \tag{20}$$

Multiply Eq. (19) by R

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} - \lambda R = 0. \tag{21}$$

This O.D.E. has a general solution

$$R = Ar^n + Br^{-n-1}. \tag{22}$$

Without loss of generality we may set $\lambda = n(n+1)$. Next we factor $Y(\theta,\phi) = P(\theta)E(\phi)$ in Eq. (20)

$$\frac{1}{P\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P}{\partial\theta}\right) + \frac{1}{E\sin^2\theta}\frac{\partial^2 E}{\partial\phi^2} = -n(n+1). \tag{23}$$

Multiply by P

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P}{\partial\theta}\right) + n(n+1)P + \frac{P}{E\sin^2\theta}\frac{\partial^2 E}{\partial\phi^2} = 0. \tag{24}$$

Separation of variables

$$
\begin{aligned}
\frac{1}{E}\frac{\partial^2 E}{\partial \phi^2} &= -m^2, &(25)\\
\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P}{\partial\theta}\right) + n(n+1)P &= \frac{m^2 P}{\sin^2\theta}. &(26)
\end{aligned}
$$

Multiply Eq. (25) by E

$$
\frac{d^2 E}{d\phi^2} + m^2 E = 0. \tag{27}
$$

This O.D.E. has a general solution

$$
E = e^{im\phi}. \tag{28}
$$

Next we change variables $x = \cos\theta$ in Eq. (26)

$$
\frac{d}{dx}(1-x^2)\frac{dP}{dx} + n(n+1)P - \frac{m^2}{1-x^2}P = 0. \tag{29}
$$

This is the general Legendre equation. When $m = 0$ (azimuthally symmetric) it becomes Legendre's equation

$$
\frac{d}{dx}(1-x^2)\frac{dP}{dx} + n(n+1)P = 0, \tag{30}
$$

where the solution is the Legendre polynomial

$$
P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \tag{31}
$$

The canonical solution to the general Legendre equation (29) is the associated Legendre polynomial

$$
P_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}(P_n(x)). \quad (m \geq 0) \tag{32}
$$

The general Legendre equation (29) is invariant under a change in sign of m. By substituting Eq. (31) into Eq. (32) the associated Legendre polynomial can be expressed in the form

$$
P_n^m(x) = \frac{(-1)^m}{2^n n!}(1-x^2)^{m/2}\frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n. \tag{33}
$$

Therefore, we may extend the range of m to $-n \leq m \leq n$ by finding the proportionality constants C_n^m to equate both sides of $P_n^{-m} = C_n^m P_n^m$, hence

$$
\frac{d^{n-m}}{dx^{n-m}}(x^2-1)^n = C_n^m(1-x^2)^m\frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n. \tag{34}
$$

From this we obtain

$$C_n^m = (-1)^m \frac{(n-m)!}{(n+m)!}, \tag{35}$$

and therefore

$$P_n^{-m}(x) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(x). \tag{36}$$

Since $Y(\theta,\phi) = P(\theta)E(\phi)$ is the product of Eqs. (28) and (32) it can be written as

$$Y_n^m(\theta,\phi) = P_n^m(\cos\theta)e^{im\phi}. \tag{37}$$

for $0 \le m \le n$. For $-n \le m \le n$ we may use Eq. (36) to obtain

$$Y_n^m(\theta,\phi) = \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta)e^{im\phi} \tag{38}$$

This definition of spherical harmonics satisfies the property

$$Y_n^{m*}(\theta,\phi) = (-1)^m Y_n^{-m}(\theta,\phi) \tag{39}$$

If we redefine the spherical harmonics to be

$$Y_n^m(\theta,\phi) = (-1)^m \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta)e^{im\phi} \tag{40}$$

it will have conjugate symmetry

$$Y_n^{m*}(\theta,\phi) = Y_n^{-m}(\theta,\phi) \tag{41}$$

From Eq. 22 we can add back the radial component $u(r,\theta,\phi) = R(r)Y(\theta,\phi)$. We define the harmonic outer function O_n^m and inner function I_n^m

$$O_n^m(r,\theta,\phi) = \frac{(-1)^n i^{|m|}}{A_n^m} \frac{Y_n^m(\theta,\phi)}{r^{n+1}} \tag{42}$$

$$I_n^m(r,\theta,\phi) = i^{-|m|} A_n^m r^n Y_n^m(\theta,\phi) \tag{43}$$

where

$$A_n^m = A_n^{-m} = \frac{(-1)^n}{\sqrt{(n-m)!(n+m)!}} \tag{44}$$