FMM CMSC 878R/AMSC 698R

Lecture 20

Outline

- 3D Laplace equation
- Multipole and local expansions
- Special functions
  - Legendre polynomials
  - Associated Legendre functions
  - Spherical harmonics
- Translations of elementary solutions
- Rotations of elementary solutions
- Coaxial Translation-Rotation decomposition

Translation and Differentiation Properties for Laplace Equation

If

$$\nabla^2\Phi(\mathbf{r}) = 0, \quad \mathbf{r} \in \Omega.$$

then shifted function $\Phi(\mathbf{r} - \mathbf{r}_0)$ also satisfies the Laplace equation

$$\nabla^2\Phi(\mathbf{r} - \mathbf{r}_0) = 0, \quad \mathbf{r} - \mathbf{r}_0 \in \Omega.$$

Also the Laplace operator is commutative with differential operators

$$D_x = \frac{\partial}{\partial x}, \quad D_y = \frac{\partial}{\partial y}, \quad D_z = \frac{\partial}{\partial z}, \quad \text{or} \quad D_{\mathbf{t}} = \mathbf{t} \cdot \nabla,$$

So

$$D_{\mathbf{t}}\nabla^2\Phi(\mathbf{r}) = \nabla^2 D_{\mathbf{t}}\Phi(\mathbf{r}).$$

Introduction of Multipoles for Laplace Equation

$$\Phi_n(\mathbf{r}) = (-1)^n D_{\mathbf{t}_1} D_{\mathbf{t}_2} \ldots D_{\mathbf{t}_n} \Phi(\mathbf{r})$$

also satisfy the Laplace equation. In case when $\Phi(\mathbf{r}) = G(\mathbf{r}) = |\mathbf{r}|^{-1}$ functions

$$G_n(\mathbf{r}) = (-1)^n D_{\mathbf{t}_1} D_{\mathbf{t}_2} \ldots D_{\mathbf{t}_n} \frac{1}{|\mathbf{r}|}, \quad |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2} \neq 0$$

are called MULTIPOLES OF DEGREE n centered at $\mathbf{r} = \mathbf{0}$. Vectors $\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_n$ are called multole generating vectors. Also $G_n(\mathbf{r})$ can be represented as

$$G_n(\mathbf{r}) = \sum_{i+j+k=n} Q_{ijk}^{(n)} \frac{\partial^n}{\partial x^i \partial y^j \partial z^k} \frac{1}{|\mathbf{r}|},$$

where $Q_{ijk}^{(n)}$ are called 'components of the multipole momentum'.

$n = 0$: 'monopole'

$n = 1$: 'dipole'

$n = 2$: 'quadrupole'

$n = 3$: 'octupole'.

Multipole Expansion of Laplace Equation Solutions

$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty} b_n G_n(\mathbf{r}),$$

$$G_n(\mathbf{r}) = \sum_{i+j+k=n} Q_{ijk}^{(n)} \frac{\partial^n}{\partial x^i \partial y^j \partial z^k} \frac{1}{|\mathbf{r}|}.$$

Legendre Polynomials

Legendre polynomials $P_n(\mu)$ can be introduced via generating function

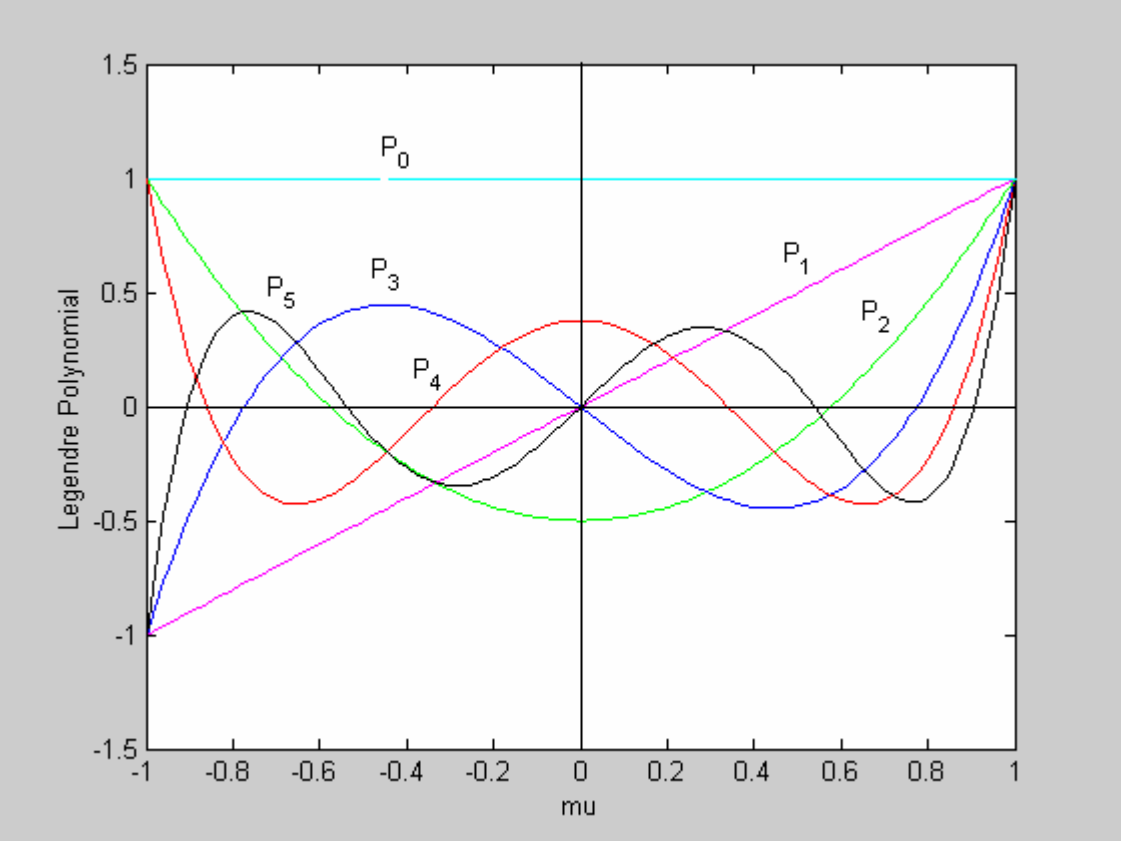
$$\frac{1}{\sqrt{1-2\mu x+x^2}} = \begin{cases} \sum_{n=0}^{\infty} P_n(\mu)x^n, & |x|<1, \\ \sum_{n=0}^{\infty} P_n(\mu)x^{-n-1}, & |x|>1. \end{cases}$$

First few polynomials

$$P_0(\mu) = 1,$$
$$P_1(\mu) = \mu = \cos\theta,$$
$$P_2(\mu) = \frac{1}{2}(3\mu^2-1) = \frac{1}{4}(3\cos 2\theta + 1),$$
$$\ldots$$

Legendre Polynomials (2)

First six polynomials ($n = 0,\ldots,5$):



Legendre Polynomials (3)

Some Properties:

- The Rodrigues' formula

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

- Form orthogonal complete basis in $L_2[-1,1]$:

$$\int_{-1}^{1} P_n(\mu)P_m(\mu)d\mu = \begin{cases} \frac{2}{2n+1}, & m = n, \\ 0, & m \neq n. \end{cases}$$

A lot of other nice properties!

Expansion/Translation of Fundamental Solution

$$G(\mathbf{r}) = \frac{1}{r}, \quad r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2},$$

then

$$G(\mathbf{r} - \mathbf{r}_0) = \frac{1}{|\mathbf{r} - \mathbf{r}_0|} = \frac{1}{\sqrt{(\mathbf{r} - \mathbf{r}_0) \cdot (\mathbf{r} - \mathbf{r}_0)}} = \frac{1}{\sqrt{r^2 - 2\mathbf{r} \cdot \mathbf{r}_0 + r_0^2}}$$

$$= \frac{1}{\sqrt{r^2 - 2rr_0 \cos\theta + r_0^2}} = \frac{1}{\sqrt{r^2 - 2\mu r r_0 + r_0^2}}$$

$$= \begin{cases} r_0^{-1} \sum_{n=0}^{\infty} P_n(\mu)(r/r_0)^n, & r < r_0, \\ r^{-1} \sum_{n=0}^{\infty} P_n(\mu)(r_0/r)^n = r_0^{-1} \sum_{n=0}^{\infty} P_n(\mu)(r/r_0)^{-n-1}, & r > r_0. \end{cases}$$

At $r = r_0$ the series also converges, if $\cos\theta \neq 1$ ($\mathbf{r} \neq \mathbf{r}_0$).

Addition Theorem for Spherical Harmonics

Spherical Harmonics

$$P_n(\cos\theta) = \frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_n^{-m}(\theta',\varphi')Y_n^m\left(\hat{\theta},\hat{\varphi}\right),$$

order

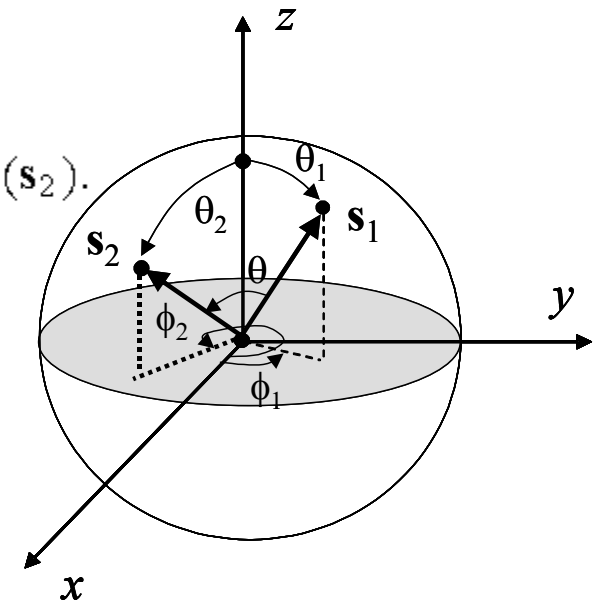
$$Y_n^m(\theta,\varphi) = (-1)^m\sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}P_n^{|m|}(\mu)e^{im\varphi}, \quad \mu = \cos\theta.$$

where θ is the angle between two points on a sphere with spherical angles (θ',φ') and $\left(\hat{\theta},\hat{\varphi}\right)$.

degree

$$P_n(\mathbf{s}_1\cdot\mathbf{s}_2) = \frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_n^{-m}(\mathbf{s}_1)Y_n^m(\mathbf{s}_2) = \frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_n^m(\mathbf{s}_1)Y_n^{-m}(\mathbf{s}_2).$$

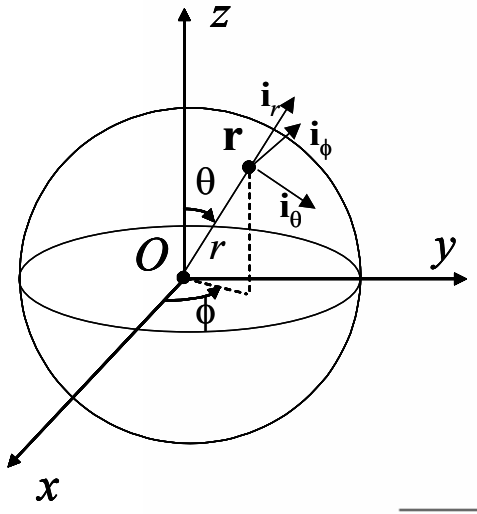
Vector form of the addition theorem



S- and R- expansions of Fundamental Solution

$$\frac{1}{|\mathbf{r}-\mathbf{r}_0|} = \frac{4\pi}{r_0}\sum_{n=0}^{\infty}\frac{1}{2n+1}\left(\frac{r}{r_0}\right)^n\sum_{m=-n}^{n}Y_n^{-m}(\theta',\varphi')Y_n^m\left(\hat{\theta},\hat{\varphi}\right), \quad r<r_0,$$

$$\frac{1}{|\mathbf{r}-\mathbf{r}_0|} = \frac{4\pi}{r_0}\sum_{n=0}^{\infty}\frac{1}{2n+1}\left(\frac{r_0}{r}\right)^{n+1}\sum_{m=-n}^{n}Y_n^{-m}(\theta',\varphi')Y_n^m\left(\hat{\theta},\hat{\varphi}\right), \quad r>r_0.$$



$$\mathbf{r} = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta),$$

$$R_n^m(\mathbf{r}) = r^n Y_n^m(\theta,\varphi),$$

$$S_n^m(\mathbf{r}) = r^{-n-1} Y_n^m(\theta,\varphi),$$

Multipole (!)

$$\frac{1}{4\pi|\mathbf{r}-\mathbf{r}_0|} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{1}{2n+1}S_n^{-m}(\mathbf{r}_0)R_n^m(\mathbf{r}), \quad r<r_0,$$

$$\frac{1}{4\pi|\mathbf{r}-\mathbf{r}_0|} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{1}{2n+1}R_n^{-m}(\mathbf{r}_0)S_n^m(\mathbf{r}), \quad r>r_0.$$

`Multipole expansion` means S-expansion

Compare

$$\frac{1}{4\pi|\mathbf{r}-\mathbf{r}_0|}=\sum_{n=0}^{\infty}b_nG_n(\mathbf{r}),\quad G_n(\mathbf{r})=\sum_{i+j+k=n}Q_{ijk}^{(n)}\frac{\partial^n}{\partial x^i\partial y^j\partial z^k}\frac{1}{|\mathbf{r}|}.$$

and

$$\frac{1}{4\pi|\mathbf{r}-\mathbf{r}_0|}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{1}{2n+1}R_n^{-m}(\mathbf{r}_0)S_n^m(\mathbf{r}),\quad r>r_0.$$

$$b_n\sum_{i+j+k=n}Q_{ijk}^{(n)}\frac{\partial^n}{\partial x^i\partial y^j\partial z^k}\frac{1}{|\mathbf{r}|}=\sum_{m=-n}^{n}\frac{1}{2n+1}R_n^{-m}(\mathbf{r}_0)S_n^m(\mathbf{r}).$$

Generally

$$\sum_{i+j+k=n}Q_{ijk}^{(n)}\frac{\partial^n}{\partial x^i\partial y^j\partial z^k}\frac{1}{|\mathbf{r}|}=\sum_{m=-n}^{n}q_n^mS_n^m(\mathbf{r})=\frac{1}{r^{n+1}}\sum_{m=-n}^{n}q_n^mY_n^m(\theta,\varphi).$$

Associated Legendre Functions

$$P_n^m(\mu) = \frac{(-1)^m}{2^m}\frac{(n+m)!}{(n-m)!m!}(1-\mu^2)^{m/2}F\left(m-n, m+n+1; m+1; \frac{1-\mu}{2}\right)$$

$$= \frac{(-1)^m}{2^m}\frac{(n+m)!}{(n-m)!m!}(1-\mu^2)^{m/2}\sum_{l=0}^{n-m}\frac{(-1)^l(n-m-l+1)_l(n+m+1)_l}{2^l l!(m+1)_l}(1-\mu)^l,$$

where $(n)_l$ is the Pochhammer's symbol:

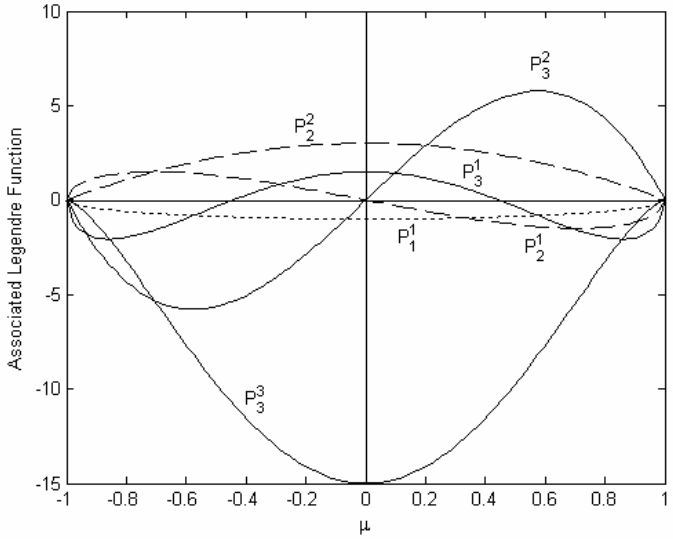
$$(n)_0 = 1, \quad (n)_l = \frac{(n+l-1)!}{(n-1)!}.$$

This formula yields the following particular functions:

$$P_1^1(\mu) = -(1-\mu^2)^{1/2}, \quad P_2^1(\mu) = -3\mu(1-\mu^2)^{1/2}, \quad P_2^2(\mu) = 3(1-\mu^2).$$

$$(P_n^m, P_l^m) = \int_{-1}^{1} P_n^m(\mu)P_l^m(\mu)\mathrm{d}\mu = \frac{2}{2n+1}\frac{(n+m)!}{(n-m)!}\delta_{nl}.$$

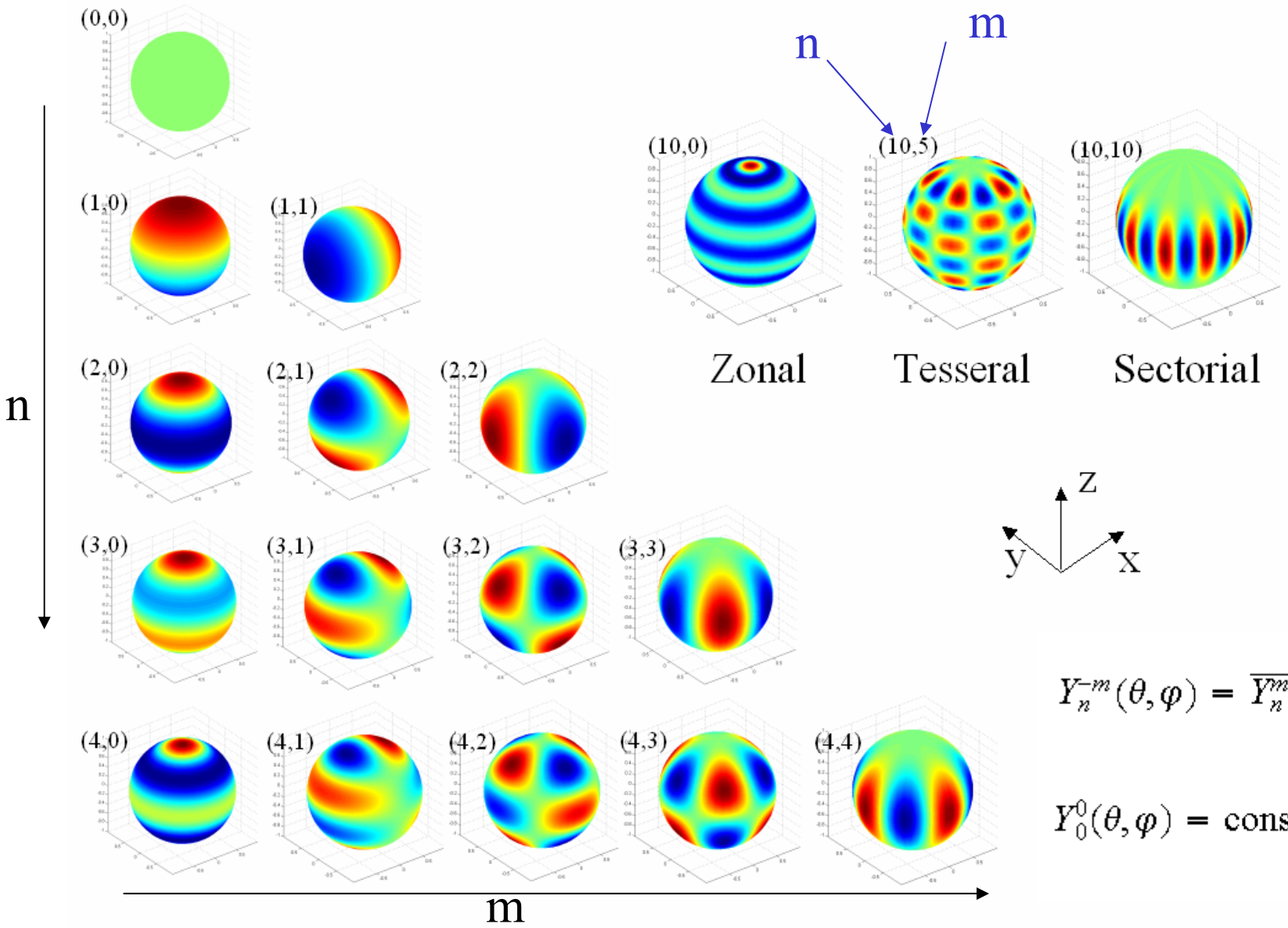
Orthogonal!



Spherical Harmonics

$$Y_n^m(\theta,\varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}\, P_n^{|m|}(\cos\theta) e^{im\varphi},$$

$$n = 0, 1, 2, \ldots; \qquad m = -n, \ldots, n.$$



$$Y_n^{-m}(\theta,\varphi) = \overline{Y_n^m(\theta,\varphi)}.$$

$$Y_0^0(\theta,\varphi) = \text{const} = \sqrt{\frac{1}{4\pi}}.$$

Orthonormality of Spherical Harmonics

The scalar product of two spherical harmonics in $L_2(S_u)$ is

$$\left(Y_n^m, Y_{n'}^{m'}\right) = \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} Y_n^m(\theta,\varphi)\bar{Y}_{n'}^{m'}(\theta,\varphi)\mathrm{d}\varphi = \delta_{mm'}\delta_{nn'}.$$

Expansion of an arbitrary surface function over the basis of spherical harmonics:

$$F(\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m Y_n^m(\theta,\varphi).$$

$$\left(F, Y_{n'}^{m'}\right) = \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} F(\theta,\varphi)\bar{Y}_{n'}^{m'}(\theta,\varphi)d\varphi.$$

$$\left(F, Y_{n'}^{m'}\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m\left(Y_n^m, Y_{n'}^{m'}\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m\delta_{mm'}\delta_{nn'} = F_{n'}^{m'}.$$

$$F_{n'}^{m'} = \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} F(\theta,\varphi)\bar{Y}_{n'}^{m'}(\theta,\varphi)\mathrm{d}\varphi.$$

R- and S- expansions of arbitrary solutions of the 3D Laplace equation

$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} [A_n^m R_n^m(\mathbf{r}) + B_n^m S_n^m(\mathbf{r})],$$

Functions regular at $\mathbf{r} = \mathbf{0}$:

$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} A_n^m R_n^m(\mathbf{r}),$$

Functions decaying at $|\mathbf{r}| \to \infty$:

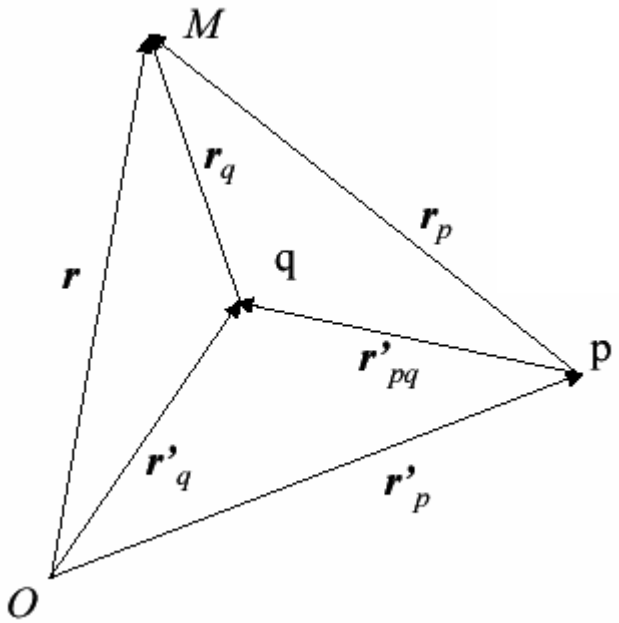
$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} B_n^m S_n^m(\mathbf{r}).$$

Translations of elementary solutions of the 3D Laplace equation

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}(\mathbf{r}'_{pq})R_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| < |\mathbf{r}'_{pq}|, \quad p \neq q.$$

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|S)_{ln}^{sm}(\mathbf{r}'_{pq})S_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| > |\mathbf{r}'_{pq}|,$$

$$R_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(R|R)_{ln}^{sm}(\mathbf{r}'_{pq})R_l^s(\mathbf{r}_q).$$



Renormalized S- and R- functions

Definition:

$$\widetilde{S}_n^m(\mathbf{r}) = O_n^m(\mathbf{r}) = \frac{(-1)^n i^{|m|}}{\alpha_n^m}\sqrt{\frac{4\pi}{2n+1}}\,S_n^m(\mathbf{r}) = \frac{(-1)^n i^{|m|}}{\alpha_n^m}\sqrt{\frac{4\pi}{2n+1}}\,\frac{1}{r^{n+1}}\,Y_n^m(\theta,\varphi),$$

$$\widetilde{R}_n^m(\mathbf{r}) = I_n^m(\mathbf{r}) = i^{-|m|}\alpha_n^m\sqrt{\frac{4\pi}{2n+1}}\,R_n^m(\mathbf{r}) = i^{-|m|}\alpha_n^m\sqrt{\frac{4\pi}{2n+1}}\,r^n\,Y_n^m(\theta,\varphi),$$

where

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

In the renormalized basis translation matrices are simple

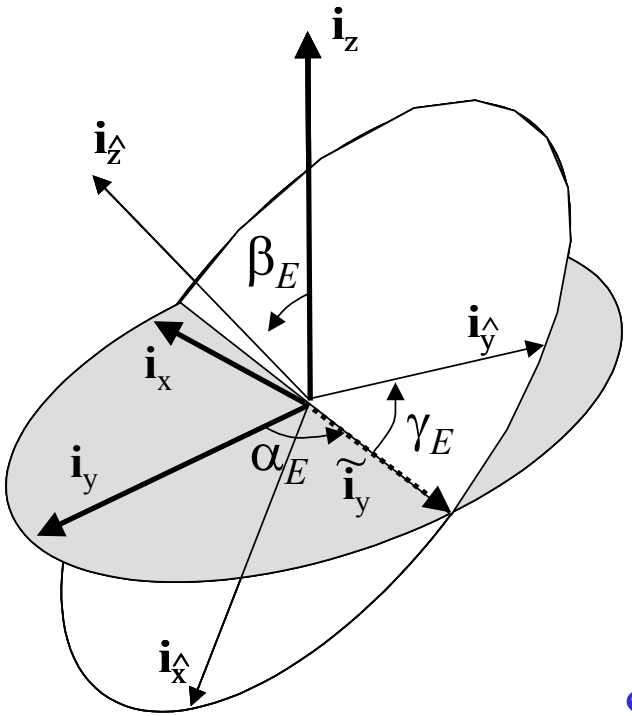
$$\left(\widetilde{S}|\widetilde{R}\right)_{n'n}^{m'm}(\mathbf{t}) = (O|\Gamma)_{n'n}^{m'm}(\mathbf{t}) = O_{n+n'}^{m-m'}(\mathbf{t}) = \widetilde{S}_{n+n'}^{m-m'}(\mathbf{t}),$$

$$\left(\widetilde{S}|\widetilde{S}\right)_{n'n}^{m'm}(\mathbf{t}) = (O|O)_{n'n}^{m'm}(\mathbf{t}) = I_{n'-n}^{m-m'}(\mathbf{t}) = \widetilde{R}_{n'-n}^{m-m'}(\mathbf{t}),$$

$$\left(\widetilde{R}|\widetilde{R}\right)_{n'n}^{m'm}(\mathbf{t}) = (I|\Gamma)_{n'n}^{m'm}(\mathbf{t}) = I_{n-n'}^{m-m'}(\mathbf{t}) = \widetilde{R}_{n-n'}^{m-m'}(\mathbf{t}).$$

These are structured matrices (2D Toeplitz-Hankel type)
Fast translation procedures are possible
(e.g. see $O(p^2 \log p)$ algorithm in **W.D. Elliott & J.A. Board, Jr.:**
``Fast Fourier Transform Accelerated Fast Multipole Algorithm"
SIAM J. Sci. Comput. Vol. 17, No. 2, pp. 398-415, 1996).

Rotations of coordinates



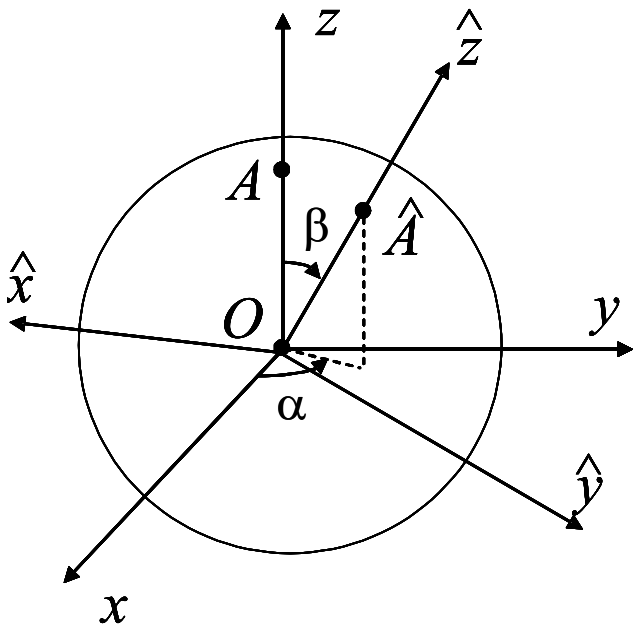
Rotation Matrix

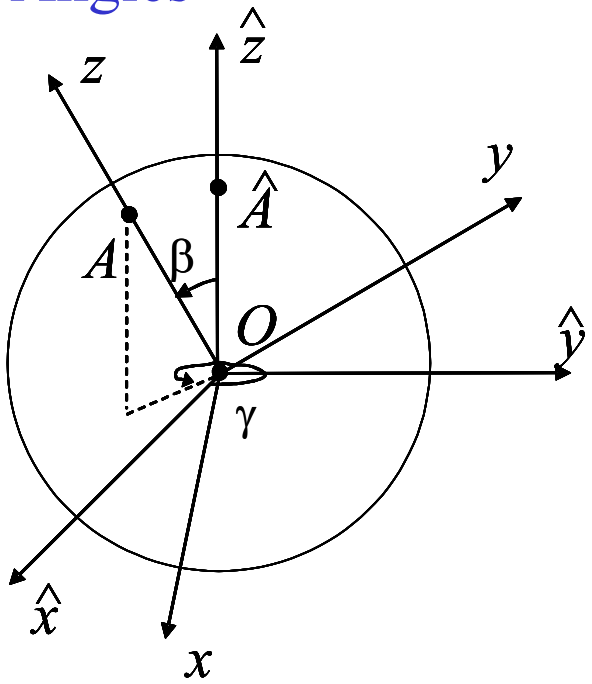
$$Q = \begin{bmatrix} \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_z \end{bmatrix}$$

Euler Angles

$$\alpha_E = \pi - \alpha, \quad \beta_E = \beta, \quad \gamma_E = \gamma.$$

Spherical Polar Angles





Rotations of elementary solutions of the 3D Laplace equation

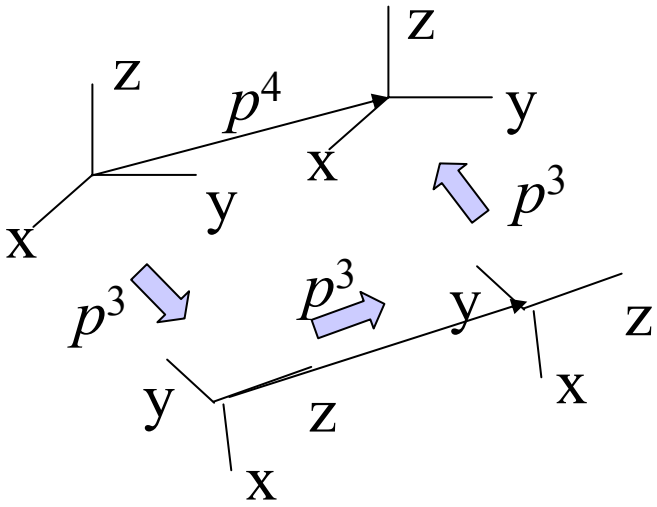
Rotations

$$Y_n^m(\theta,\varphi) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q) Y_n^{\nu}\left(\hat{\theta},\hat{\varphi}\right),$$

$$S_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q) S_n^{\nu}(\hat{\mathbf{r}}_p), \qquad |\hat{\mathbf{r}}_p| = |\mathbf{r}_p|,$$

$$R_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q) R_n^{\nu}(\hat{\mathbf{r}}_p), \qquad |\hat{\mathbf{r}}_p| = |\mathbf{r}_p|,$$

Rotation-Coaxial Translation Decomposition



Coaxial Translation

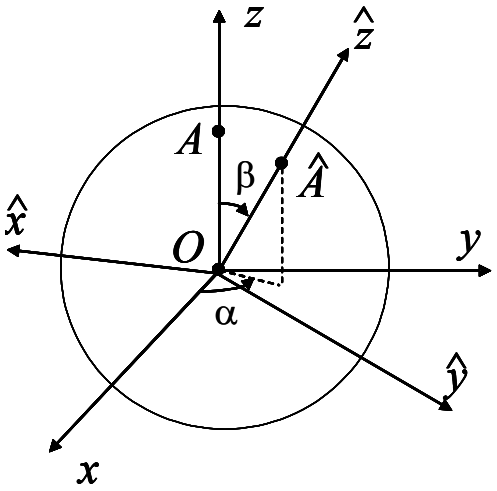
$$S_n^m(\vec{\mathbf{r}}+\mathbf{i}_z d)=\sum_{l=|m|}^{\infty}(S|R)_{ln}^m(d)R_l^m(\vec{\mathbf{r}}),\qquad |\vec{\mathbf{r}}|<d,$$

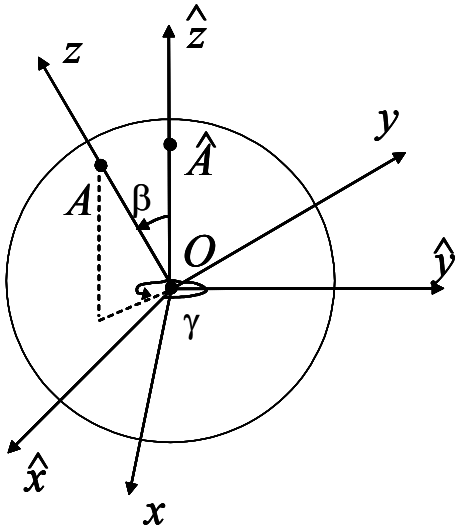
$$S_n^m(\vec{\mathbf{r}}+\mathbf{i}_z d)=\sum_{l=|m|}^{\infty}(S|S)_{ln}^m(d)S_l^m(\vec{\mathbf{r}}),\qquad |\vec{\mathbf{r}}|>d,$$

$$R_n^m(\vec{\mathbf{r}}+\mathbf{i}_z d)=\sum_{l=|m|}^{\infty}(R|R)_{ln}^m(d)R_l^m(\vec{\mathbf{r}}).$$

$$(E|F)_{ln}^m(d)=\left[(E|F)_{ln}^{mm}(\mathbf{d})\right]_{\theta'_{\mathbf{d}}=0},\qquad E,F=S,R.$$

Rotation





$$Y_n^m(\theta,\varphi)=\sum_{\nu=n}^{n}T_n^{\nu m}(\mathcal{Q})Y_n^{\nu}\left(\hat{\theta},\hat{\varphi}\right),$$

$$\mathcal{Q}=\begin{bmatrix}\mathbf{i}_{\hat{x}}\cdot\mathbf{i}_x & \mathbf{i}_{\hat{x}}\cdot\mathbf{i}_y & \mathbf{i}_{\hat{x}}\cdot\mathbf{i}_z\\ \mathbf{i}_{\hat{y}}\cdot\mathbf{i}_x & \mathbf{i}_{\hat{y}}\cdot\mathbf{i}_y & \mathbf{i}_{\hat{y}}\cdot\mathbf{i}_z\\ \mathbf{i}_{\hat{z}}\cdot\mathbf{i}_x & \mathbf{i}_{\hat{z}}\cdot\mathbf{i}_y & \mathbf{i}_{\hat{z}}\cdot\mathbf{i}_z\end{bmatrix}.$$

Decomposition into Subspaces

$$\Phi^p(\mathbf{r}) = \sum_{n=0}^{p}\sum_{m=-n}^{n} A_n^m F_n^m(\mathbf{r}) = \sum_{m=-p}^{p}\sum_{n=|m|}^{p} A_n^m F_n^m(\mathbf{r}) = \mathbf{A}\cdot\mathbf{F}, \quad F = S,R.$$

$$\mathbf{A} = \mathbf{A}^0 \oplus \mathbf{A}^{\pm 1} \oplus \ldots = \sum_{m=-\infty}^{\infty} \oplus \mathbf{A}^m,$$

where

$$\mathbf{A}^m = \left(A_{|m|}^m, A_{|m|+1}^m, A_{|m|+2}^m, \ldots\right)^T, \quad m = 0, \pm 1, \pm 2, \ldots,$$

and as the direct sum of finite blocks $\mathbf{A}_n$ corresponding to degree m :

$$\mathbf{A} = \mathbf{A}_0 \oplus \mathbf{A}_1 \oplus \ldots = \sum_{n=0}^{\infty} \oplus \mathbf{A}_n,$$

where

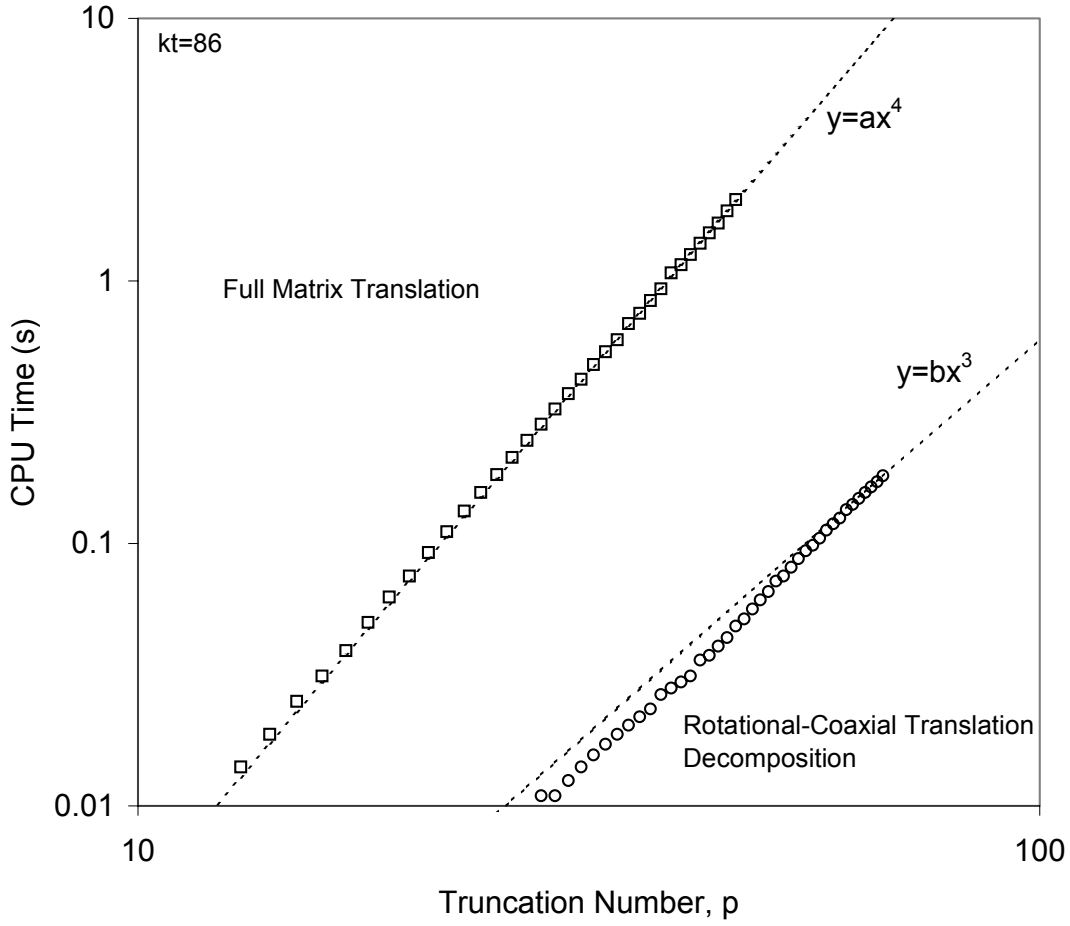
$$\mathbf{A}_n = (A_n^{-n}, \ldots, A_n^n)^T, \quad n = 0, 1, 2, \ldots.$$

So the coaxial translation operator has invariant subspaces at fixed order, *m*, while the rotation operator has invariant subspaces at fixed degree, *n*.

Coaxial Translation:

$$(\mathbf{S}|\mathbf{R})=(\mathbf{S}|\mathbf{R})^{0}\oplus(\mathbf{S}|\mathbf{R})^{\pm 1}\oplus\ldots=\sum_{m=-\infty}^{\infty}\oplus(\mathbf{S}|\mathbf{R})^{m},$$

Rotation

$$(\mathbf{S}|\mathbf{R})=(\mathbf{S}|\mathbf{R})_{0}\oplus(\mathbf{S}|\mathbf{R})_{1}\oplus\ldots=\sum_{n=0}^{\infty}\oplus(\mathbf{S}|\mathbf{R})_{n},$$

Comparison of Direct Matrix Translation and Coaxial Translation-Rotation Decomposition