MAIT 627 Fast Multipole Methods

Lecture 10

Outline

- Laplace equation in 2D and 3D: Problem statement
- Laplace equation in 2D: $O(p^2)$ method
  - Normalized basis functions
  - Translation operators
  - Error bounds
- Laplace equation in 3D: $O(p^4)$ method
  - Normalized basis functions
  - Translation operators
  - Error bounds
- Asymptotically faster translation methods
  - Use of the FFT: 2D Laplace: $O(p\log p)$, 3D Laplace: $O(p^2\log p)$
  - RCR-decomposition for 3D Laplace: $O(p^3)$
  - Reduction of asymptotic constants: Exponential forms for 2D: $O(p^2)$ and 3D: $O(p^3)$

Problems resulting in summation of large amount of singularities for Laplace equation

- Stellar and molecular dynamics
- Boundary element method (fluid dynamics, electrostatics, etc.)
- Vortex element method (fluid dynamics)
- Theory of functions of complex variable
- Many more…

Example 1: Stellar and molecular dynamics

N-body motion under Newton's gravity forces

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, j\neq i}^{N} \frac{m_j}{r_{ij}^3}(\mathbf{r}_i - \mathbf{r}_j) = G \sum_{j=1, j\neq i}^{N} m_j \nabla \frac{1}{|\mathbf{r} - \mathbf{r}_j|}\bigg|_{\mathbf{r}=\mathbf{r}_j}$$

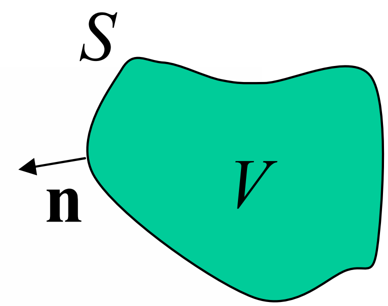
$$= \nabla \sum_{j=1, j\neq i}^{N} q_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|}\bigg|_{\mathbf{r}=\mathbf{r}_i}, \quad q_j = Gm_j.$$

or

$$\phi(\mathbf{r}) = \sum_{j=1, \mathbf{r}\neq\mathbf{r}_j}^{N} q_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|}, \quad \ddot{\mathbf{r}}_i = \nabla\phi(\mathbf{r}_i).$$

Similarly potential for Coulomb electrostatic forces.

Example 2: Boundary element method



$$\nabla^2 \phi(\mathbf{x}) = 0, \quad \mathbf{x} \in V,$$

$$\alpha\phi + \beta\frac{\partial \phi}{\partial n} = \gamma, \quad \mathbf{x} \in S.$$

$$\phi(\mathbf{y}) = \int_S \left(G(\mathbf{x},\mathbf{y})\frac{\partial \phi(\mathbf{x})}{\partial n(\mathbf{x})} - \phi(\mathbf{x})\frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})} \right) dS(\mathbf{x}), \quad \mathbf{y} \in V,$$

$$\frac{1}{2}\phi(\mathbf{y}) = \int_S \left(G(\mathbf{x},\mathbf{y})\frac{\partial \phi(\mathbf{x})}{\partial n(\mathbf{x})} - \phi(\mathbf{x})\frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})} \right) dS(\mathbf{x}), \quad \mathbf{y} \in S,$$

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}, \quad d = 3,$$

$$G(\mathbf{x},\mathbf{y}) = \ln\frac{1}{|\mathbf{x}-\mathbf{y}|}, \quad d = 2.$$

Boundary element method(2)

Surface discretization: $$\int_S = \sum_{i=1}^{N} \int_{S_i}$$

$$\int_{S_i} G(\mathbf{x},\mathbf{y}) \frac{\partial \phi(\mathbf{x})}{\partial n(\mathbf{x})} dS(\mathbf{x}) \approx \frac{\partial \phi(\mathbf{x}_i)}{\partial n(\mathbf{x}_i)} S_i K_i(\mathbf{y}),$$

$$\int_{S_i} \phi(\mathbf{x}) \frac{\partial G(\mathbf{x},\mathbf{y})}{\partial n(\mathbf{x})} dS(\mathbf{x}) \approx \phi(\mathbf{x}_i) S_i L_i(\mathbf{y}),$$

$$K_i(\mathbf{y}) \approx G(\mathbf{x}_i,\mathbf{y}), \quad L_i(\mathbf{y}) \approx \frac{\partial G(\mathbf{x}_i,\mathbf{y})}{\partial n(\mathbf{x}_i)}, \quad |\mathbf{x}_i - \mathbf{y}| > R.$$

System to solve:

$$\frac{1}{2}\phi(\mathbf{x}_j) = \sum_{i=1}^{N} K_i(\mathbf{x}_j) S_i \frac{\partial \phi(\mathbf{x}_i)}{\partial n(\mathbf{x}_i)} - \sum_{i=1}^{N} L_i(\mathbf{x}_j) S_i \phi(\mathbf{x}_i),$$

$$\alpha(\mathbf{x}_j)\phi(\mathbf{x}_j) + \beta(\mathbf{x}_j)\frac{\partial \phi(\mathbf{x}_j)}{\partial n} = \gamma(\mathbf{x}_j), \quad j = 1,\ldots,N.$$

Use iterative methods with fast matrix-vector multiplier:

$$\sum_{i=1}^{N} K_{ji} u_i = \sum_{|\mathbf{x}_i - \mathbf{x}_j| \leqslant R} K_{ji} u_i + \sum_{|\mathbf{x}_i - \mathbf{x}_j| > R} K_{ji} u_i = \sum_{|\mathbf{x}_i - \mathbf{x}_j| \leqslant R} K_{ji} u_i + \sum_{|\mathbf{x}_i - \mathbf{x}_j| > R} G(\mathbf{x}_i,\mathbf{x}_j) u_i$$

Non-FMM'able, but sparse — FMM'able, dense

2D Laplace Equation

2D Laplace equation

Laplace equation: $$\nabla^2 \Phi = 0, \quad (x, y) \in \Omega,$$

Cauchy-Riemann conditions: $$\frac{\partial \Psi}{\partial y} = \frac{\partial \Phi}{\partial x}, \quad \frac{\partial \Psi}{\partial x} = -\frac{\partial \Phi}{\partial y},$$

Complex potential: $$g(z) = \Phi(x, y) + i\Psi(x, y), \quad z = x + iy, \quad i^2 = -1,$$

Problem of summation of sources: $$g(z) = \sum_{j=1}^{N} q_j G(z - z_j), \quad G(z) = \ln \frac{1}{z}.$$

Green's function

Normalized basis functions

$$R_n(z) = \frac{(-1)^n}{n!} z^n, \quad n = 0, 1, \ldots, \quad z = x + iy,$$

$$S_0(z) = \ln \frac{1}{z}, \quad S_n(z) = \frac{(n-1)!}{z^n}, \quad n = 1, 2, \ldots.$$

Green's function expansion

$$G(z - z_0) = \ln \frac{1}{z - z_0} = \sum_{n=0}^{\infty} R_n(-z_0) S_n(z), \quad |z| > |z_0|,$$

Prove that! (Hint: $\ln(1 - x) = -(x + x^2/2 + \ldots + x^n/n + \ldots)$), $|x| < 1$).

R|R-translation operator

$$R_n(z+t) = \sum_{m=0}^{\infty} (R|R)_{mn}(t) R_m(z),$$

$$R_n(z+t) = \frac{(-1)^n (z+t)^n}{n!} = \sum_{m=0}^{n} \frac{n!\,(-1)^n}{n!\,m!(n-m)!} z^m t^{n-m}$$

$$= \sum_{m=0}^{n} \left(\frac{(-1)^m}{m!} z^m \right) \left(\frac{(-1)^{n-m}}{(n-m)!} t^{n-m} \right) = \sum_{m=0}^{n} R_{n-m}(t) R_m(z).$$

$$(R|R)_{mn}(t) = \begin{cases} R_{n-m}(t), & n \geqslant m \\ 0, & n < m. \end{cases}$$

S|S-translation operator

$$S_n(z+t) = \sum_{m=0}^{\infty} (S|S)_{mn}(t) S_m(z), \qquad |t| < |z|.$$

$n = 0$:

$$S_0(z+t) = \ln \frac{1}{z+t} = \sum_{n=0}^{\infty} R_n(t) S_n(z), \quad |t| < |z|.$$

$n > 0$:

$$S_n(z+t) = \frac{(n-1)!}{(z+t)^n} = \sum_{m=0}^{\infty} \frac{(n-1)!\,(m+n-1)!\,(-1)^m t^m}{(n-1)!m!z^{m+n}} = \sum_{m=n}^{\infty} \frac{(m-1)!(-1)^{m-n} t^{m-n}}{(m-n)!z^m} =$$

$$= \sum_{m=n}^{\infty} \left(\frac{(-1)^{m-n} t^{m-n}}{(m-n)!} \right) \left(\frac{(m-1)!}{z^m} \right) = \sum_{m=n}^{\infty} R_{m-n}(t) S_m(z), \qquad |t| < |z|.$$

$$(S|S)_{mn}(t) = \begin{cases} R_{m-n}(t), & m \geqslant n \\ 0, & m < n. \end{cases} = (R|R)_{nm}(t).$$

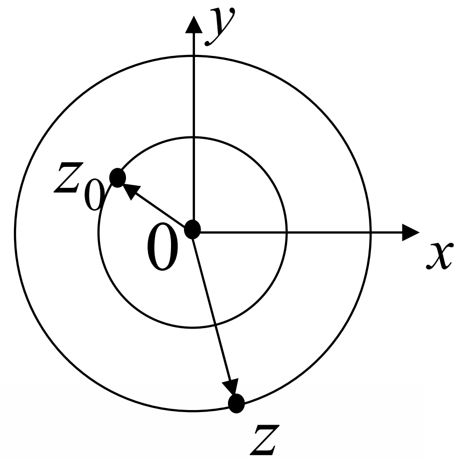
S|R-translation operator

$$S_n(z+t) = \sum_{m=0}^{\infty} (S|R)_{mn}(t) R_m(z), \qquad |z| < |t|.$$

$$S_n(z+t) = \sum_{m=n}^{\infty} R_{m-n}(z) S_m(t) = \sum_{m=0}^{\infty} S_{m+n}(t) R_m(z)$$

$$(S|R)_{mn}(t) = S_{m+n}(t).$$

Error bounds



Error of the S-expansion:

$$G(z-z_0) = \ln\frac{1}{z-z_0} = \sum_{n=0}^{\infty} R_n(-z_0)S_n(z) = \ln\frac{1}{z} + \sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{z_0}{z}\right)^n, \quad |z| > |z_0|,$$

$$|\epsilon_p| = \left|G(z-z_0) - \ln\frac{1}{z} - \sum_{n=1}^{p-1}\frac{1}{n}\left(\frac{z_0}{z}\right)^n\right| = \left|\sum_{n=p}^{\infty}\frac{1}{n}\left(\frac{z_0}{z}\right)^n\right|$$

$$\leqslant \sum_{n=p}^{\infty}\frac{1}{n}\left|\frac{z_0}{z}\right|^n = \left[\frac{1}{p}\left|\frac{z_0}{z}\right|^p + \sum_{n=1}^{\infty}\frac{1}{n+p}\left|\frac{z_0}{z}\right|^{n+p}\right]$$

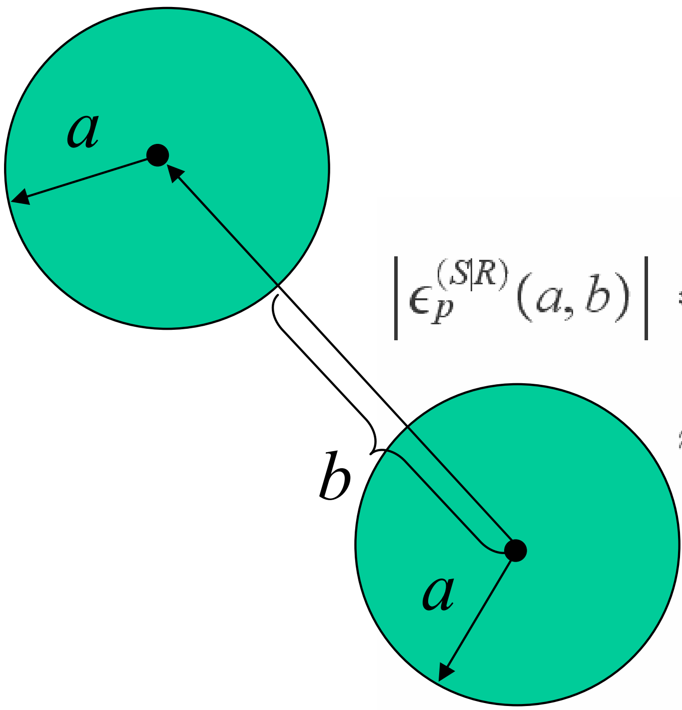
$$< \left|\frac{z_0}{z}\right|^p\left[\frac{1}{p} + \sum_{n=1}^{\infty}\frac{1}{n}\left|\frac{z_0}{z}\right|^n\right] = \left|\frac{z_0}{z}\right|^p\left[\frac{1}{p} - \ln\left(1-\left|\frac{z_0}{z}\right|\right)\right].$$

In the FMM with 1-neighborhoods:

$$\left|\frac{z_0}{z}\right| < \frac{\sqrt{2}}{3} < 0.471405, \quad |\epsilon_p| < (0.471405)^p\left[\frac{1}{p} + 0.637532\right].$$

Error bounds (2)

Translation errors: No error in S|S and R|R translations.



The error of the truncated S|R-translation can be evaluated from the theorem on the error bound of the truncated translation:

$$\left|\epsilon_p^{(S|R)}(a,b)\right| \leqslant \left[\left(1+\left|\epsilon_p^{(S)}(a,b)\right|\right)^2 - 1\right] = 2\left|\epsilon_p^{(S)}(a,b)\right| + O\left(\left|\epsilon_p^{(S)}(a,b)\right|^2\right)$$

$$\approx 2\left|\epsilon_p^{(S)}(a,b)\right| < 2\left|\frac{a}{b}\right|^p \left[\frac{1}{p} + \ln\frac{1}{1-|a/b|}\right].$$

$$\frac{a}{b} = \frac{\sqrt{2}}{2\left(2-\sqrt{2}/2\right)} = \frac{1}{2\sqrt{2}-1} < 0.54692.$$

$$\left|\epsilon_p^{(S|R)}(a,b)\right| \lesssim 2(0.54692)^p\left[\frac{1}{p} + 0.79168\right].$$

3D Laplace Equation

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

$$P_0(\mu) = 1,$$

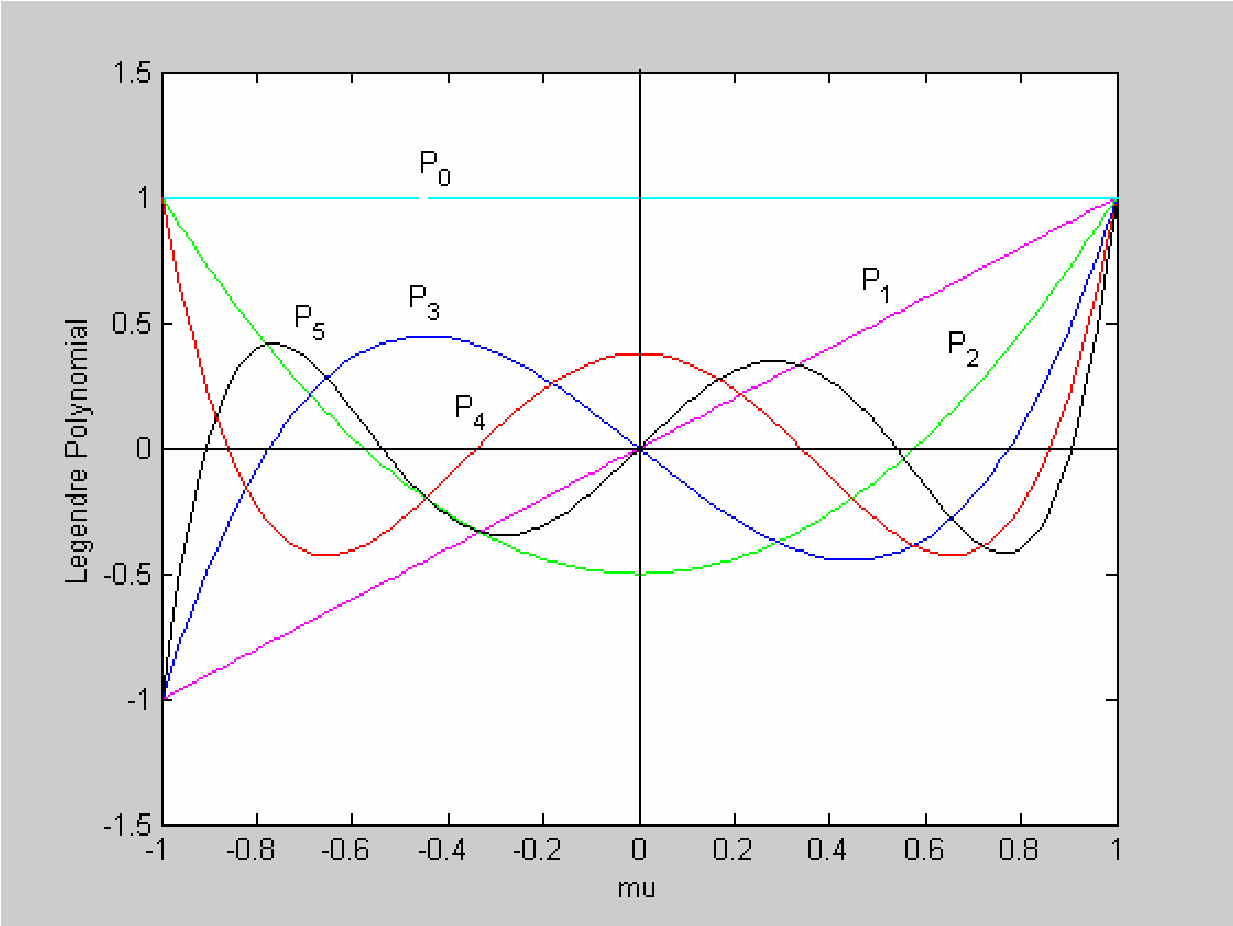
$$P_1(\mu) = \mu = \cos\theta,$$

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

$$\dots$$

Legendre Polynomials (2)

First six polynomials (n = 0,…,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

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

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

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

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

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

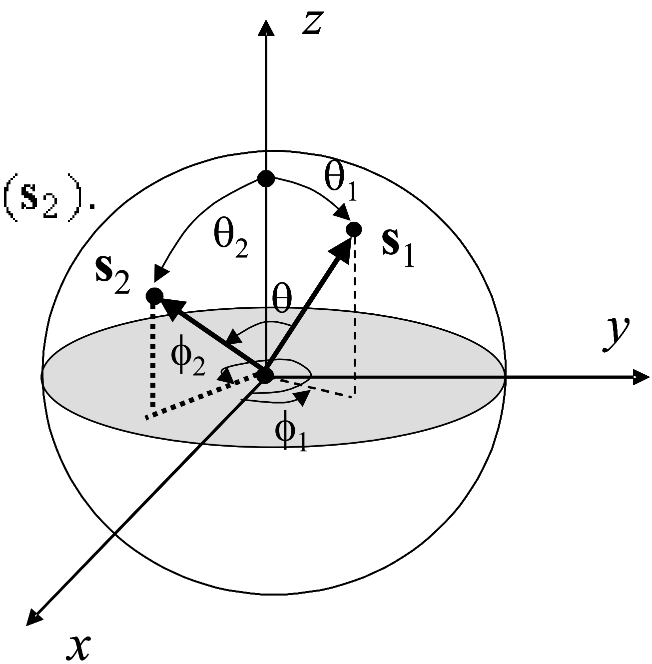
order

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

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

degree

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

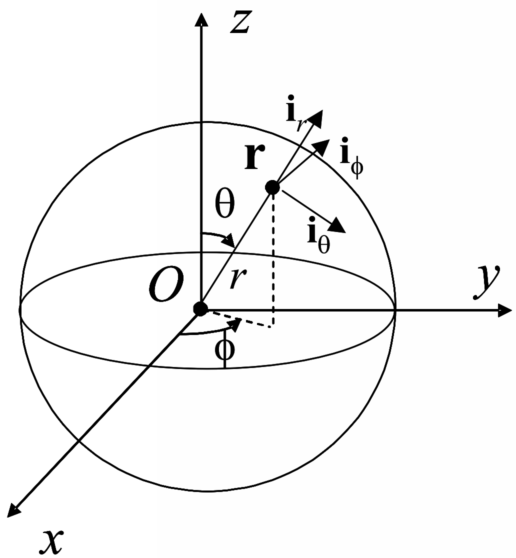


Vector form of the addition theorem

S- and R- expansions of Fundamental Solution

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

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



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

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

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

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

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

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

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:

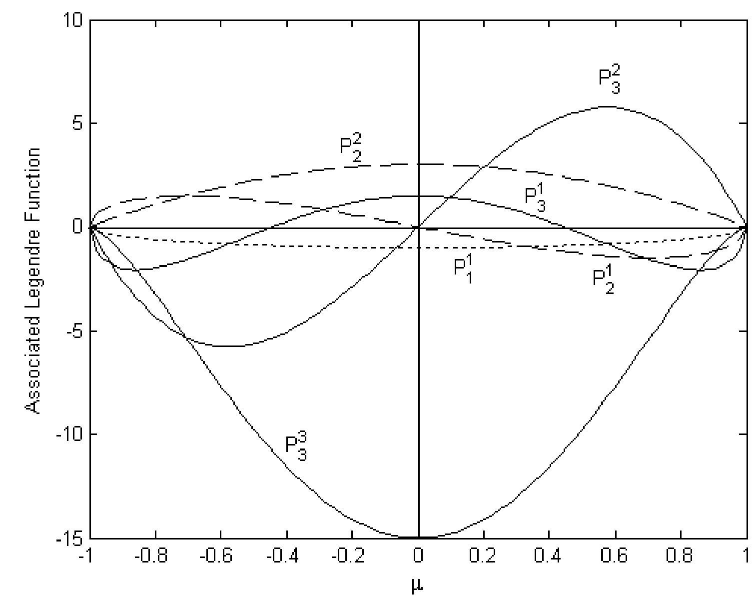
$$(n)_0 = 1, \quad (n)_l = \frac{(n+l-1)!}{(n-1)!}.$$

This formula yields the following particular functions:

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

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

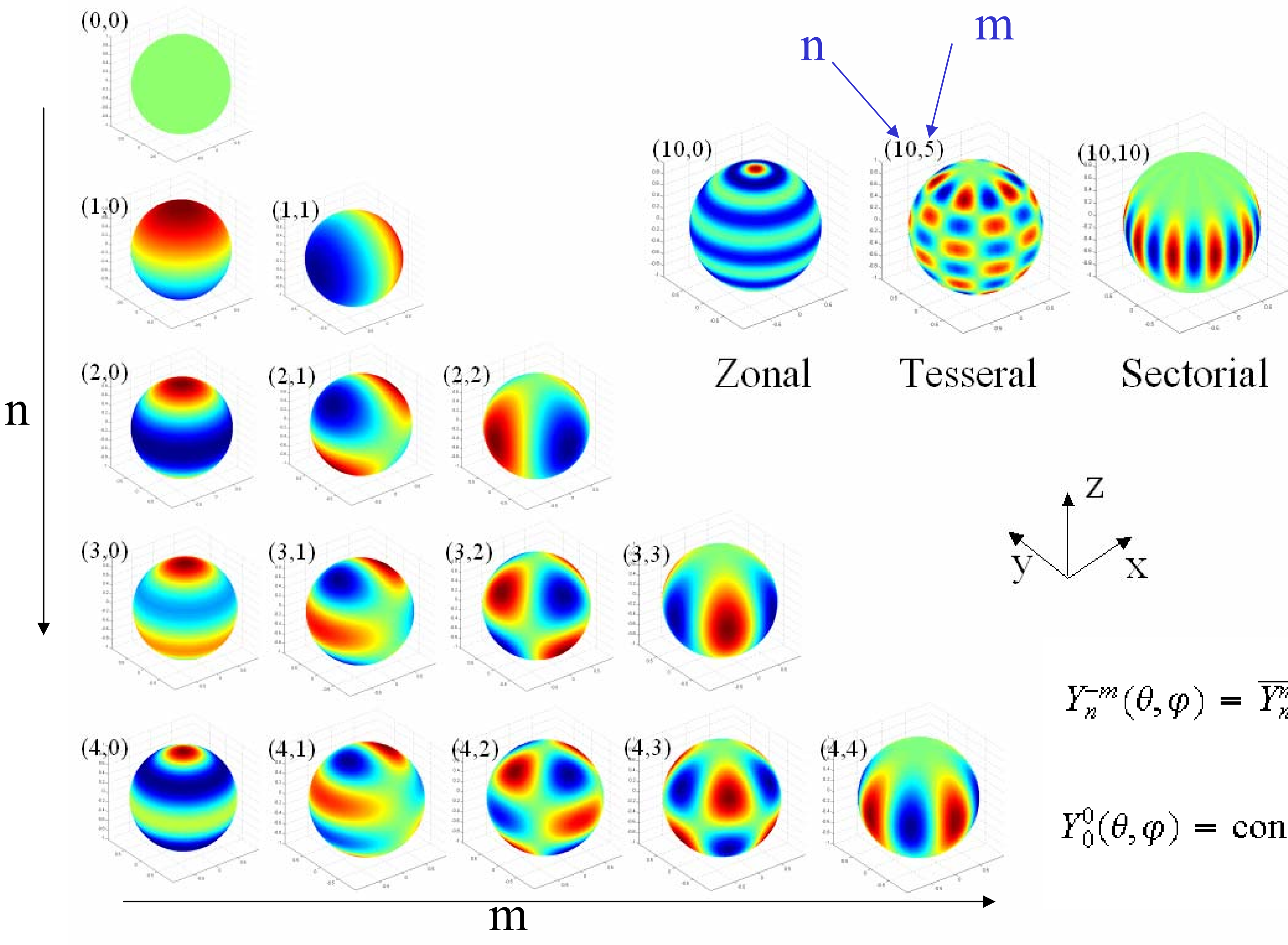
Orthogonal!



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:

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

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

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

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

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 $|\mathbf{r}| \to \infty$:

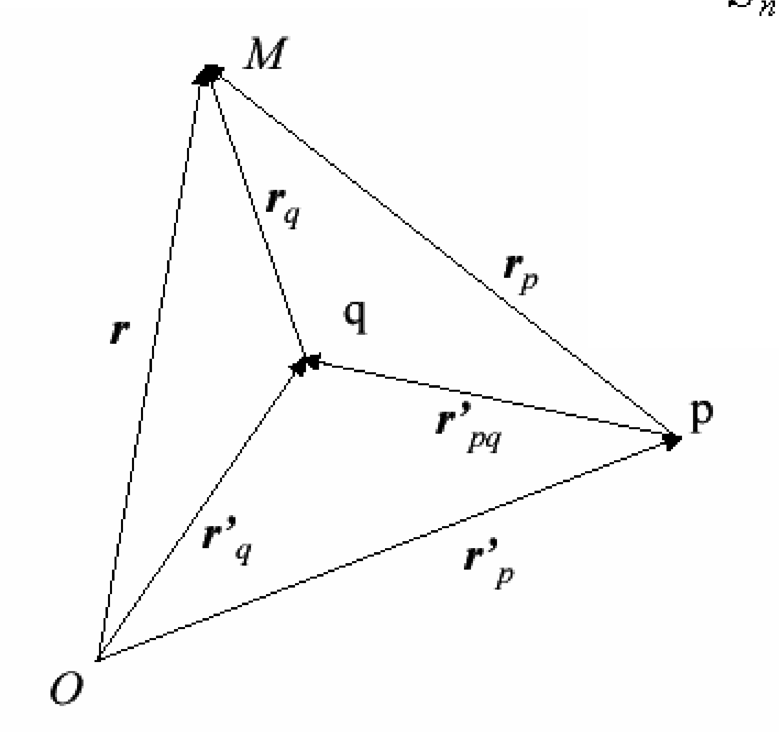
$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} B_n^m S_n^m(\mathbf{r}).$$

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

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

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

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

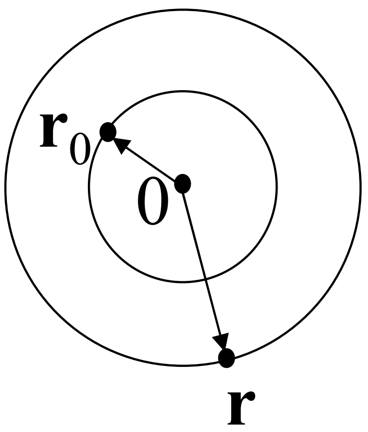
Derivation of these relations can be found in

M.A. Epton and B. Dembart,

Multipole translation theory for the three-dimensional Laplace and Helmholtz equations, *SIAM J. Sci. Comput.*, **16**(4), 1995, 865-897.

(Also in the thesis of Greengard (1988), MIT Press).

Error bounds



Error of the S-expansion:

$$G(\mathbf{r}-\mathbf{r}_0) = \frac{1}{|\mathbf{r}-\mathbf{r}_0|} = \frac{1}{r_0}\sum_{n=0}^{\infty}\left(\frac{r_0}{r}\right)^n P_n(\mu), \quad r > r_0, \quad \mu = \cos\theta = \frac{\mathbf{r}_0 \cdot \mathbf{r}}{r_0 r}.$$

$$|\epsilon_p| = \left|G(\mathbf{r}-\mathbf{r}_0) - \frac{1}{r}\sum_{n=0}^{\infty}\left(\frac{r_0}{r}\right)^n P_n(\mu)\right| = \frac{1}{r}\left|\sum_{n=p}^{\infty}\left(\frac{r_0}{r}\right)^n P_n(\mu)\right|$$

$$\leqslant \frac{1}{r}\sum_{n=p}^{\infty}\left(\frac{r_0}{r}\right)^n |P_n(\mu)| \leqslant \frac{1}{r}\sum_{n=p}^{\infty}\left(\frac{r_0}{r}\right)^n = \frac{1}{r}\left(\frac{r_0}{r}\right)^p \frac{1}{1-r_0/r}$$

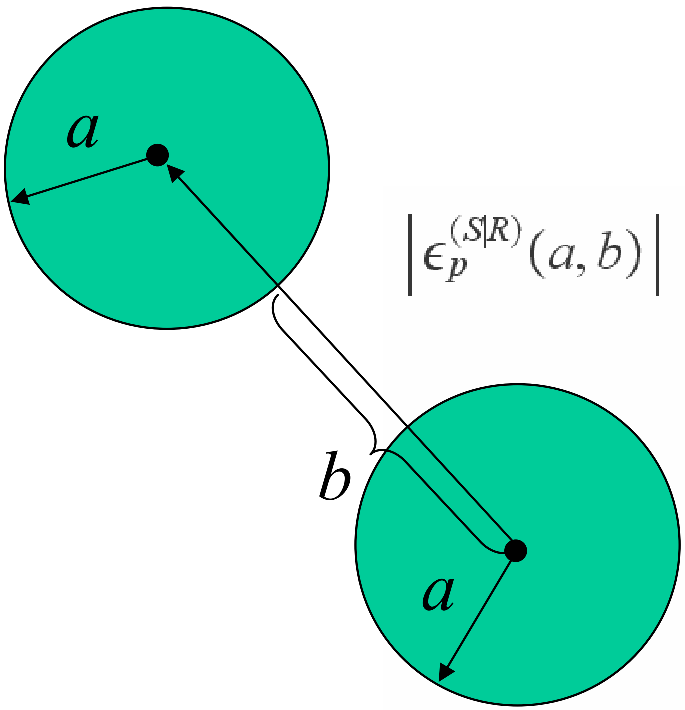
$$= \frac{1}{r-r_0}\left(\frac{r_0}{r}\right)^p \leqslant \frac{1}{|\mathbf{r}-\mathbf{r}_0|}\left(\frac{r_0}{r}\right)^p = \left(\frac{r_0}{r}\right)^p G(\mathbf{r}-\mathbf{r}_0).$$

In the FMM with 1-neighborhoods:

$$\frac{r_0}{r} < \frac{\sqrt{3}}{3} < 0.5773503, \quad |\epsilon_p| < (0.5773503)^p G(\mathbf{r}-\mathbf{r}_0).$$

Error bounds (2)

Translation errors: No error in S|S and R|R translations.



The error of the truncated S|R-translation can be evaluated from the theorem on the error bound of the truncated translation:

$$\left|\epsilon_p^{(S|R)}(a,b)\right| \leqslant \left[\left(1+\left|\epsilon_p^{(S)}(a,b)\right|\right)^2-1\right] = 2\left|\epsilon_p^{(S)}(a,b)\right| + O\left(\left|\epsilon_p^{(S)}(a,b)\right|^2\right)$$

$$\approx 2\left|\epsilon_p^{(S)}(a,b)\right| < \frac{2}{b-a}\left(\frac{a}{b}\right)^p.$$

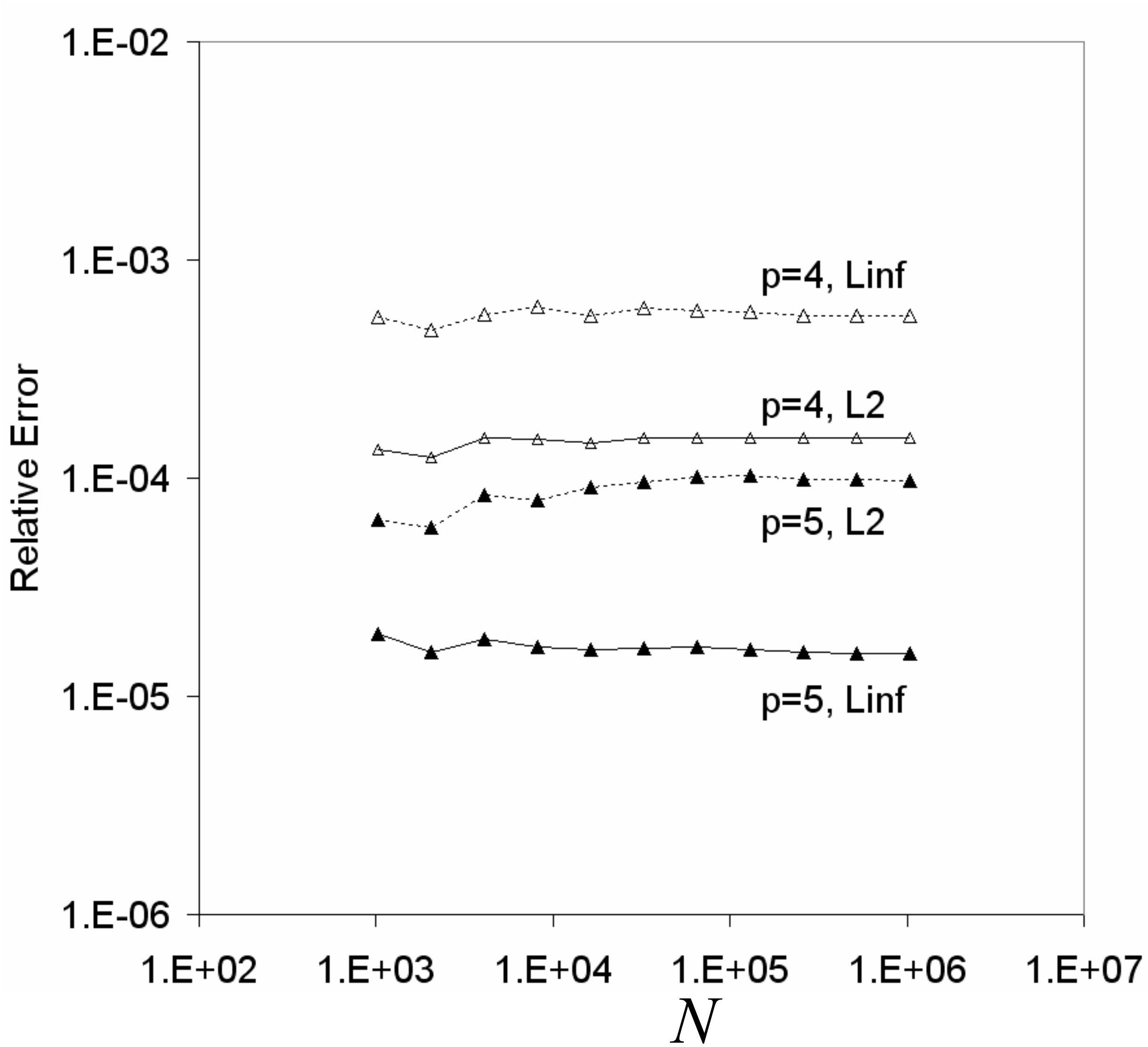
$$\frac{a}{b} = \frac{\sqrt{3}}{2\left(2-\sqrt{3}/2\right)} = \frac{1}{4/\sqrt{3}-1} < 0.763708.$$

$$\left|\epsilon_p^{(S|R)}(a,b)\right| \lesssim \frac{2}{b-a}(0.763708)^p.$$

Error bounds (3)

Normally algorithms with moderate p, much smaller than this perform well. Real example:

100 random points are selected to evaluate the error.



$$\epsilon_{\infty}^{(abs)} = \max_{j=1,\ldots,M} |\phi_{exact}(\mathbf{r}_j) - \phi_{approx}(\mathbf{r}_j)|,$$

$$\epsilon_{2}^{(abs)} = \left[\frac{1}{M} \sum_{j=1}^{M} |\phi_{exact}(\mathbf{r}_j) - \phi_{approx}(\mathbf{r}_j)|^2 \right]^{1/2},$$

$$\|\phi_{exact}(\mathbf{r})\|_2 = \left[\frac{1}{M} \sum_{j=1}^{M} |\phi_{exact}(\mathbf{r}_j)|^2 \right]^{1/2}.$$

$$\epsilon_{\infty} = \frac{\epsilon_{\infty}^{(abs)}}{\|\phi_{exact}(\mathbf{r})\|_2}, \quad \epsilon_2 = \frac{\epsilon_2^{(abs)}}{\|\phi_{exact}(\mathbf{r})\|_2}.$$

Asymptotically faster translation methods

Fast Toeplitz matrix-vector multiplication(1)

$$B_m = \sum_{n=0}^{N} W_{mn} A_n, \quad m = 0, \ldots, M$$

$$W_{mn} = U_{m-n}.$$

$$\mathbf{W} = \{W_{mn}\} = \begin{pmatrix} W_{00} & W_{01} & \ldots & W_{0N} \\ W_{10} & W_{11} & \ldots & W_{1N} \\ \ldots & \ldots & \ldots & \ldots \\ W_{M0} & W_{M1} & \ldots & W_{MN} \end{pmatrix} = \begin{pmatrix} U_0 & U_{-1} & \ldots & U_{-N} \\ U_1 & U_0 & \ldots & U_{1-N} \\ \ldots & \ldots & \ldots & \ldots \\ U_M & U_{M-1} & \ldots & U_{M-N} \end{pmatrix}.$$

Fast Toeplitz matrix-vector multiplication(2)

$$u(t) = \sum_{l=-N}^{M} U_l e^{ilt}, \quad b(t) = \sum_{m=0}^{M} B_m e^{imt}, \quad a(t) = \sum_{n=0}^{N} A_n e^{int}.$$

$$a(t)u(t) = \sum_{n=0}^{N} A_n e^{int} \sum_{l=-N}^{M} U_l e^{ilt} = \sum_{n=0}^{N} \sum_{l=-N}^{M} A_n U_l e^{i(n+l)t}$$

$$= \sum_{m=-N}^{-1} e^{imt} \sum_{n=0}^{N+m} A_n U_{m-n} + \sum_{m=0}^{M} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} + \sum_{m=M+1}^{M+N} e^{imt} \sum_{n=m-M-1}^{N} A_n U_{m-n}$$

$$= \sum_{m=-N}^{-1} e^{imt} \sum_{n=0}^{N+m} A_n U_{m-n} + b(t) + \sum_{m=M+1}^{M+N} e^{imt} \sum_{n=m-M-1}^{N} A_n U_{m-n}.$$

So to get $b(t)$ we should perform inverse FFT of $\{A_n\}, \{U_l\}$, multiply $a(t)u(t)$, perform the forward FFT, and then take take harmonics from 0 to M which are $\{B_m\}$.

Fast Hankel matrix-vector multiplication(1)

$$B_m = \sum_{n=0}^{N} W_{mn} A_n, \quad m = 0, \ldots, N$$

$$W_{mn} = U_{m+n}.$$

$$\mathbf{W} = \{W_{mn}\} = \begin{pmatrix} W_{00} & W_{01} & \ldots & W_{0N} \\ W_{10} & W_{11} & \ldots & W_{1N} \\ \ldots & \ldots & \ldots & \ldots \\ W_{N0} & W_{N1} & \ldots & W_{NN} \end{pmatrix} = \begin{pmatrix} U_0 & U_1 & \ldots & U_N \\ U_1 & U_2 & \ldots & U_{N+1} \\ \ldots & \ldots & \ldots & \ldots \\ U_N & U_{N+1} & \ldots & U_{2N} \end{pmatrix}$$

Fast Hankel matrix-vector multiplication(2)

$$u(t) = \sum_{l=0}^{2N} U_l e^{ilt}, \quad b(t) = \sum_{m=0}^{N} B_m e^{imt}, \quad a(t) = \sum_{n=0}^{N} \overline{A_n} e^{int}.$$

$$\begin{aligned}
\overline{a(t)}u(t) &= \sum_{n=0}^{N} A_n e^{-int} \sum_{l=0}^{2N} U_l e^{ilt} = \sum_{n=0}^{N} \sum_{l=0}^{2N} A_n U_l e^{i(l-n)t} \\
&= \sum_{m=-N}^{2N} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} \\
&= \sum_{m=-N}^{-1} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} + \sum_{m=0}^{N} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} + \sum_{m=N+1}^{2N} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} \\
&= \sum_{m=-N}^{-1} e^{imt} \sum_{n=0}^{N} A_n U_{m+n} + b(t) + \sum_{m=N+1}^{2N} e^{imt} \sum_{n=0}^{N} A_n U_{m+n}.
\end{aligned}$$

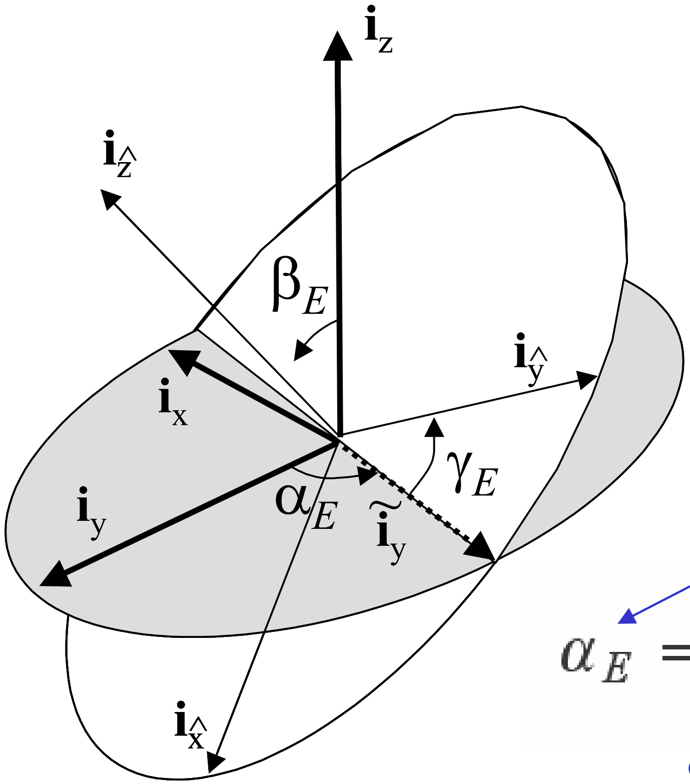
So to get $b(t)$ we should perform inverse FFT of $\{\overline{A_n}\}$, $\{U_l\}$, multiply $\overline{a(t)}u(t)$, perform the forward FFT, and then take take harmonics from 0 to M which are $\{B_m\}$.

Use of the FFT in the FMM

- 1D Toeplitz-Hankel structure of translation operators for 2D Laplace; 2D Toeplitz-Hankel structure for 3D Laplace (convolution should be properly modified, e.g. see **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).
- Doing straightforward for 2D Laplace, one needs 3FFTs per translation (27*3=81 FFTs for S|R-translation in the E4-neighborhood);
- How to save on FFTs:
  - Transform translation operators into Fourier domain and save (one time precomputation step); This cost can be dropped from operations count as it can be precomputed and stored forever);
  - For translation: Transform coefficients into Fourier domain ($O(p\log p)$) for each box from which translation should be performed (27 FFTs);
  - Perform point-by-point matrix vector multiplication for each translation ($27p$);
  - Consolidate transforms in the Fourier domain ($27p$);
  - Pad with zeros ($27p$);
  - Perform one Fourier transform for the translated box (1 FFT);
  - Total: 28 FFTs (about 1 FFT per translation);

RCR-decomposition (**R**otation- **C**oaxial translation- **R**otation) for 3D Laplace

Rotations of coordinates



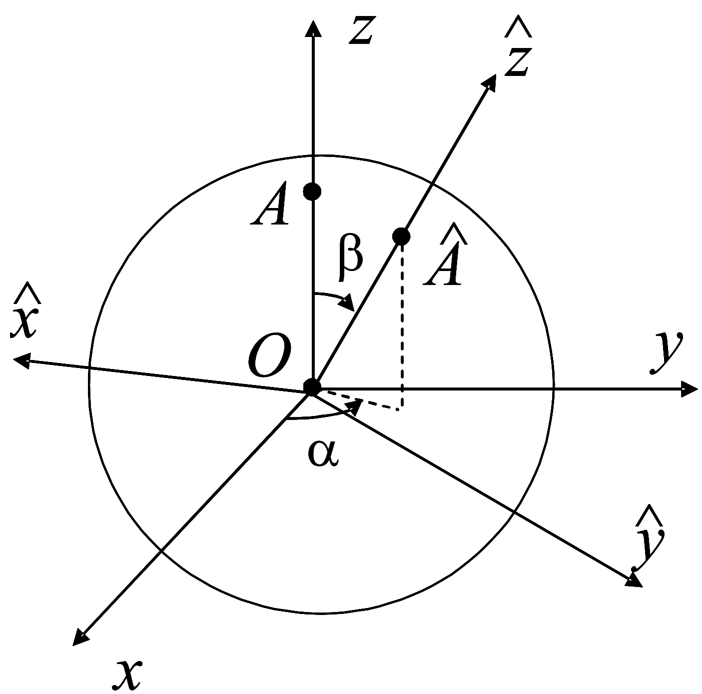
Rotation Matrix

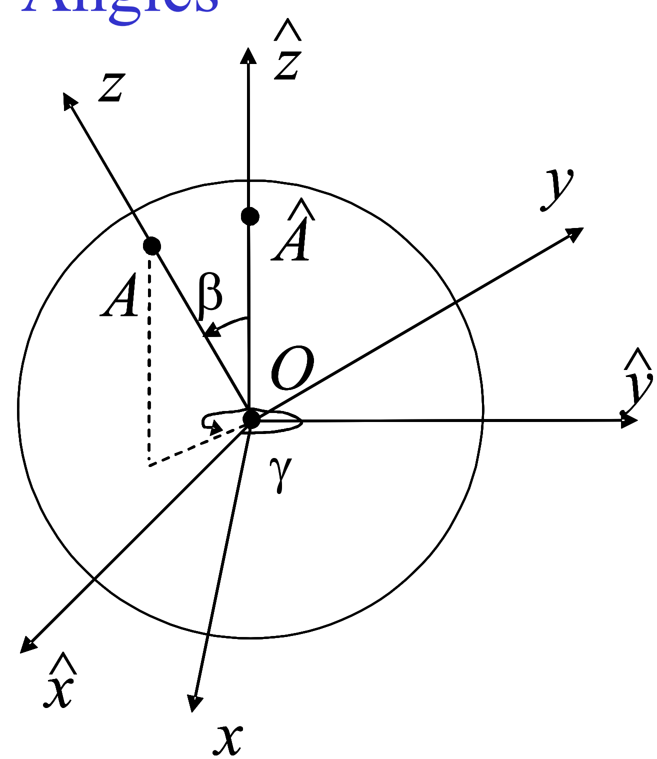
$$Q = \begin{bmatrix} \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{z}} \cdot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

Euler Angles

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

Spherical Polar Angles





Rotations of elementary solutions of the 3D Laplace equation

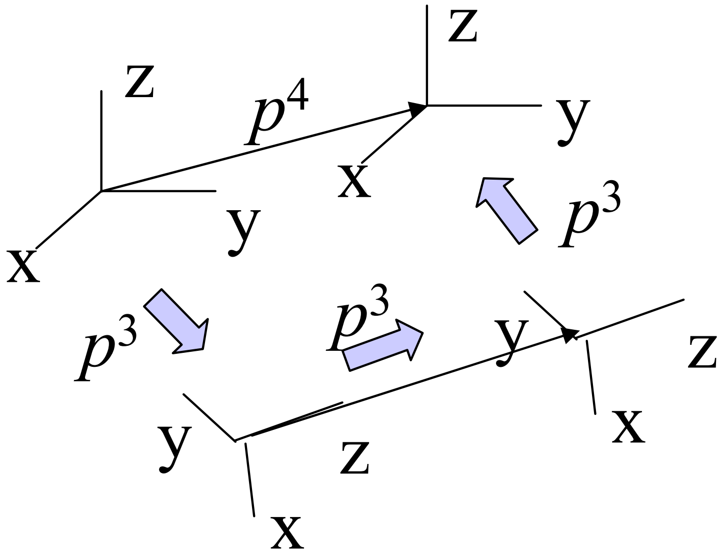
Rotations

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

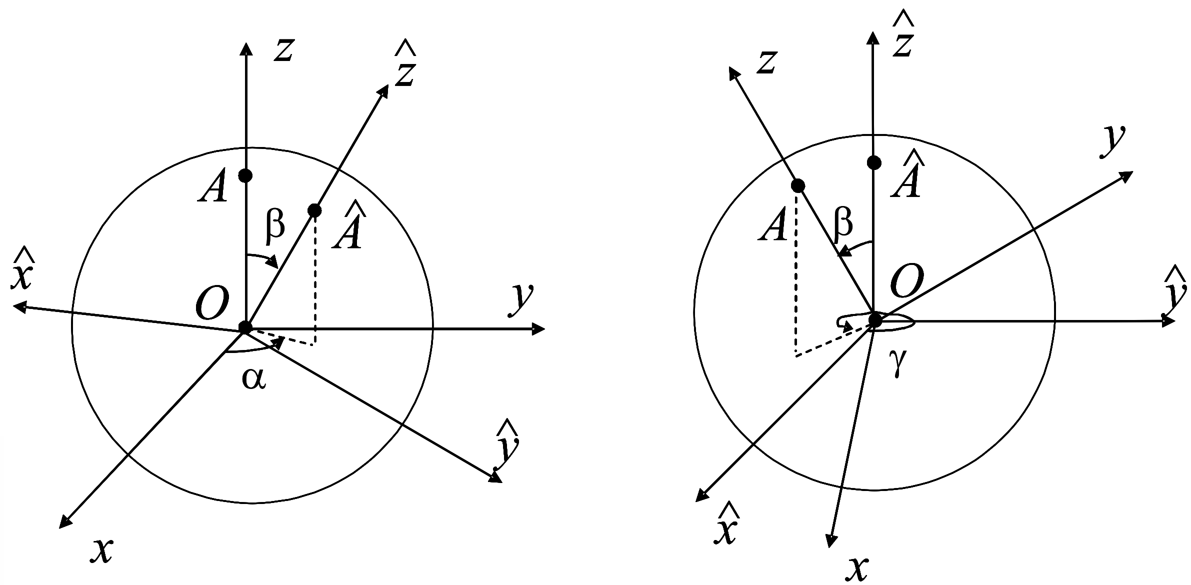
$$S_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q) S_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|,$$

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

Rotation-Coaxial Translation Decomposition



Rotation



Coaxial Translation

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

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

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

$$(E|F)_{ln}^m(d) = (E|F)_{ln}^{mm}(\mathbf{d})\big|_{\theta_{pq}=0}, \qquad E, F = S, R.$$

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

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

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:

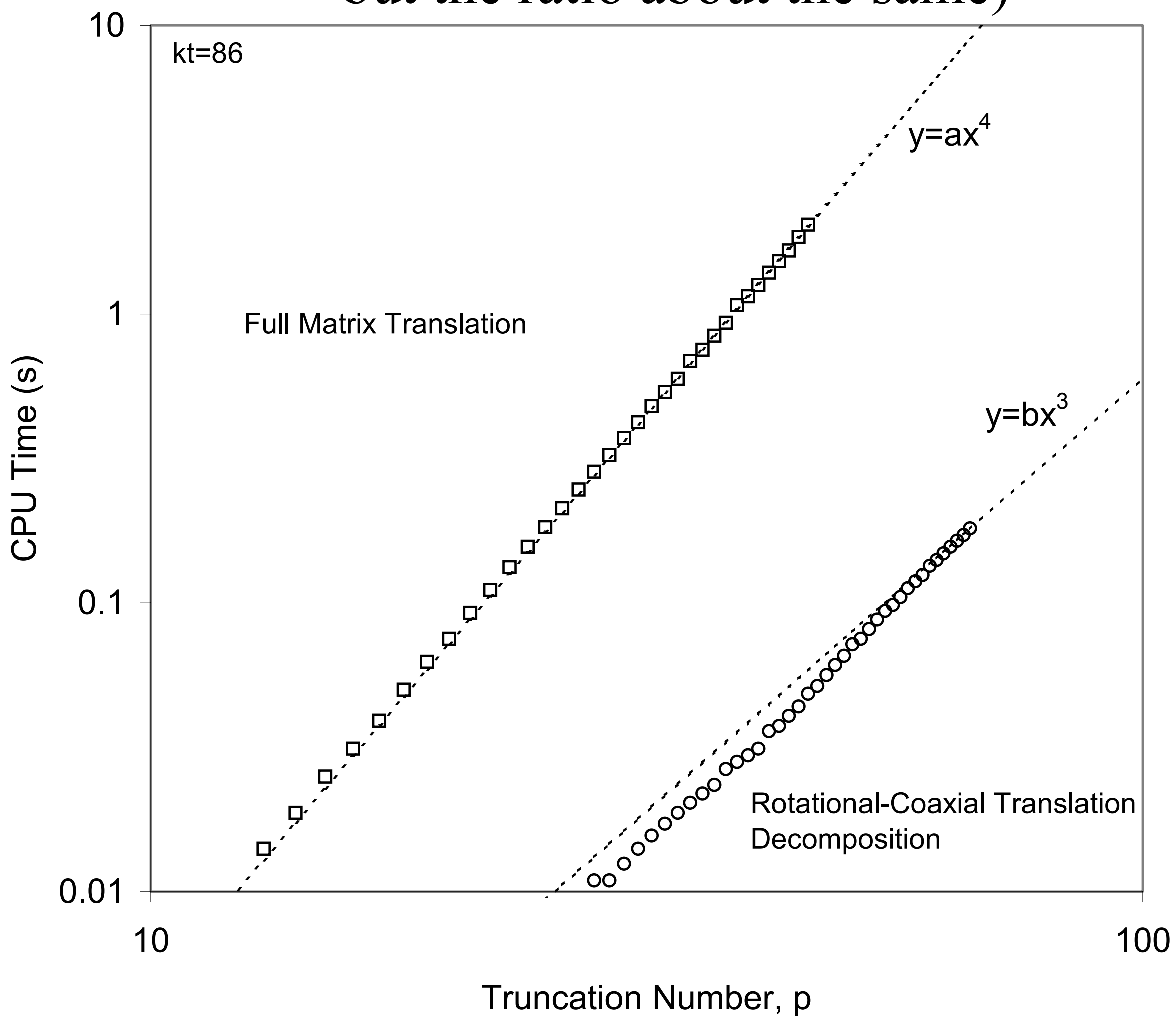
$$(\mathbf{S}|\mathbf{R}) = (\mathbf{S}|\mathbf{R})^{0} \oplus (\mathbf{S}|\mathbf{R})^{\pm 1} \oplus \ldots = \sum_{m=-\infty}^{\infty} \oplus (\mathbf{S}|\mathbf{R})^{m},$$

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

(Figure for the Helmholtz equation; for the Laplace CPU time is different, but the ratio about the same)



Exponential form for the S|R-translation ("Plane wave expansion").

L. Greengard and V. Rokhlin, A new version of the fast multipole method for the Laplace equation in three dimensions, Acta Numerica, 6, 1997, 229-269.

H. Cheng, L. Greengard, and V. Rokhlin, A fast adaptive multipole algorithm in three dimensions, J. Comput. Phys., 155, 1999, 468-498.

Expansions of the Greens function and arbitrary harmonic function

$$G(\mathbf{r},\mathbf{r}_0) = \frac{1}{8\pi^2}\int_0^\infty e^{-\lambda(z-z_0)}\int_0^{2\pi} e^{i\lambda[(x-x_0)\cos\alpha+(y-y_0)\sin\alpha]}d\alpha d\lambda,$$

$$\mathbf{r} = (x,y,z), \quad \mathbf{r}_0 = (x_0,y_0,z_0), \quad z > z_0.$$

For

$$a \leqslant z-z_0 \leqslant b, \sqrt{(x-x_0)^2+(y-y_0)^2} \leqslant c, \quad (a=1, b=4, c=4\sqrt{2}):$$

$$G(\mathbf{r},\mathbf{r}_0) = \frac{1}{4\pi}\sum_{k=1}^{S(\epsilon)}\frac{w_k}{M_k}e^{-\lambda_k(z-z_0)}\sum_{j=1}^{M_k} e^{i\lambda_k[(x-x_0)\cos\alpha_{jk}+(y-y_0)\sin\alpha_{jk}]},$$

$$\phi(\mathbf{r}) = \sum_{k=1}^{S(\epsilon)}\sum_{j=1}^{M_k} W_{kj}e^{-\lambda_k z}e^{i\lambda_k(x\cos\alpha_{jk}+y\sin\alpha_{jk})},$$

$$S_{\exp} = \sum_{k=1}^{S(\epsilon)} M_k = \sigma p^2, \quad S(\epsilon) = \kappa p.$$

S|R-translation

$$\phi(\mathbf{r}+\mathbf{t}) = \sum_{k=1}^{S(\epsilon)}\sum_{j=1}^{M_k} W_{kj} e^{-\lambda_k t_z} e^{i\lambda_k (t_x \cos\alpha_{jk} + t_y \sin\alpha_{jk})} e^{-\lambda_k z} e^{i\lambda_k (x\cos\alpha_{jk} + y\sin\alpha_{jk})}$$

$$= \sum_{k=1}^{S(\epsilon)}\sum_{j=1}^{M_k} \widehat{W}_{kj} e^{-\lambda_k z} e^{i\lambda_k (x\cos\alpha_{jk} + y\sin\alpha_{jk})} = \hat{\phi}(\mathbf{r}),$$

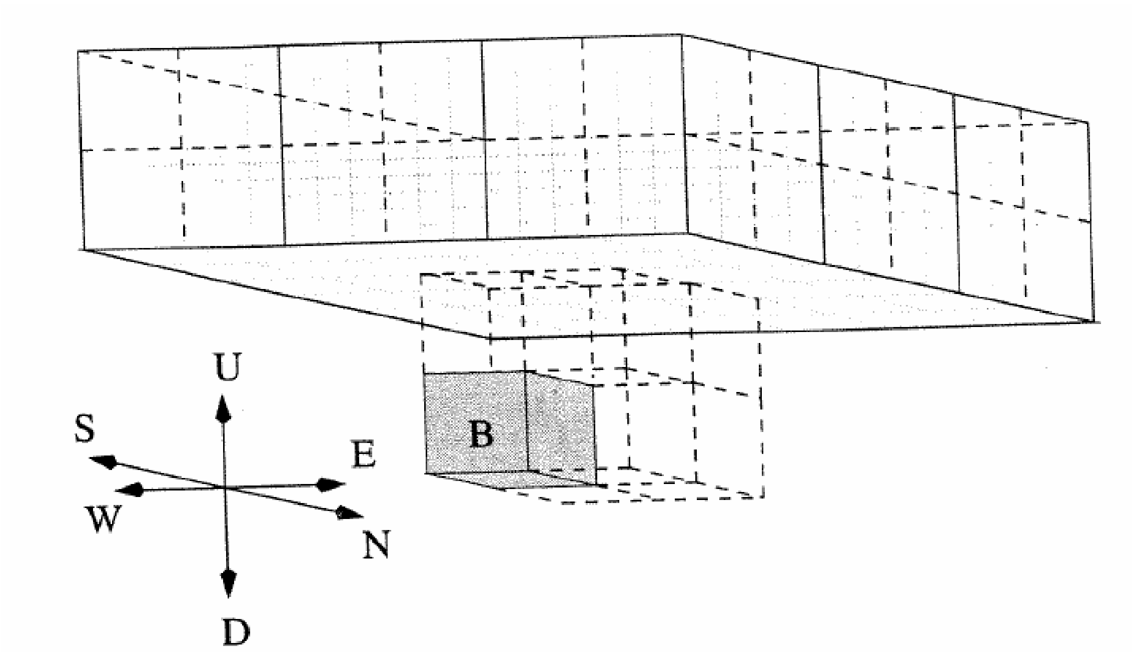
$$\widehat{W}_{kj} = E_{kj} W_{kj}, \quad E_{kj} = e^{-\lambda_k t_z} e^{i\lambda_k (t_x \cos\alpha_{jk} + t_y \sin\alpha_{jk})}, \quad \mathbf{t} = (t_x, t_y, t_z).$$

$$W_{kj} = \frac{w_k}{M_k d} \sum_{m=-(p-1)}^{p-1} e^{im\alpha_{jk}} \sum_{n=|m|}^{p-1} \frac{1}{\beta_n^m \beta_{(1)n}^m} \left(\frac{\lambda_k}{d}\right)^n \phi_n^m, \quad k = 1,..,s(\epsilon), \quad j = 1,\ldots,M_k,$$

$$\phi_n^m = \alpha_n^m \alpha_{(1)n}^m \sum_{k=1}^{S(\epsilon)} \left(\frac{\lambda_k}{d}\right)^n \sum_{j=1}^{M_k} W_{kj} e^{-im\alpha_{jk}},$$

$$N^{(E|R)} = N^{(S|E)} \approx (\kappa + 4\sigma) p^3.$$

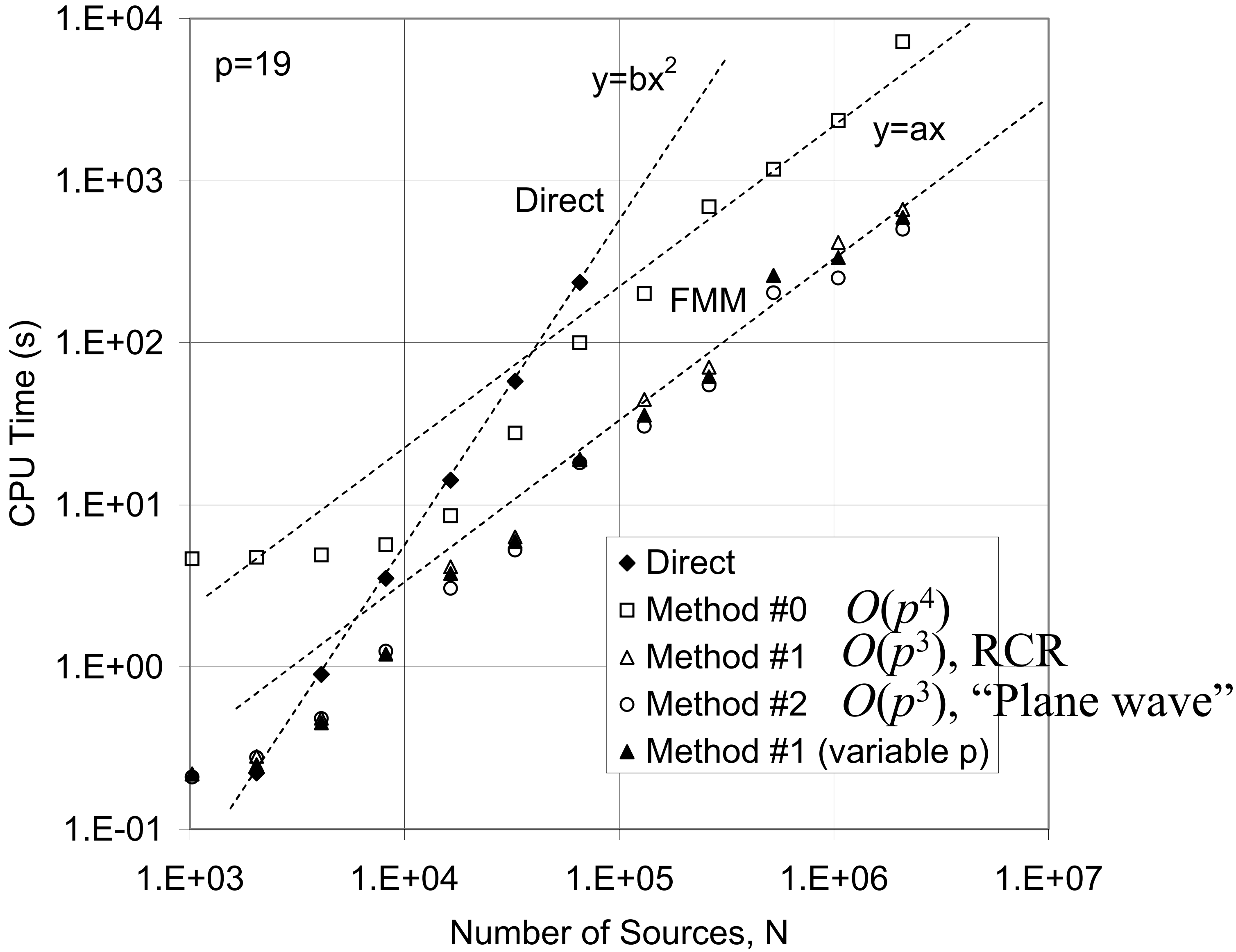
Translation scheme



Needs also 6 translation directions;
Performed by rotation transforms (axis flips);
$O(p^3)$ complexity;

(From Greengard & Rokhlin, 1997)

Comparison of translation methods (for the same accuracy)



Theory of Signature Function

Translation Kernels

$$\Lambda_r(z;\alpha) = \sum_{n=0}^{\infty} e^{in\alpha} R_n(z),$$

$$\Lambda_s^{(p)}(z;\alpha) = \sum_{n=0}^{p-1} e^{-in\alpha} S_n(z).$$

$$\Lambda_r(z;\alpha) = \sum_{n=0}^{\infty} e^{in\alpha} R_n(z) = \sum_{n=0}^{\infty} \frac{(-ze^{i\alpha})^n}{n!} = e^{-ze^{i\alpha}}.$$

Integral representation of basis functions(1)

$$R_n(z) = \frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\Lambda_r(z;\alpha)d\alpha, \quad n = 0,1,\ldots, \quad 0 \leqslant |z| < \infty.$$

Indeed:

$$\frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\Lambda_r(z;\alpha)d\alpha = \frac{1}{2\pi}\int_0^{2\pi} e^{-in\alpha}\sum_{m=0}^{\infty} e^{im\alpha}R_m(z)d\alpha$$

$$= \sum_{m=0}^{\infty} R_m(z)\frac{1}{2\pi}\int_0^{2\pi} e^{i(m-n)\alpha}d\alpha$$

$$= \sum_{m=0}^{\infty} R_m(z)\delta_{mn} = R_n(z).$$

Integral representation of basis functions(2)

$$S_n(z) = \frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\Lambda_s^{(p)}(z;\alpha)d\alpha, \quad n = 0,1,\ldots,p-1, \quad 0 < |z| < \infty.$$

Indeed:

$$\frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\Lambda_s^{(p)}(z;\alpha)d\alpha = \frac{1}{2\pi}\int_0^{2\pi} e^{in\alpha}\sum_{m=0}^{p-1} e^{-im\alpha}S_m(z)d\alpha$$

$$= \sum_{m=0}^{p-1} S_m(z)\frac{1}{2\pi}\int_0^{2\pi} e^{i(n-m)\alpha}d\alpha$$

$$= \sum_{m=0}^{p-1} S_m(z)\delta_{mn} = S_n(z).$$

R-signature function