MAIT 627 Fast Multipole Methods

Lecture 16

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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

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

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

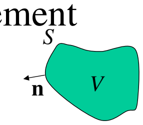
$$= \nabla\sum_{j=1,j\neq i}^{N} q_j\frac{1}{|\mathbf{r}-\mathbf{r}_j|}\bigg|_{\mathbf{r}=\mathbf{r}_i}, \quad q_j = Gm_j.$$

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



$$\nabla^2\phi(\mathbf{x}) = 0, \quad \mathbf{x} \in V,$$
$$\alpha\phi + \beta\frac{\partial\phi}{\partial n} = \gamma, \quad \mathbf{x} \in S.$$

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

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}, \quad d = 3,$$
$$G(\mathbf{x},\mathbf{y}) = \frac{1}{2\pi}\ln\frac{1}{|\mathbf{x}-\mathbf{y}|}, \quad d = 2.$$

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

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

$n = 0$:

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

$n > 0$:

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

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

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

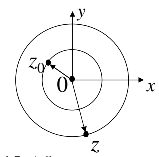
S|R-translation operator

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

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

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

Error bounds



Error of the S-expansion:

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

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

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

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

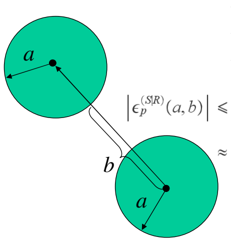
In the FMM with 1-neighborhoods:

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

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:



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

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

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

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

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

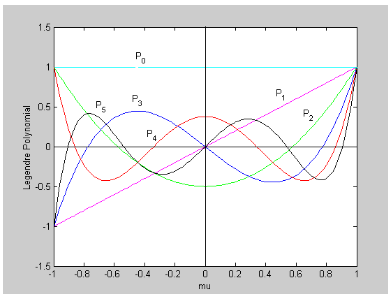
$$\frac{1}{\sqrt{1-2\mu x + x^2}} = \begin{cases} \sum_{n=0}^{\infty} P_n(\mu) x^n, & |x| < 1, \\ \sum_{n=0}^{\infty} P_n(\mu) x^{-n-1}, & |x| > 1. \end{cases}$$

First few polynomials

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

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

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

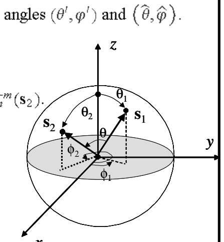
order

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

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

degree

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

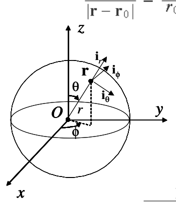


Vector form of the addition theorem

S- and R- expansions of Fundamental Solution

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

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



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

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

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

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:

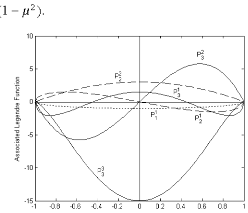
$$(n)_0 = 1, \quad (n)_l = \frac{(n+l-1)!}{(n-1)!}.$$

This formula yields the following particular functions:

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

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

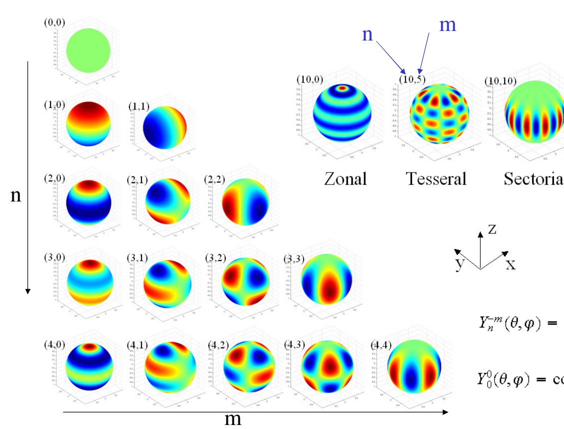
Orthogonal!



Spherical Harmonics

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

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



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

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

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

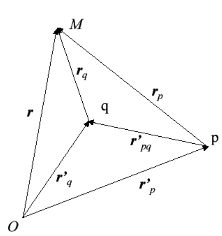
$$\Phi(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} B_n^m S_n^m(\mathbf{r}).$$

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

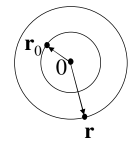
$$\left(\widetilde{S}|\widetilde{R}\right)^{m'm}_{n'n}(\mathbf{t}) = (O|I)^{m'm}_{n'n}(\mathbf{t}) = O^{m-m'}_{n+n'}(\mathbf{t}) = \widetilde{S}^{m-m'}_{n+n'}(\mathbf{t}),$$

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

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

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:

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

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

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

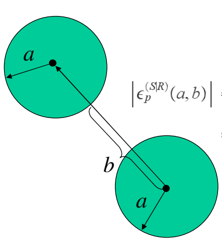
$$= \frac{1}{r-r_0}\left(\frac{r_0}{r}\right)^p \leqslant \frac{1}{|\mathbf{r}-\mathbf{r}_0|}\left(\frac{r_0}{r}\right)^p = \left(\frac{r_0}{r}\right)^p G(\mathbf{r}-\mathbf{r}_0).$$

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:

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

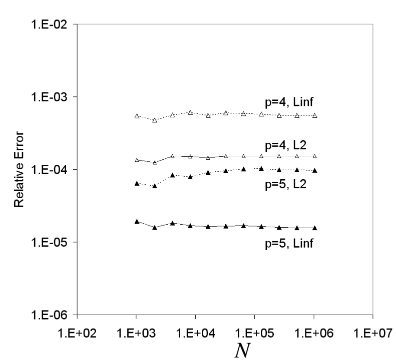
$$\approx 2\left|\epsilon_p^{(S)}(a,b)\right| < \frac{2}{b-a}\left(\frac{a}{b}\right)^p.$$

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

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

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.

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

$$\epsilon_2^{(abs)} = \left[\frac{1}{M}\sum_{j=1}^{M}\left|\phi_{exact}(\mathbf{r}_j) - \phi_{approx}(\mathbf{r}_j)\right|^2\right]^{1/2},$$

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

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