Fast Multipole Methods for The Laplace Equation

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Outline

- 3D Laplace equation and Coulomb potentials
- Multipole and local expansions
- Special functions
  - Legendre polynomials
  - Associated Legendre functions
  - Spherical harmonics
- Translations of elementary solutions
- Complexity of FMM
- Reducing complexity
- Rotations of elementary solutions
- Coaxial Translation-Rotation decomposition
- Faster Translation techniques

Review

$$\mathbf{v} = \mathbf{\Phi u},$$

- FMM aims at accelerating the matrix vector product
- Matrix entries determined by a set of source points and evaluation points (possibly the same)
- Function Φ has following point-centered representations about a given point x_*
  - Local (valid in a neighborhood of a given point)
  - Far-field or multipole (valid outside a neighborhood of a given point)
  - In many applications Φ is singular
- Representations are usually series
  - Could be integral transform representations
- Representations are usually approximate
  - Error bound guarantees the error is below a specified tolerance

$$\mathbf{\Phi} = \begin{pmatrix} \Phi(\mathbf{y}_1,\mathbf{x}_1) & \Phi(\mathbf{y}_1,\mathbf{x}_2) & \dots & \Phi(\mathbf{y}_1,\mathbf{x}_N) \\ \Phi(\mathbf{y}_2,\mathbf{x}_1) & \Phi(\mathbf{y}_2,\mathbf{x}_2) & \dots & \Phi(\mathbf{y}_2,\mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ \Phi(\mathbf{y}_M,\mathbf{x}_1) & \Phi(\mathbf{y}_M,\mathbf{x}_2) & \dots & \Phi(\mathbf{y}_M,\mathbf{x}_N) \end{pmatrix}.$$

$$\mathsf{X} = \{\mathbf{x}_1,\mathbf{x}_2,\dots,\mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathsf{R}^d, \quad i = 1,\dots,N,$$
$$\mathsf{Y} = \{\mathbf{y}_1,\mathbf{y}_2,\dots,\mathbf{y}_M\}, \quad \mathbf{y}_j \in \mathsf{R}^d, \quad j = 1,\dots,M.$$

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j,\mathbf{x}_i), \quad j = 1,\dots,M.$$

Review

$$\Phi(\mathbf{y}_j,\mathbf{x}_i) = \sum_{m=0}^{p-1} A_m(\mathbf{x}_i) F_m(\mathbf{y}_j) + Error(p,\mathbf{x}_i,\mathbf{y}_j).$$

- One representation, valid in a given domain, can be converted to another valid in a subdomain contained in the original domain
- Factorization trick is at core of the FMM speed up

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j,\mathbf{x}_i) = \sum_{i=1}^{N} u_i \sum_{m=0}^{p-1} A_m(\mathbf{x}_i) F_m(\mathbf{y}_j) + \sum_{i=1}^{N} u_i Error(p,\mathbf{x}_i,\mathbf{y}_j)$$
$$= \sum_{m=0}^{p-1} B_m F_m(\mathbf{y}_j) + Error_j(p,N), \quad j = 1,\dots,M.$$

- Representations we use are factored … separate points x_i and y_j
- Data is partitioned to organize the source points and evaluation points so that for each point we can separate the points over which we can use the factorization trick, and those we cannot.
- Hierarchical partitioning allows use of different factorizations for different groups of points
- Accomplished via MLFMM discussed yesterday
- Today concrete example for Laplace equation/Coulomb potentials

Solution of Laplace’s equation

- Green’s function for Laplace’s equation

$$\nabla^2 G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}) \qquad G(\mathbf{x},\mathbf{y}) = -\frac{1}{4\pi \mathbf{x}-\mathbf{y}}$$

- Green’s formula

$$\begin{aligned}\phi(\mathbf{y}) &= \int_\Omega \phi(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})d^3x = \int_\Omega \phi(\mathbf{x})\nabla^2 G(\mathbf{x},\mathbf{y})d^3x \\ &= -\int_\Omega \nabla\phi(\mathbf{x})\cdot\nabla G(\mathbf{x},\mathbf{y})d^3x + \int_{\partial\Omega}\phi(\mathbf{x})\mathbf{n}\cdot\nabla G(\mathbf{x},\mathbf{y})dS_x \\ &= \int_\Omega \nabla^2\phi(\mathbf{x})\nabla G(\mathbf{x},\mathbf{y})d^3x + \int_{\partial\Omega}\left[\phi(\mathbf{x})\mathbf{n}\cdot\nabla G(\mathbf{x},\mathbf{y}) - \mathbf{n}\cdot\nabla\phi(\mathbf{x})G(\mathbf{x},\mathbf{y})\right]dS_x\end{aligned}$$

- Goal solve Laplace’s equation with given boundary conditions
  - E.g. $\nabla^2 \phi = 0$ in Ω $\qquad \partial \phi / \partial n = f$ on $\partial \Omega$

$$\phi(\mathbf{y}) - \int_{\partial\Omega}\phi(\mathbf{x})\frac{\partial G}{\partial n}(\mathbf{x},\mathbf{y}) = -\int_{\partial\Omega} f(\mathbf{x})G(\mathbf{x},\mathbf{y})dS_x$$

- Upon discretization yields system of type that can be solved iteratively, with matrix vector products accelerated by FMM

Molecular and stellar dynamics

- Many particles distributed in space
- Particles are moving and exert a force on each other
- Simplest case this force obeys an inverse-square law (gravity, coulombic interaction)
- Goal of computations compute the dynamics $\frac{d^2\mathbf{x}_i}{dt^2} = F_i,$
- Force is

$$F_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} q_i q_j \frac{(\mathbf{x}_i - \mathbf{x}_j)}{|\mathbf{x}_i - \mathbf{x}_j|^3}$$

- After time step, particles move
- Recompute force and iterate

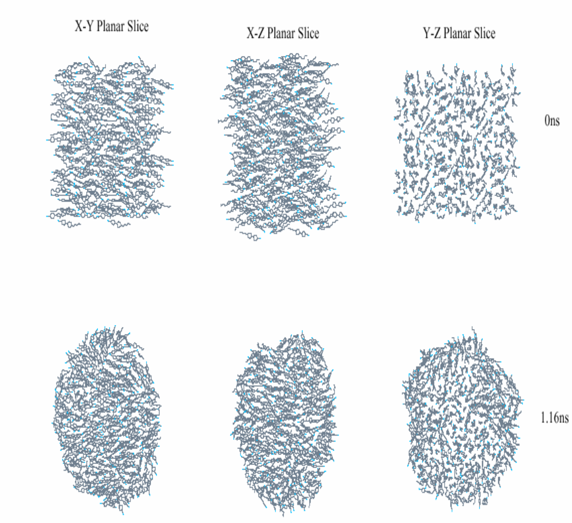


Figure 10: Slice views of the 5CB cluster at time 0 and 1.16 *ns*. The slices are passing the spheric center with thickness of 20 Å

What is needed for the FMM

- Local expansion
- Far-field or multipole expansion
- Translations
  - Multipole-to-multipole (S|S)
  - Local-to-local (R|R)
  - Multipole-to-local (S|R)
- Error bounds

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

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

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

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

are called MULTIPOLES OF DEGREE n centered at $\mathbf{r} = \mathbf{0}$. Vectors $\mathbf{t}_1, \mathbf{t}_2, ..., \mathbf{t}_n$ 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

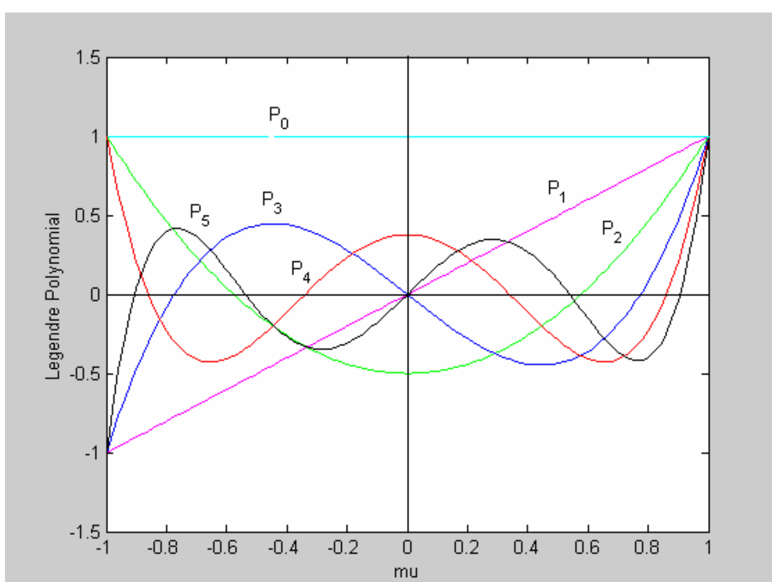
$$\frac{1}{\sqrt{1-2\mu x+x^2}} = \begin{cases} \sum_{n=0}^{\infty} P_n(\mu) x^n, & |x| < 1, \\ \sum_{n=0}^{\infty} P_n(\mu) x^{-n-1}, & |x| > 1. \end{cases}$$

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):



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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

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

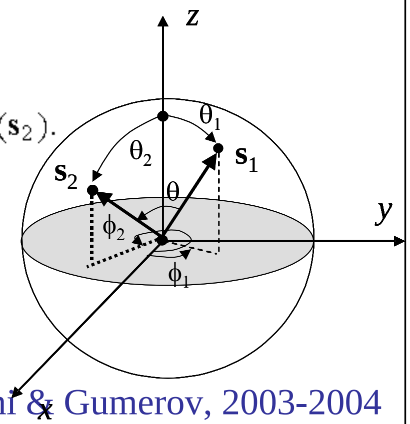
order

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

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

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

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:

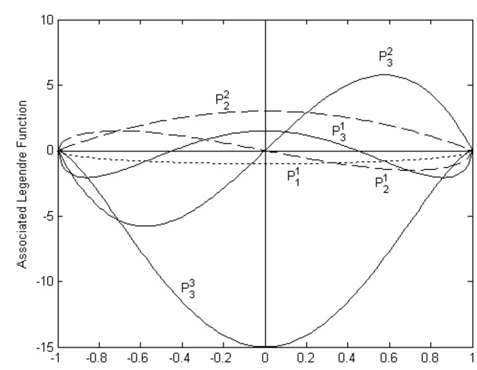
$$(n)_0 = 1, \quad (n)_l = \frac{(n+l-1)!}{(n-1)!}.$$

This formula yields the following particular functions:

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

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

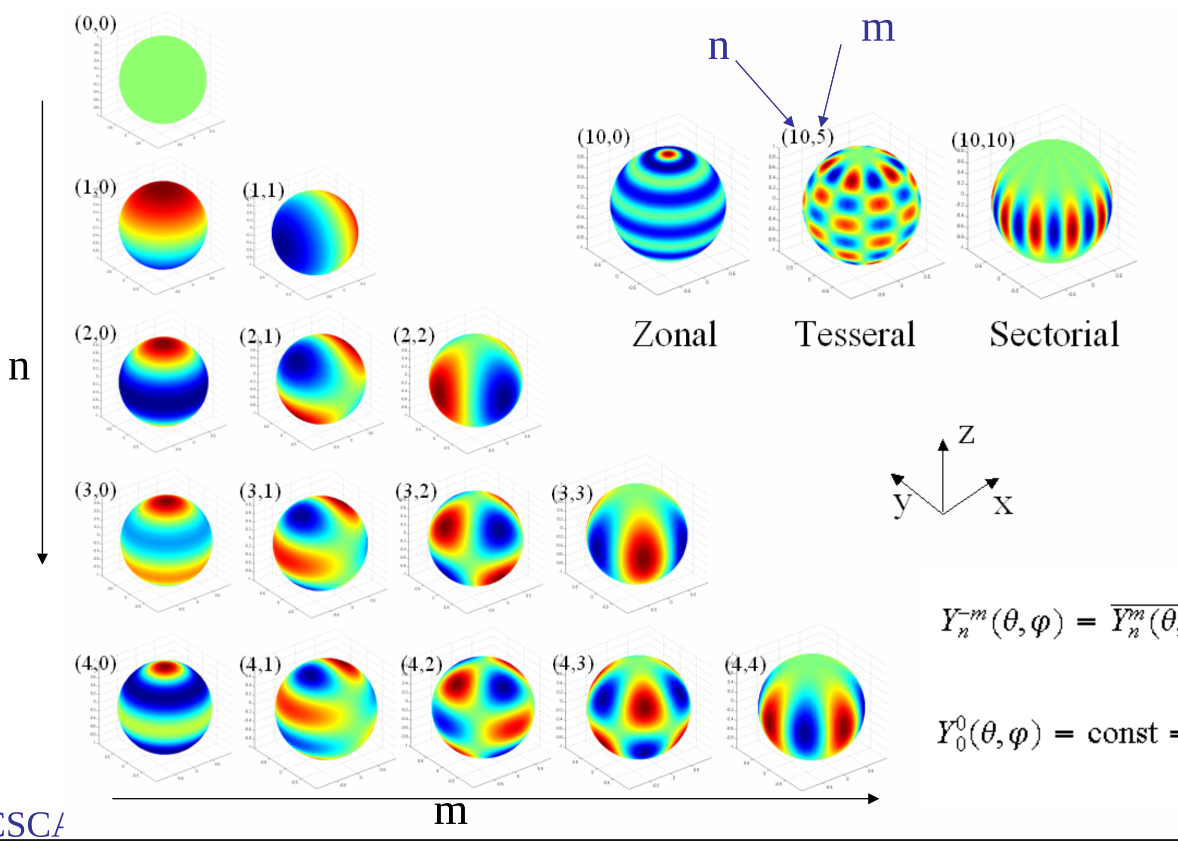
Orthogonal!



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:

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

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

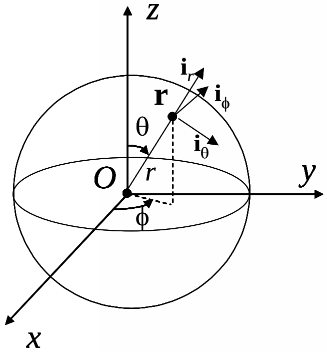
$$\left(F, Y_{n'}^{m'}\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m \left(Y_n^m, Y_{n'}^{m'}\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m \delta_{mm'}\delta_{nn'} = F_{n'}^{m'}.$$

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

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 (!)

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

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

Error bound

- Series converge rapidly
  - E.g,. For multipole expansion we have

$$\Phi(P) = \sum_{i=1}^{k}\frac{q_i}{\|P_i - P\|}$$

potential due to a set of k sources of strengths $\{q_i,\ i = 1,\ldots,k\}$ at $\{P_i = (r_i,\theta_i,\phi_i),\ i = 1,\ldots,k\}$, with $|r_i| < a$. Then for $P = (r,\theta,\phi) \in R^3$ with $|r| > a$,

$$\Phi(P) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{M_n^m}{r^{n+1}}Y_n^m(\theta,\phi),$$

$$M_n^m = \sum_{i=1}^{k}(-1)^m q_i * r_i^n * Y_n^{-m}(\theta_i,\phi_i)\,.$$

$$\left|\Phi(P) - \sum_{n=0}^{p}\sum_{m=-n}^{n}\frac{M_n^m}{r^{n+1}}Y_n^m(\theta,\phi)\right| \le \frac{A}{r-a}\left(\frac{a}{r}\right)^{p+1},$$

$$A = \sum_{i=1}^{k}|q_i|.$$

`Multipole expansion` is 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

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

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

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

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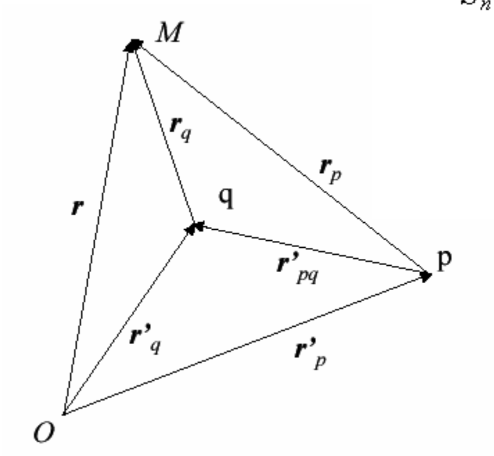
Translations of elementary solutions of the 3D Laplace equation

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

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



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

For a p-truncated expansion *(E|F)* is a $p^2 \times p^2$ matrix

See Tang 03 or Greengard 89 for explicit expressions

Translation of a Multipole Expansion

Let

$$\Phi(P) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{O_n^m}{r'^{n+1}}Y_n^m(\theta',\phi'),$$

Where $P - Q = (r', \theta', \phi')$. Then the potential ϕ can be expressed as,

$$\Phi(P) = \sum_{j=0}^{\infty}\sum_{k=-j}^{j}\frac{M_j^k}{r^{j+1}}Y_j^k(\theta,\phi),$$

$$M_j^k = \sum_{n=0}^{j}\sum_{m=\max(k+n-j,-n)}^{\min(k+j-n,n)}\frac{O_{j-n}^{k-m}i^{|k|-|m|-|k-m|}A_n^m A_{j-n}^{k-m}\rho^n Y_n^{-m}(\alpha,\beta)}{A_j^k},$$

$$A_n^m = \frac{(-1)^n}{\sqrt{(n-m)!(n+m)!}}. \qquad M = SS(\rho,\alpha,\beta) * O$$

Translation of a Local Expansion

Suppose that

$$\Phi(P) = \sum_{n=0}^{p} \sum_{m=-n}^{n} O_n^m r'^n Y_n^m(\theta', \phi')$$

is a local expansion centered at $Q = (\rho, \alpha, \beta)$,
Where $P = (r, \theta, \phi)$, and $P - Q = (r', \theta', \phi')$.
Then the local expansion centered at origin is

$$\Phi(P) = \sum_{j=0}^{p} \sum_{k=-j}^{j} L_j^k r^j Y_j^k(\theta, \phi),$$

where

$$L_j^k = \sum_{n=j}^{p} \sum_{m=k-n+j}^{k-j+n} \frac{O_n^m i^{|m|-|m-k|-|k|} A_j^k A_{n-j}^{m-k} \rho^{n-j} Y_{n-j}^{m-k}(\alpha, \beta)}{(-1)^{n+j} A_n^m},$$

$$L = RR(\rho, \alpha, \beta) * O$$

Complexity Analysis

Step 1,Forming Expansions $O(Np^2)$.
Step 2, Upward pass with Matrix based S|S translations

$$\sum_{l=2}^{n-1} 8 * 8^l * p^4 = \frac{8^3 - 8^{n+1}}{1-8} p^4 \approx \frac{8}{7} 8^n p^4 = \frac{8}{7} \frac{N}{s} p^4.$$

Step 3, Downward pass with matrix based S|R and R|R translations

$$\sum_{l=2}^{n} 8^l * p^4 + \sum_{l=2}^{n} 8^l * p^4 * 189 \approx \frac{8}{7} * 8^n * 190 p^4 = \frac{1520}{7} \frac{N}{s} p^4.$$

Step 4, Evaluate R expansions at points$O(Np^2)$
Step 5, Sum missed neighbor points $O(27Ns)$
The total cost for all five steps is approximately

$$2Np^2 + \frac{1528}{7} \frac{N}{s} p^4 + 27Ns.$$

With $s \approx \sqrt{\frac{1528}{189}} p^2$, the total number of operations is approximately $156Np^2$.

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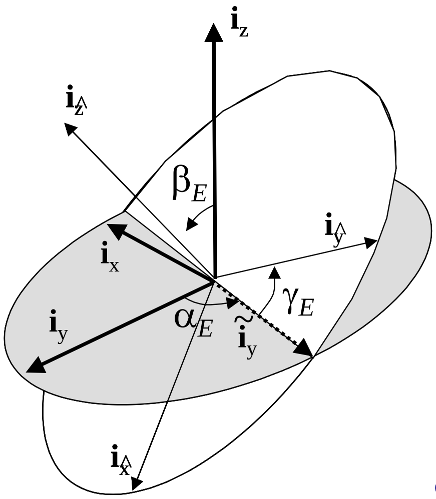


Rotations of coordinates

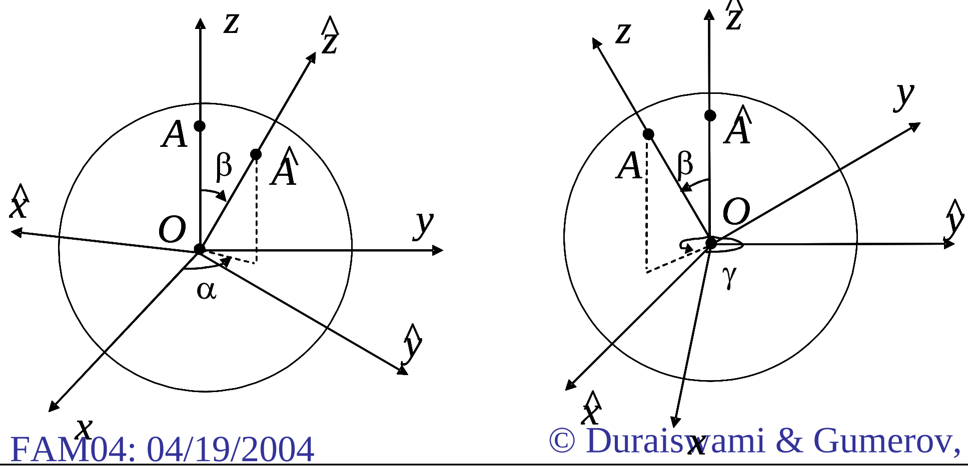
Rotation Matrix

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

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

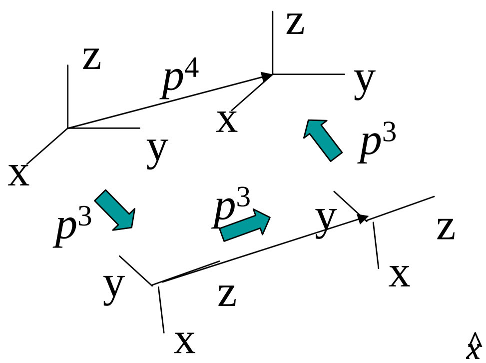
Rotations

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

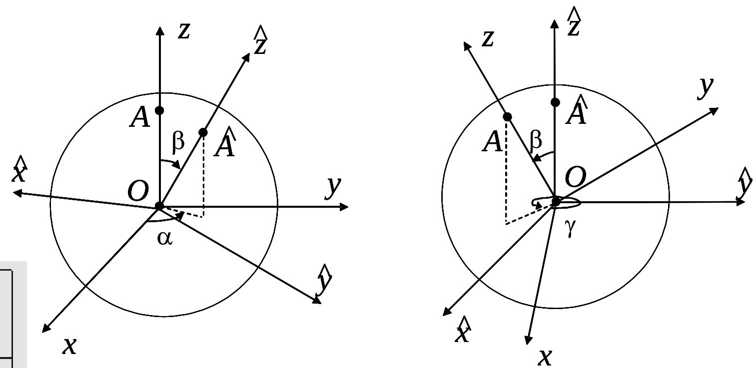
$$S_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q) S_n^{\nu}(\hat{\mathbf{r}}_p), \qquad |\hat{\mathbf{r}}_p| = |\mathbf{r}_p|,$$

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

Rotation-Coaxial Translation Decomposition



Rotation



Coaxial Translation

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

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

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

$$(E|F)_{ln}^m(d) = (E|F)_{ln}^{mm}(\mathbf{d})|_{\theta'_{pq}=0}, \quad E,F = S,R.$$

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

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

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

Coaxial Translation:

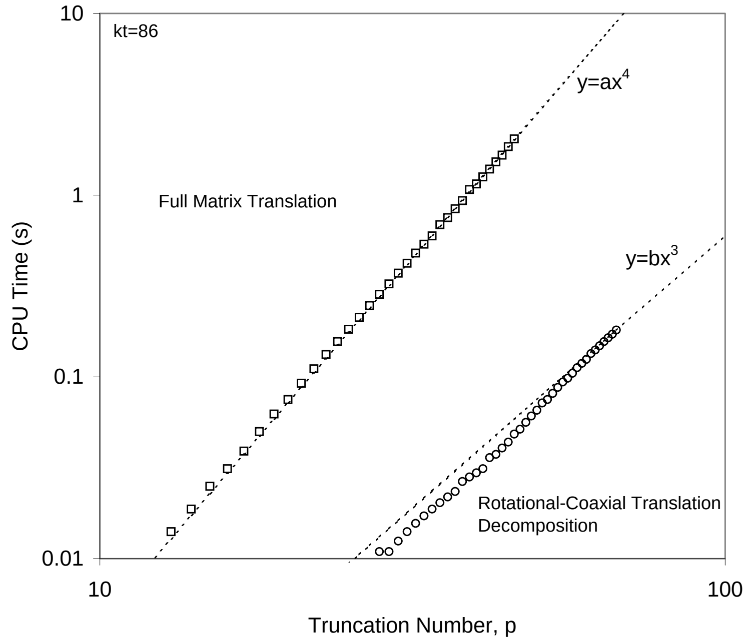
$$(\mathbf{S}|\mathbf{R}) = (\mathbf{S}|\mathbf{R})^0 \oplus (\mathbf{S}|\mathbf{R})^{\pm 1} \oplus \ldots = \sum_{m=-\infty}^{\infty} \oplus (\mathbf{S}|\mathbf{R})^m,$$

Rotation

$$(\mathbf{S}|\mathbf{R}) = (\mathbf{S}|\mathbf{R})_0 \oplus (\mathbf{S}|\mathbf{R})_1 \oplus \ldots = \sum_{n=0}^{\infty} \oplus (\mathbf{S}|\mathbf{R})_n,$$

Each can be done in *p* operations which cost $O(p^2)$ resulting in $O(p^3)$ complexity

Comparison of Direct Matrix Translation and Coaxial Translation-Rotation Decomposition



Other Fast translation schemes: Elliot and Board (1996)

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

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

Other Fast translation schemes: Elliot and Board (1996)

In the renormalized basis translation matrices are simple

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

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

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

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).
However, there are some stability issues reported.

Structured matrix based translation

- Tang 03
- Idea: use the rotation-coaxial translation method, and decompose resulting matrices into structured matrices
- Cost $O(p^2 \log p)$
- Details in Tang's thesis.

http://www.umiacs.umd.edu/~ramani/pubs/zhihui_thesis.pdf

Complexity

The total cost of the original algorithm is

$$2Np^2 + \frac{1528}{7}\frac{N}{s}p^4 + 27Ns.$$

With $s \approx \sqrt{\frac{1528}{189}}p^2$, it is $156Np^2$.
In Tang's algorithm, the total cost is

$$2Np^2 + \frac{1528}{7}\frac{N}{s} * \frac{85}{4}p^2\log(4p) + 9Ns.$$

With $s \approx \frac{\sqrt{228480p^2\log(4p)}}{21}$, it is

$$2Np^2 + 410\sqrt{\log(4p)}Np.$$

According to this result, the break even p is 5.

Cheng et al 1999

- H. Cheng,¤ L. Greengard,*y* and V. Rokhlin, A Fast Adaptive Multipole Algorithm in Three Dimensions, Journal of Computational Physics **155,** 468–498 (1999)
- Convert to a transform representation ("plane-wave")
  - at a cost of O(p^2 log p)
  - Expansion formula

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

- Discretize integrals

$$\left|\frac{1}{r} - \sum_{k=1}^{s(\varepsilon)}\frac{w_k}{M_k}\sum_{j=1}^{M_k} e^{-\lambda_k\cdot(z-z_0)}\cdot e^{i\lambda_k\cdot[(x-x_0)\cdot\cos(\alpha_{j,k}+(y-y_0)\cdot\sin(\alpha_{j,k})]}\right| < \varepsilon,$$

- Trans
- Convert back