

# The FMM for 3D Helmholtz Equation

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CSCAMM FAM04: 04/19/2004

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## Reference

N.A. Gumerov & R. Duraiswami

Fast Multipole Methods for Solution of the Helmholtz Equation in Three Dimensions

Academic Press, Oxford (2004)  
(in process).

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# Content

- Helmholtz Equation
- Expansions in Spherical Coordinates
- Matrix Translations
- Complexity and Modifications of the FMM
- Fast Translation Methods
- Error Bounds
- Multiple Scattering Problem

## Helmholtz Equation

# Helmholtz Equation

$$\nabla^2 \psi + k^2 \psi = 0$$

- Wave equation in frequency domain
  - ❑ Acoustics
  - ❑ Electromagnetics (Maxwell equations)
  - ❑ Diffusion/heat transfer/boundary layers
  - ❑ Telegraph, and related equations
  - ❑  $k$  can be complex
- Quantum mechanics
  - ❑ Klein-Gordan equation
  - ❑ Shroedinger equation
- Relativistic gravity (Yukawa potentials,  $k$  is purely imaginary)
- Molecular dynamics (Yukawa)
- Appears in many other models

## Boundary Value Problems

● Dirichlet:

$$\psi|_S = 0,$$

● Neumann:

$$\left. \frac{\partial \psi}{\partial n} \right|_S = 0,$$

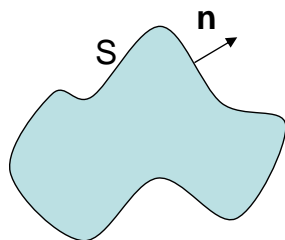
● Robin:

$$\left( \frac{\partial \psi}{\partial n} + i\sigma \psi \right) \Big|_S = 0.$$

● Sommerfield Radiation Condition (for external problems):

$$\psi = \psi_{in} + \psi_{scat}$$

$$\lim_{r \rightarrow \infty} \left[ r \left( \frac{\partial \psi_{scat}}{\partial r} - ik \psi_{scat} \right) \right] = 0.$$



# Green's Function and Identity

Free space Green's function:

$$\nabla^2 G(\mathbf{x}, \mathbf{y}) + k^2 G(\mathbf{x}, \mathbf{y}) = -\delta(\mathbf{x} - \mathbf{y}),$$

$$G(\mathbf{x}, \mathbf{y}) = \frac{\exp(ik|\mathbf{x} - \mathbf{y}|)}{4\pi|\mathbf{x} - \mathbf{y}|}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3.$$

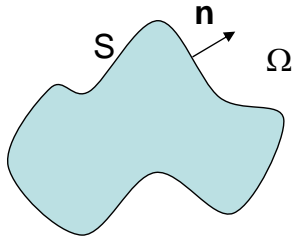
Green's formula:

$$\psi(\mathbf{y}) = \int_S \left[ \psi(\mathbf{x}) \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{x})} - G(\mathbf{x}, \mathbf{y}) \frac{\partial \psi(\mathbf{x})}{\partial n(\mathbf{x})} \right] dS(\mathbf{x}), \quad \mathbf{y} \in \Omega.$$

Boundary integral equation

$$\alpha \psi(\mathbf{y}) = \int_S \left( \psi(\mathbf{x}) \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{x})} - G(\mathbf{x}, \mathbf{y}) \frac{\partial \psi(\mathbf{x})}{\partial n(\mathbf{x})} \right) dS(\mathbf{x}),$$

$$\alpha = \begin{cases} \frac{1}{2} & \mathbf{y} \text{ on a smooth part of the boundary} \\ \frac{\gamma}{4\pi} & \mathbf{y} \text{ at a corner on the boundary} \\ 1 & \mathbf{y} \text{ inside the domain} \end{cases}.$$



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## Distributions of Monopoles and Dipoles

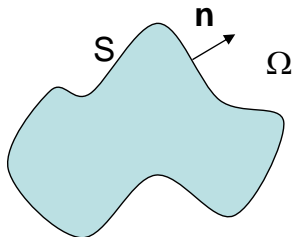
Volume source distribution:

$$\psi(\mathbf{y}) = \sum_{j=1}^N Q_j G(\mathbf{x}_j, \mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^3 \setminus \{\mathbf{x}_j\},$$

$$\psi(\mathbf{y}) = \int_{\bar{\Omega}} q(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) dV(\mathbf{x}), \quad \mathbf{y} \in \Omega, \quad \bar{\Omega} \cap \Omega = \emptyset.$$

Single layer potential:

$$\psi(\mathbf{y}) = \int_S q_\sigma(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) dS(\mathbf{x}), \quad \mathbf{y} \in \Omega, \quad S = \partial\Omega.$$



Double layer potential:

$$\psi(\mathbf{y}) = \int_S q_\mu(\mathbf{x}) \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial n(\mathbf{x})} dS(\mathbf{x}), \quad \mathbf{y} \in \Omega, \quad S = \partial\Omega.$$

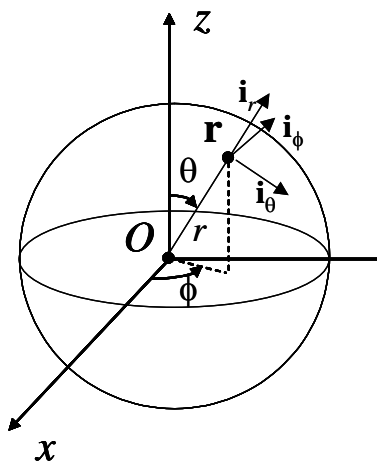
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# Expansions in Spherical Coordinates

## Spherical Basis Functions

$$x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta.$$



Spherical Coordinates

Spherical Bessel Functions

Regular Basis Functions

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

Singular Basis Functions

$$S_n^m(\mathbf{r}) = h_n(kr) Y_n^m(\theta, \varphi).$$

Spherical Hankel Functions  
of the First Kind

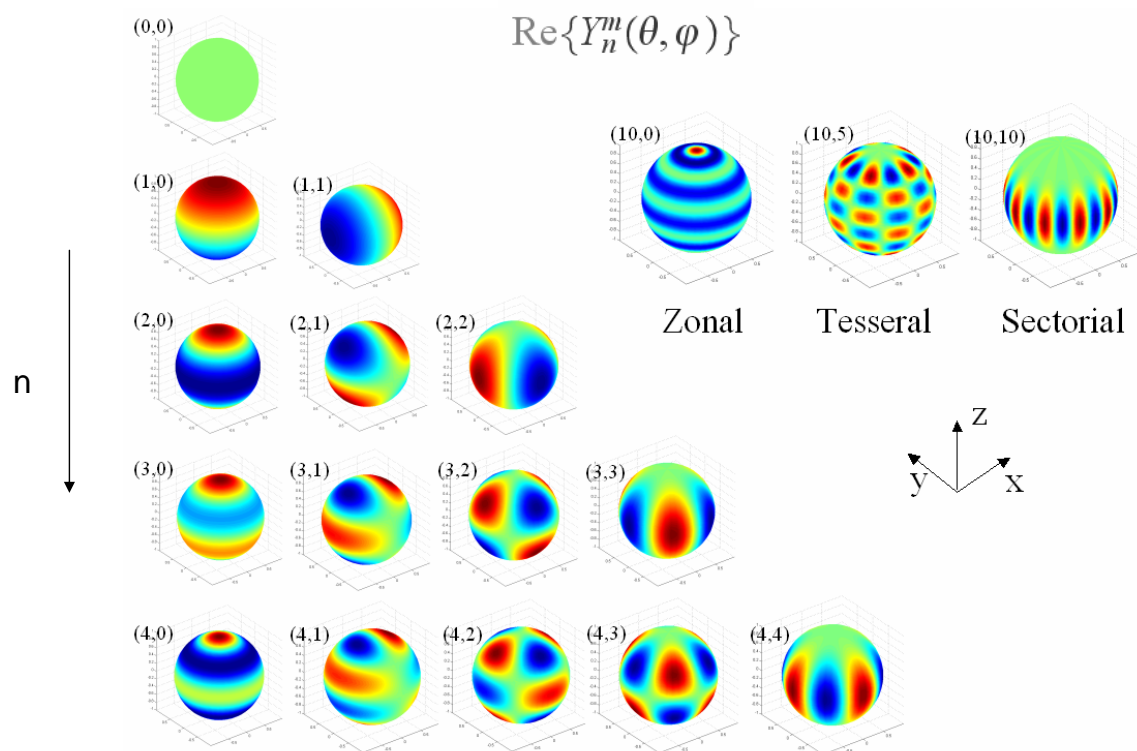
Spherical Harmonics

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

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

Associated Legendre Functions

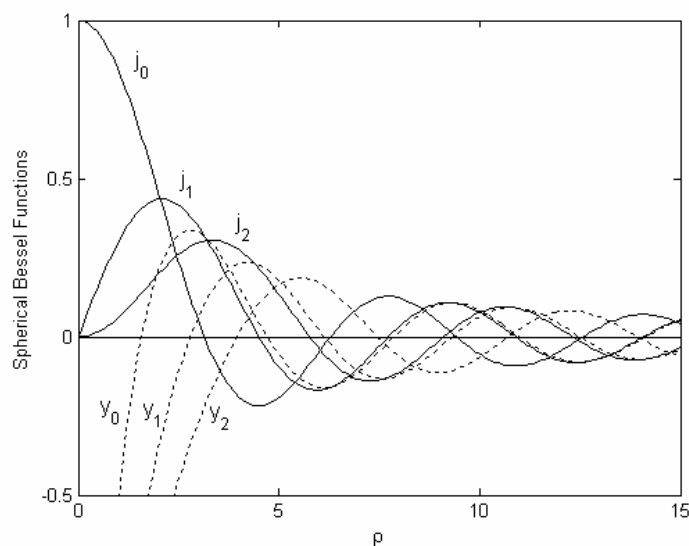
# Spherical Harmonics



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# Spherical Bessel Functions



$$h_n(\rho) = j_n(\rho) + iy_n(\rho)$$

$$j_0(\rho) = \frac{\sin \rho}{\rho}, \quad j_1(\rho) = \frac{\sin \rho}{\rho^2} - \frac{\cos \rho}{\rho},$$

$$j_2(\rho) = \left( \frac{3}{\rho^3} - \frac{1}{\rho} \right) \sin \rho - \frac{3}{\rho^2} \cos \rho,$$

$$y_0(\rho) = -\frac{\cos \rho}{\rho}, \quad y_1(\rho) = -\frac{\cos \rho}{\rho^2} - \frac{\sin \rho}{\rho},$$

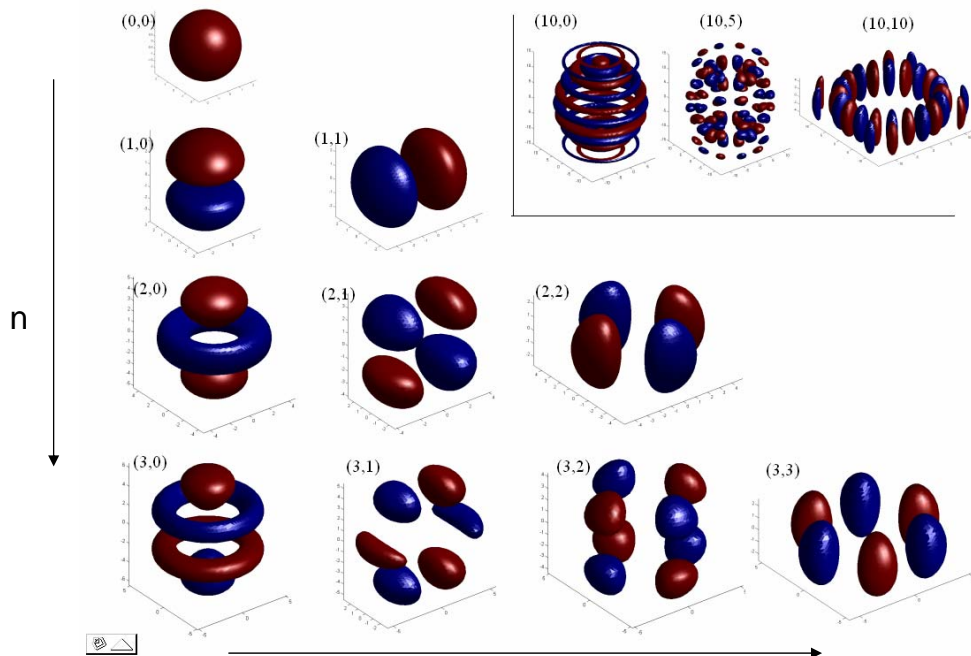
$$y_2(\rho) = \left( -\frac{3}{\rho^3} + \frac{1}{\rho} \right) \cos \rho - \frac{3}{\rho^2} \sin \rho.$$

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# Isosurfaces For Regular Basis Functions

$$\text{Re}\{R_n^m(\mathbf{r})\} = \text{const}$$



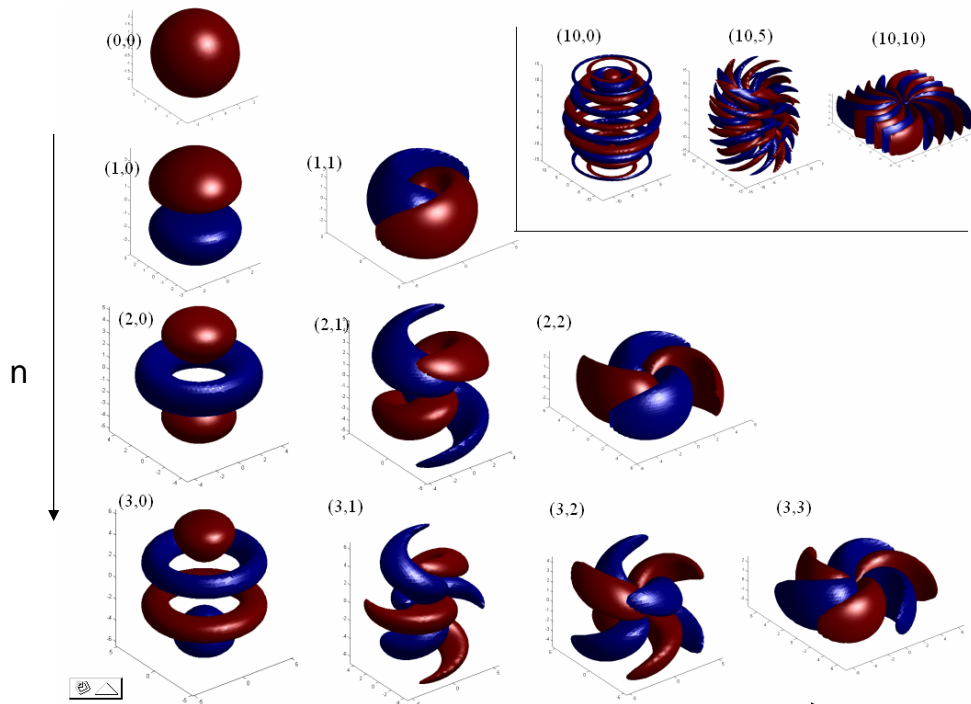
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# Isosurfaces For Singular Basis Functions

$$\text{Re}\{S_n^m(\mathbf{r})\} = \text{const}$$



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# Expansions

$$\psi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n A_n^m F_n^m(\mathbf{r}) = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} A_n^m F_n^m(\mathbf{r}), \quad F = S, R, \quad A_n^m \in \mathbb{C}.$$

Absolute and uniform convergence

$$\forall \epsilon > 0, \quad \exists p(\epsilon), \quad \left| \psi(\mathbf{r}) - \sum_{n=0}^{p-1} \sum_{m=-n}^n A_n^m F_n^m(\mathbf{r}) \right| < \epsilon, \quad \forall \mathbf{r} \in \Omega,$$

and

$$\forall \epsilon > 0, \quad \exists p(\epsilon), \quad \sum_{n=p}^{\infty} \sum_{m=-n}^n |A_n^m F_n^m(\mathbf{r})| < \epsilon, \quad \forall \mathbf{r} \in \Omega.$$

Plane Wave expansion:

$$e^{i\mathbf{k} \cdot \mathbf{r}} = 4\pi \sum_{n=0}^{\infty} \sum_{m=-n}^n i^n Y_n^{-m}(\theta_k, \varphi_k) R_n^m(\mathbf{r}),$$

$$\mathbf{k} = ks, \quad \mathbf{s} = (\sin \theta_k \cos \varphi_k, \sin \theta_k \sin \varphi_k, \cos \theta_k).$$

Wave vector

# Matrix Translations

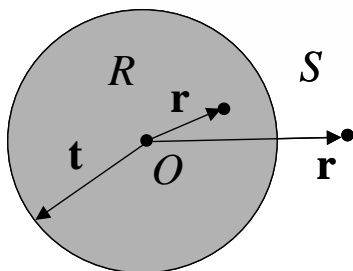
# Reexpansions of Basis Functions

$$R_n^m(\mathbf{r} + \mathbf{t}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} (R|R)_{n'n}^{m'm}(\mathbf{t}) R_{n'}^{m'}(\mathbf{r}), \quad n = 0, 1, 2, \dots, \quad m = -n, \dots, n.$$

Reexpansion Matrices

$$S_n^m(\mathbf{r} + \mathbf{t}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} \begin{cases} (S|R)_{n'n}^{m'm}(\mathbf{t}) R_{n'}^{m'}(\mathbf{r}), & |\mathbf{r}| < |\mathbf{t}| \\ (S|S)_{n'n}^{m'm}(\mathbf{t}) S_{n'}^{m'}(\mathbf{r}), & |\mathbf{r}| > |\mathbf{t}| \end{cases},$$

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



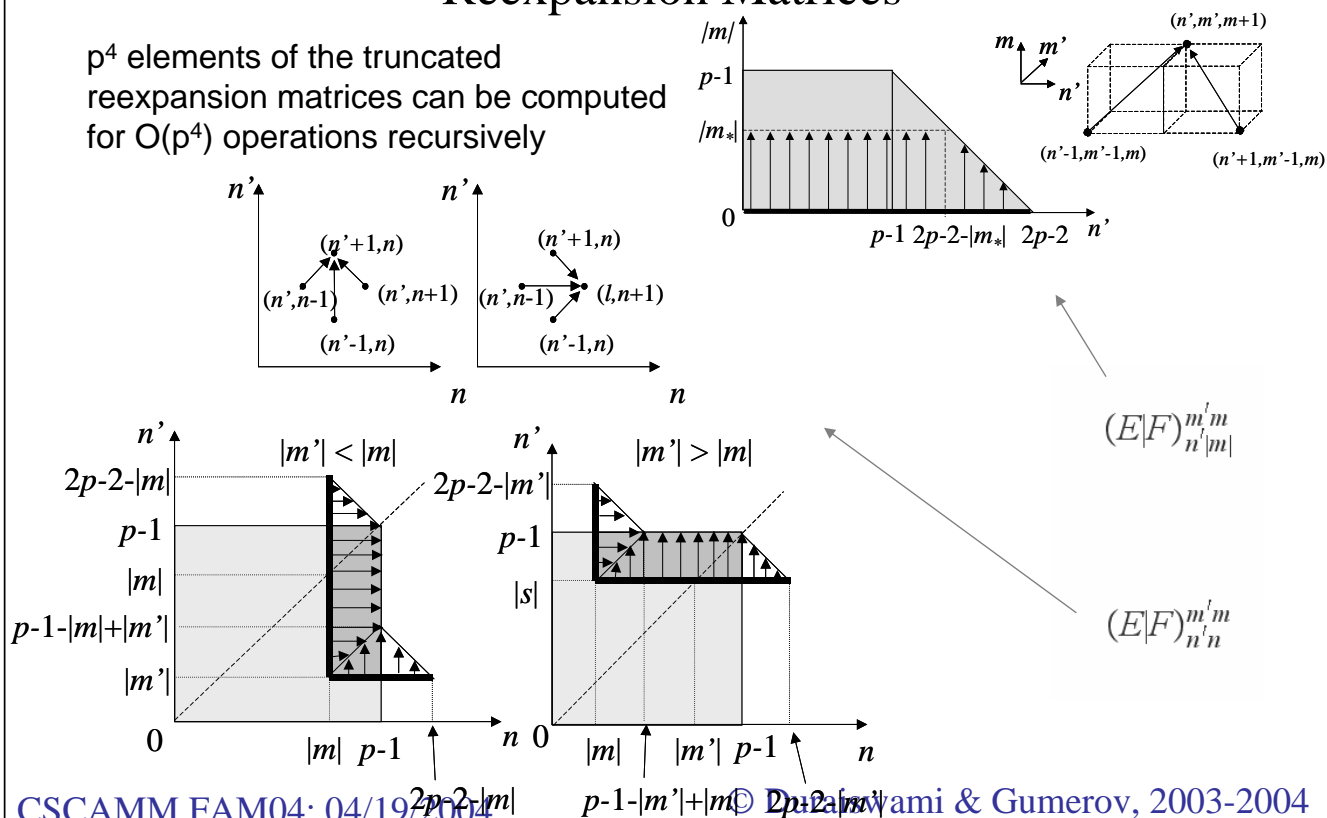
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## Recursive Computation of Reexpansion Matrices

Gumerov & Duraiswami,  
*SIAM J. Sci. Stat. Comput.*  
25(4), 1344-1381, 2003.

$p^4$  elements of the truncated reexpansion matrices can be computed for  $O(p^4)$  operations recursively



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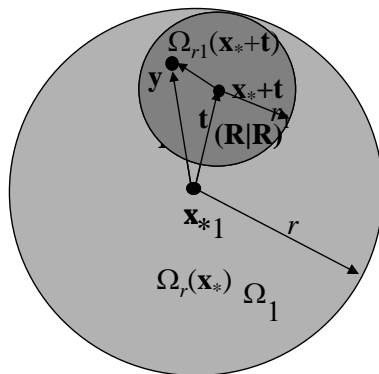
# Translations

$$\psi(\mathbf{y}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n C_n^m(\mathbf{x}_{*1}) E_n^m(\mathbf{y} - \mathbf{x}_{*1}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n C_n^m(\mathbf{x}_{*2}) F_n^m(\mathbf{y} - \mathbf{x}_{*2}),$$

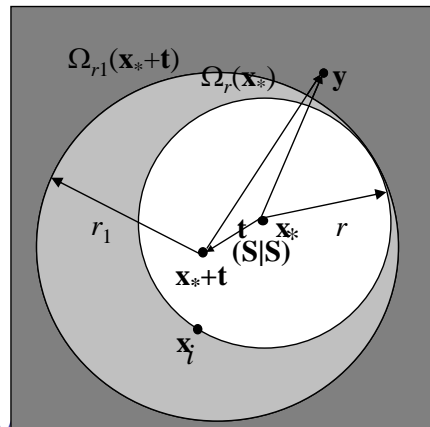
$$C_n^m(\mathbf{x}_{*2}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} (E|F)_{nm'}^{mm'}(\mathbf{t}) C_{n'}^{m'}(\mathbf{x}_{*1}), \quad \mathbf{t} = \mathbf{x}_{*2} - \mathbf{x}_{*1}$$

$$E, F = S, R, \quad n = 0, 1, \dots, \quad m = -n, \dots, n.$$

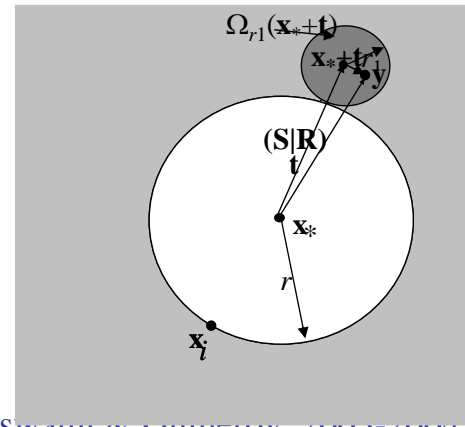
R|R



S|S



S|R



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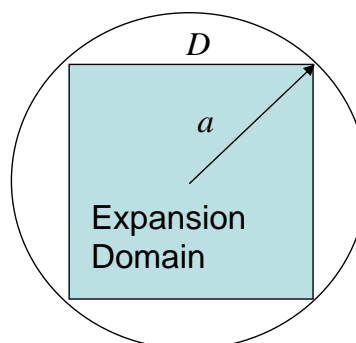
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## Problem:

- For the Helmholtz equation absolute and uniform convergence can be achieved only for

$p > ka$ . For large  $ka$  the FMM with constant  $p$  is

- very expensive (comparable with straightforward methods);
- inaccurate (since keeps much larger number of terms than required, which causes numerical instabilities).

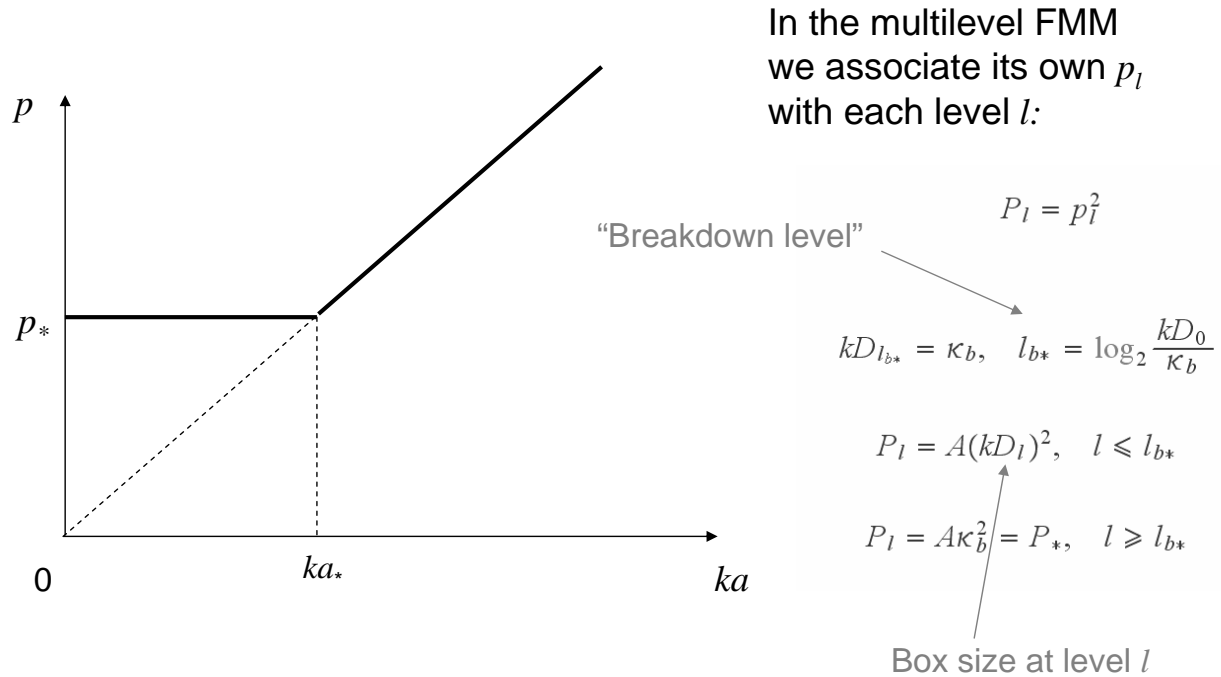


$$2a = 3^{1/2} D$$

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# Model of Truncation Number Behavior for Fixed Error



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## Complexity of Single Translation

Translation exponent

$$CostTrans(P_l) = CP_l^v = Cp_l^{2v}, \quad l = 2, \dots, l_{\max}.$$

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# Spatially Uniform Data Distributions

$$N_l \sim 8^{-l}N, \quad l_{\max} \sim \frac{1}{3} \log N$$

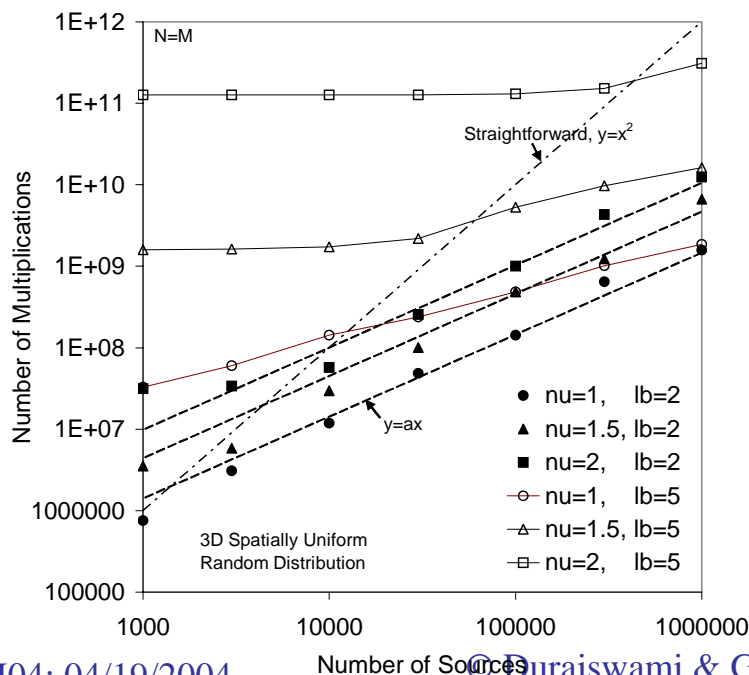
$$p_l \sim 2^{-l}kD_0,$$

$$N_{oper} \sim (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 2^{-2\nu l} 8^l = (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 2^{(3-2\nu)l}.$$

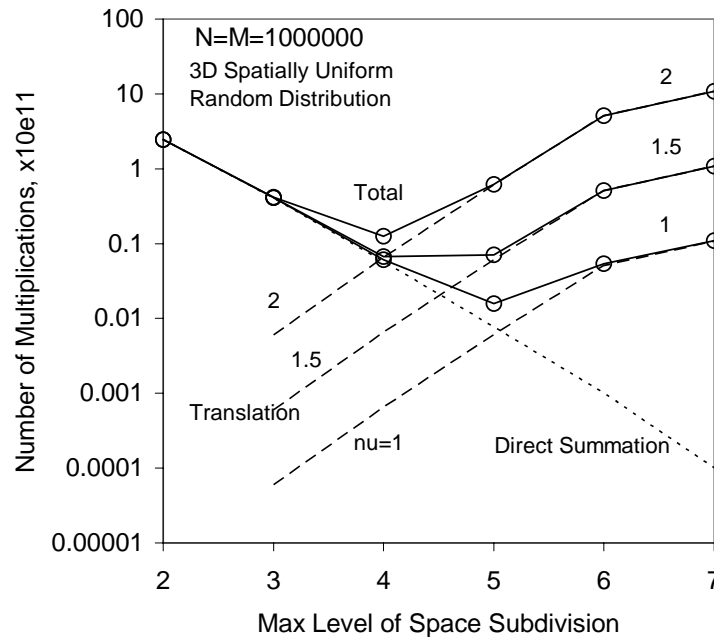
- $\nu < 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu} 2^{(3-2\nu)l_{\max}} \sim (kD_0)^{2\nu} N^{1-2\nu/3}$
- $\nu = 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu} l_{\max} \sim (kD_0)^{2\nu} \log N$
- $\nu > 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu}$

Constant!

## Complexity of the Optimized FMM for Fixed $kD_0$ and Variable $N$



# Optimum Level for Low Frequencies



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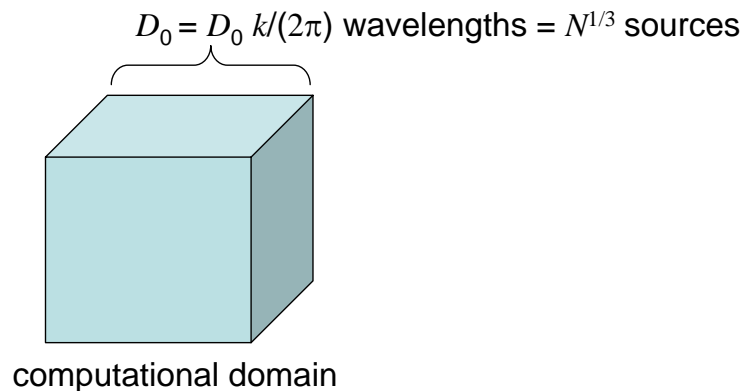
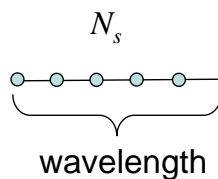
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## Volume Element Methods

$$N = \left( \frac{N_s}{2\pi} kD_0 \right)^3, \quad kD_0 \sim N^{1/3}$$

- $\nu < 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu} 2^{(3-2\nu)l_{\max}} \sim (kD_0)^{2\nu} N^{1-2\nu/3} \sim N$
- $\nu = 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu} l_{\max} \sim (kD_0)^{2\nu} \log N \sim N \log N$
- $\nu > 1.5$  :  $Complexity_{FMM} \sim (kD_0)^{2\nu} \sim N^{2\nu/3} \gg N \log N$

Critical Translation Exponent!



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# What Happens if Truncation Number is Constant for All Levels?

$$N_{oper} \sim (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 8^l = (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 2^{3l} \sim (kD_0)^{2\nu} 2^{3l_{\max}} \sim (kD_0)^{2\nu} N \sim N^{1+2\nu/3}.$$

- $\nu < 1.5$  :  $N \ll \text{ComplexityFMM} \ll N^2$
- $\nu = 1.5$  :  $\text{ComplexityFMM} \sim N^2$
- $\nu > 1.5$  :  $\text{ComplexityFMM} \sim N^{1+2\nu/3} \gg N^2$

“Catastrophic Disaster of the FMM”

## Surface Data Distributions

$$N_l \sim 4^{-l} N, \quad l_{\max} \sim \frac{1}{2} \log N$$

$$p_l \sim 2^{-l} kD_0,$$

$$N_{oper} \sim (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 2^{-2\nu l} 4^l = (kD_0)^{2\nu} \sum_{l=2}^{l_{\max}} 2^{(2-2\nu)l}.$$

- $\nu = 1$  :  $\text{ComplexityFMM} \sim (kD_0)^{2\nu} l_{\max} \sim (kD_0)^{2\nu} \log N$
- $\nu > 1$  :  $\text{ComplexityFMM} \sim (kD_0)^{2\nu}$

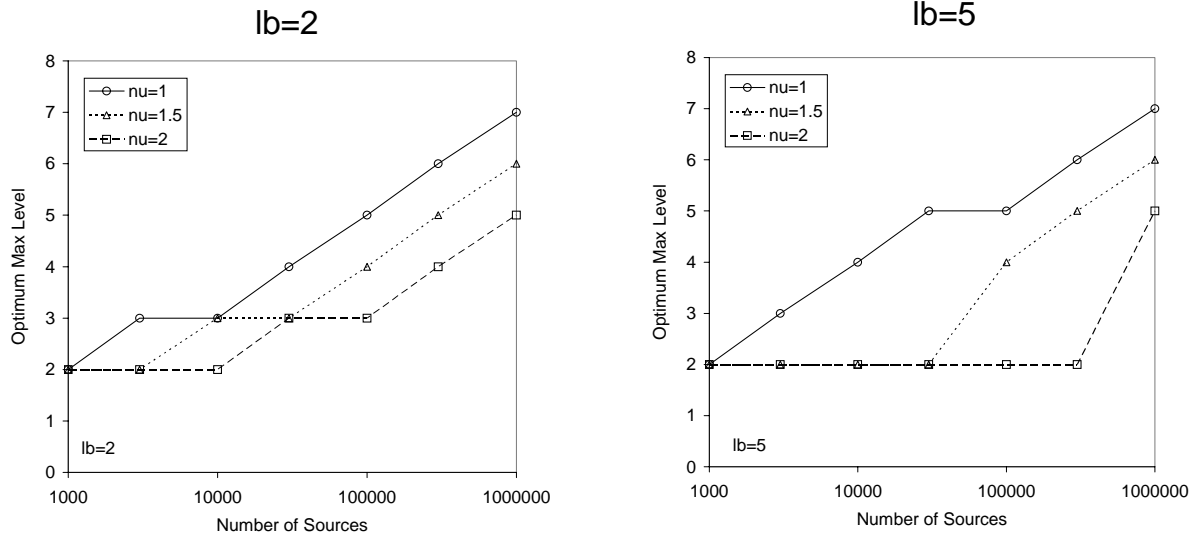
Boundary Element Methods:

$$N = \left( \frac{N_s}{2\pi} kD_0 \right)^2, \quad kD_0 \sim N^{1/2}$$

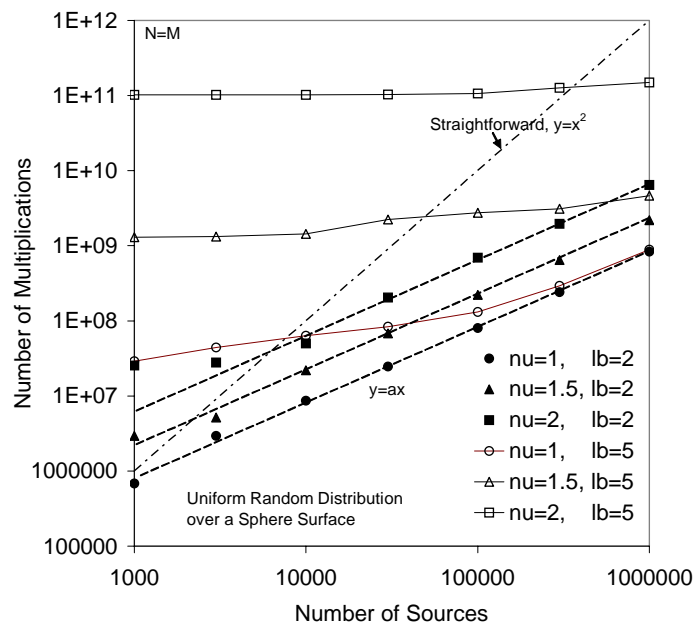
- $\nu = 1$  :  $\text{ComplexityFMM} \sim (kD_0)^{2\nu} l_{\max} \sim (kD_0)^{2\nu} \log N \sim N \log N$
- $\nu > 1$  :  $\text{ComplexityFMM} \sim (kD_0)^{2\nu} \sim N^\nu \gg N \log N.$

Critical Translation Exponent!

# Optimum Level of Space Subdivision

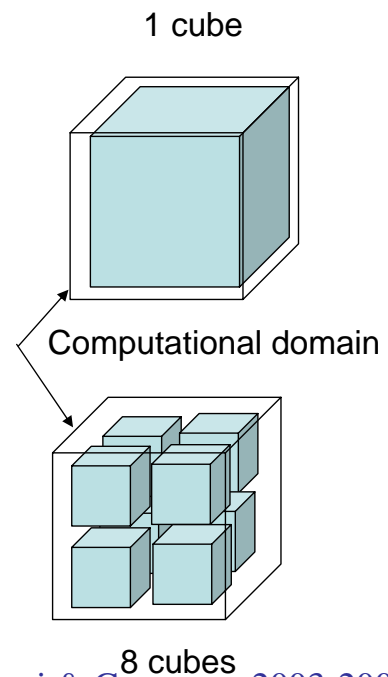
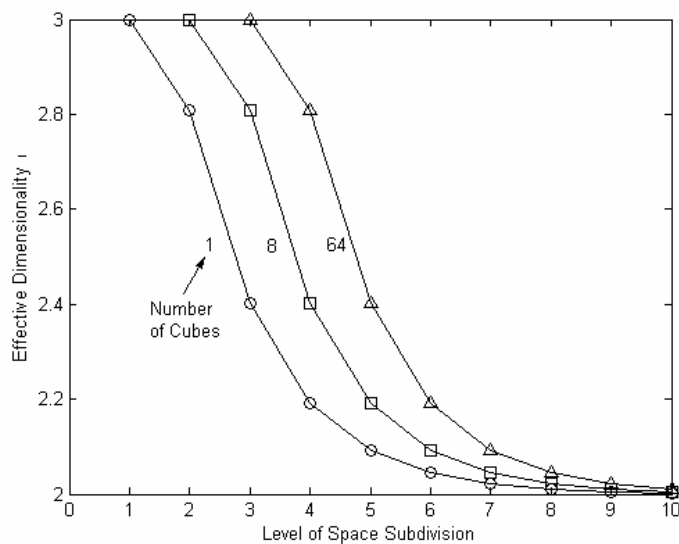


# Performance of the MLFMM for Surface Data Distributions



# Effective Dimensionality of the Problem

$$d_{\text{eff}}(l) = \log_2 \frac{N_{\text{non-empty}}(l)}{N_{\text{non-empty}}(l-1)}, \quad l = 1, 2, \dots$$



## Fast Translation Methods

# Translation Methods

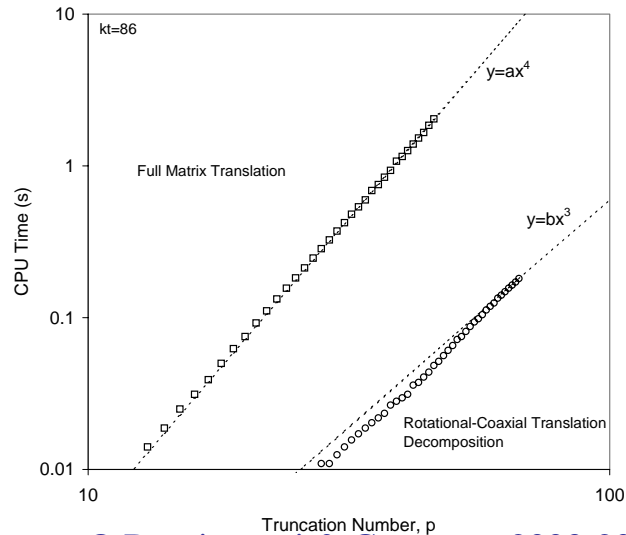
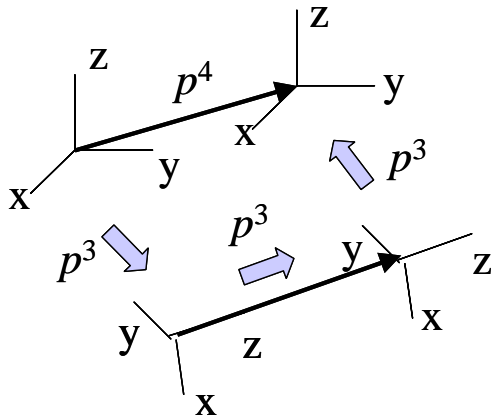
- $O(p^5)$ : Matrix Translation with Computation of Matrix Elements Based on Clebsch-Gordan Coefficients;
- $O(p^4)$  (Low Asymptotic Constant): Matrix Translation with Recursive Computation of Matrix Elements
- $O(p^3)$  (Low Asymptotic Constants):
  - ❑ Rotation-Coaxial Translation Decomposition with Recursive Computation of Matrix Elements;
  - ❑ Sparse Matrix Decomposition;
- $O(p^2 \log^b p)$ 
  - ❑ Rotation-Coaxial Translation Decomposition with Structured Matrices for Rotation and Fast Legendre Transform for Coaxial Translation;
  - ❑ Translation Matrix Diagonalization with Fast Spherical Transform;
  - ❑ Asymptotic Methods;
  - ❑ Diagonal Forms of Translation Operators with Spherical Filtering.

## $O(p^3)$ Methods

# Rotation - Coaxial Translation Decomposition (Complexity $O(p^3)$ )

From the group theory follows that general translation can be reduced to

$$(\mathbf{F}|\mathbf{E})(\mathbf{t}) = \mathbf{Rot}(\mathbf{Q}^{-1})(\mathbf{F}|\mathbf{E})_{(coax)}(\mathbf{t})\mathbf{Rot}(\mathbf{Q}), \quad F, E = S, R.$$



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## Sparse Matrix Decomposition

$$(\mathbf{R}|\mathbf{R})(\mathbf{t}) = (\mathbf{S}|\mathbf{S})(\mathbf{t}) = \sum_{n=0}^{\infty} \frac{(kt)^n}{n!} \mathbf{D}_t^n = e^{kt\mathbf{D}_t} = \Lambda_r(kt, -i\mathbf{D}_t)$$

$$(\mathbf{S}|\mathbf{R})(\mathbf{t}) = \Lambda_s(kt, -i\mathbf{D}_t)$$

$$\Lambda_r(kt, -i\mathbf{D}_t) = \sum_{n=0}^{\infty} (2n+1) i^n j_n(kt) P_n(-i\mathbf{D}_t)$$

$$\Lambda_s(kt, -i\mathbf{D}_t) = \sum_{n=0}^{\infty} (2n+1) i^n h_n(kt) P_n(-i\mathbf{D}_t).$$

Matrix-vector products with these matrices computed recursively

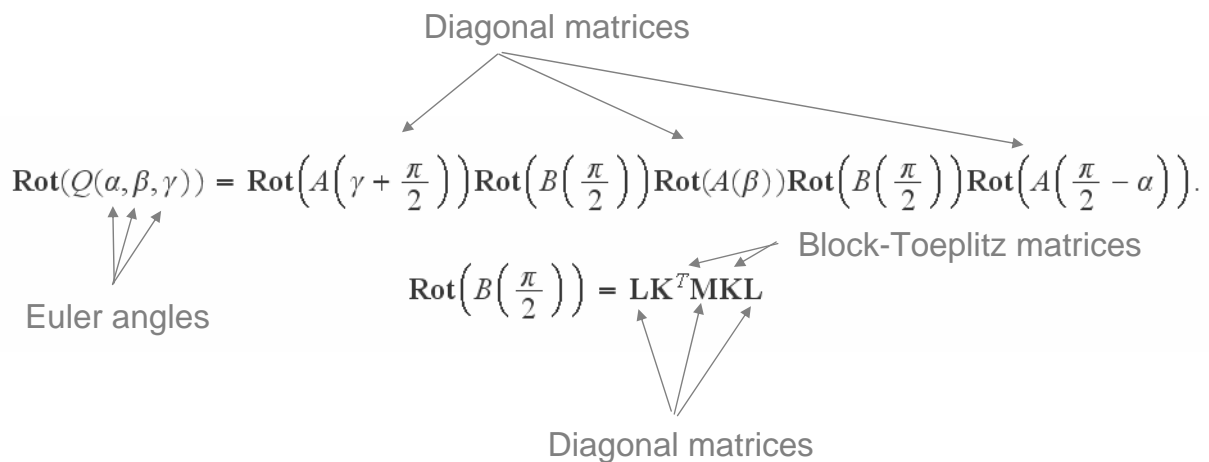
$$(\mathbf{D}_t \mathbf{C})_n^m = \frac{1}{2t} \left[ (t_x + it_y) (C_{n-1}^{m+1} b_n^m - C_{n+1}^{m+1} b_{n+1}^{m-1}) + (t_x - it_y) (C_{n-1}^{m-1} b_n^{-m} - C_{n+1}^{m-1} b_{n+1}^{m-1}) \right] \\ + \frac{t_z}{t} (a_n^m C_{n+1}^m - a_{n-1}^m C_n^m), \quad m = 0, \pm 1, \pm 2, \dots, \quad n = |m|, |m| + 1, \dots$$

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# $O(p^2 \log^{\beta} p)$ Methods

## Fast Rotation Transform



Complexity:  $O(p^2 \log p)$

# Fast Coaxial Translation

$$(\mathbf{R}|\mathbf{R})_{(coax)}^{(p,p')}(t) = (\mathbf{S}|\mathbf{S})_{(coax)}^{(p,p')}(t) = \mathbf{i}^{(p)} \mathbf{L}^{(p)} \mathbf{W} \Lambda_r^{(p+p'-1)}(kt) (\mathbf{L}^{(p')})^T \overline{\mathbf{i}^{(p')}},$$

$$(\mathbf{S}|\mathbf{R})_{(coax)}^{(p,p')}(t) = \mathbf{i}^{(p)} \mathbf{L}^{(p)} \mathbf{W} \Lambda_s^{(p+p'-1)}(kt) (\mathbf{L}^{(p')})^T \overline{\mathbf{i}^{(p')}}.$$

Legendre and  
transposed Legendre matrices

Diagonal matrices

Fast multiplication of the Legendre and transposed Legendre matrices can be performed via the forward and inverse FAST LEGENDRE TRANSFORM (FLT) with complexity  $O(p^2 \log^2 p)$

**Healy et al** *Advances in Computational Mathematics* **21**: 59-105, 2004.

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# Diagonalization of General Translation Operator

$$(\mathbf{E}|\mathbf{F})^{(p,p')}(t) = \mathbf{i}^{(p)} \mathbf{Y}^{(p)} \mathbf{W} \Lambda^{(p+p'-1)}(t) (\overline{\mathbf{Y}^{(p')}})^T \overline{\mathbf{i}^{(p')}}.$$

Matrices for the forward and  
inverse and Spherical Transform

Diagonal matrices

FAST SPHERICAL TRANSFORM (FST) can be performed with complexity  $O(p^2 \log^2 p)$

**Healy et al** *Advances in Computational Mathematics* **21**: 59-105, 2004.

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## Method of Signature Function (Diagonal Forms of the Translation Operator)

$$\psi(\mathbf{r}) = \frac{1}{4\pi} \int_{S_u} e^{iks \cdot \mathbf{r}} \Psi(\mathbf{s}) dS(\mathbf{s}), \quad \text{Regular Solution}$$

$$\psi^{(p)}(\mathbf{r}) = \frac{1}{4\pi} \int_{S_u} \Lambda_s^{(p)}(\mathbf{r}; \mathbf{s}) \Psi(\mathbf{s}) dS(\mathbf{s}), \quad \text{Singular Solution}$$

$$\Lambda_r(\mathbf{r}; \mathbf{s}) = \sum_{n=0}^{\infty} (2n+1) i^n j_n(kr) P_n\left(\frac{\mathbf{r} \cdot \mathbf{s}}{r}\right)$$

$$\Lambda_s^{(p)}(\mathbf{r}; \mathbf{s}) = \sum_{n=0}^{p-1} (2n+1) i^n h_n(kr) P_n\left(\frac{\mathbf{r} \cdot \mathbf{s}}{r}\right).$$

$$\hat{\Psi}(\mathbf{s}) = (\mathcal{S}|\mathcal{S})(\mathbf{t})[\Psi(\mathbf{s})] = (\mathcal{R}|\mathcal{R})(\mathbf{t})[\Psi(\mathbf{s})] = e^{iks \cdot \mathbf{t}} \Psi(\mathbf{s}),$$

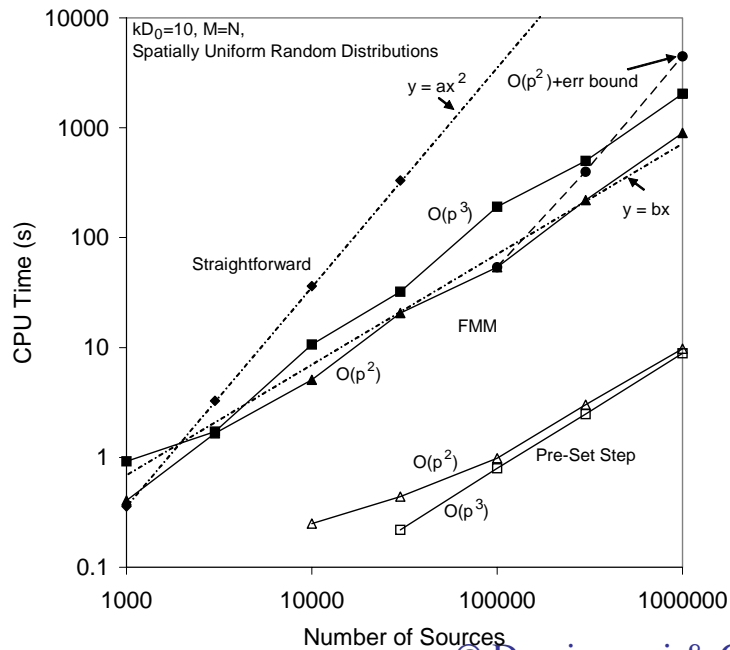
$$\hat{\Psi}_{(p)}(\mathbf{s}) = (\mathcal{S}|\mathcal{R})(\mathbf{t})[\Psi(\mathbf{s})] = \Lambda_s^{(p)}(\mathbf{t}; \mathbf{s}) \Psi(\mathbf{s}).$$

## Final Summation and Initial Expansion

$$\psi(\mathbf{r}) = \frac{1}{4\pi} \sum_{j=0}^{N_c-1} w_j e^{iks_j \cdot \mathbf{r}} \Psi(\mathbf{s}_j) + \epsilon_c, \quad \mathbf{s}_j \in S_u,$$

$$G(\mathbf{r} - \mathbf{r}_s) \rightleftharpoons \Psi_{(0)}(\mathbf{s}_j; \mathbf{r}_s - \mathbf{r}_*) = \frac{ik}{4\pi} e^{-iks_j \cdot (\mathbf{r}_s - \mathbf{r}_*)}$$

# The FMM with Band-Unlimited Signature Functions ( $O(p^2)$ method)



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## Deficiencies

- Low Frequencies;
- High Frequencies;
- Constant  $p$ ;
- Instabilities after two or three levels of translations.

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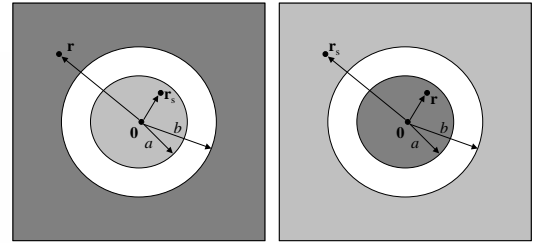
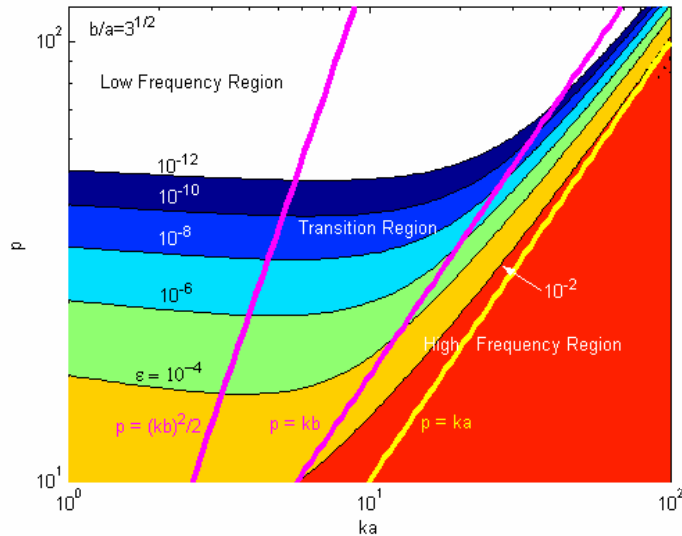
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# Methods to Fix:

- Use of Band-limited functions;
- Error control via band-limits;
- Requires filtering procedures (complexity  $O(p^2 \log^2 p)$  or  $O(p^2 \log p)$ ) with large asymptotic constants;
- The length of the representation is changed via interpolation/interpolation procedures.

# Error Bounds

# Source Expansion Errors



Low frequencies:

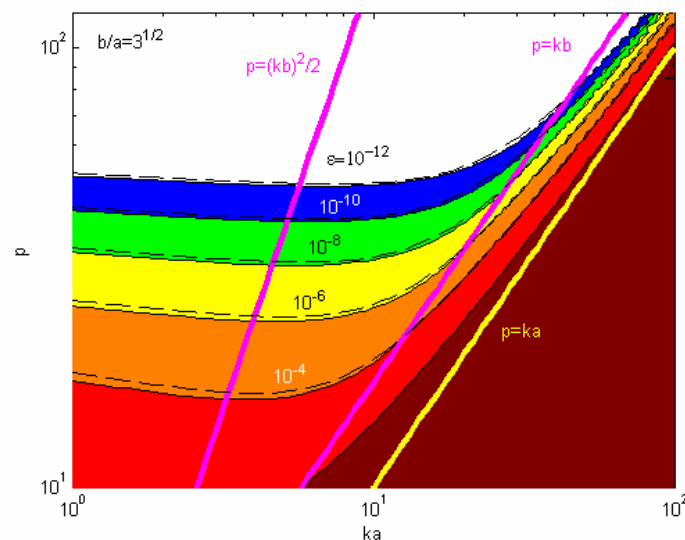
$$p = -\frac{\ln[\epsilon ka(1 - \sigma^{-1})^{3/2}]}{\ln \sigma} - 1.$$

High frequencies:

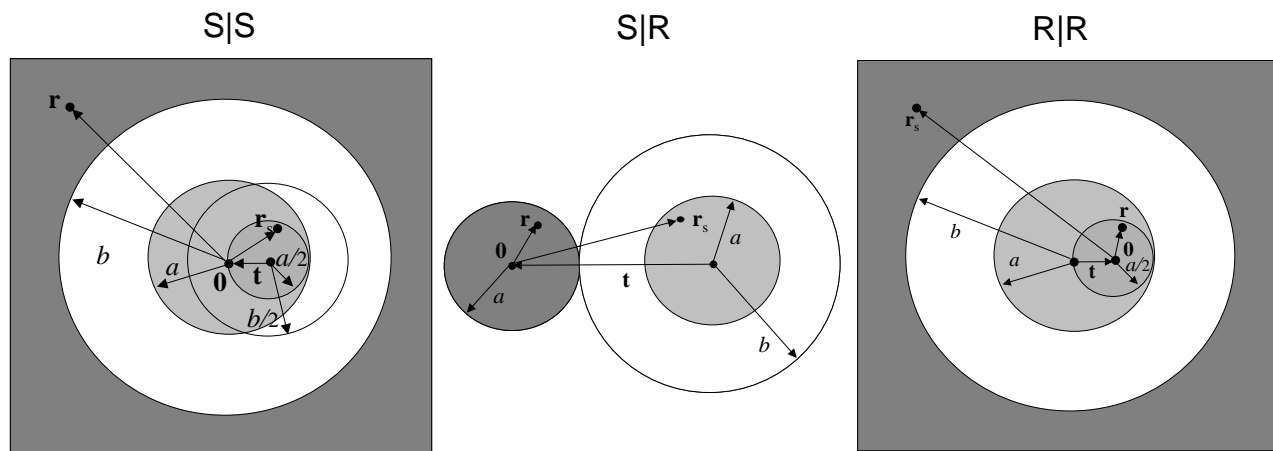
$$p = ka + \frac{1}{2} \left( 3 \ln \frac{1}{\epsilon \sigma} \right)^{2/3} (ka)^{1/3}.$$

## Approximation of the Error

$$p = \left\{ \left[ \frac{1}{\ln \sigma} \ln \frac{1}{\epsilon ka(1 - \sigma^{-1})^{3/2}} + 1 \right]^4 + \left[ ka + \frac{1}{2} \left( 3 \ln \frac{1}{\epsilon \sigma} \right)^{2/3} (ka)^{1/3} \right]^4 \right\}^{1/4}$$



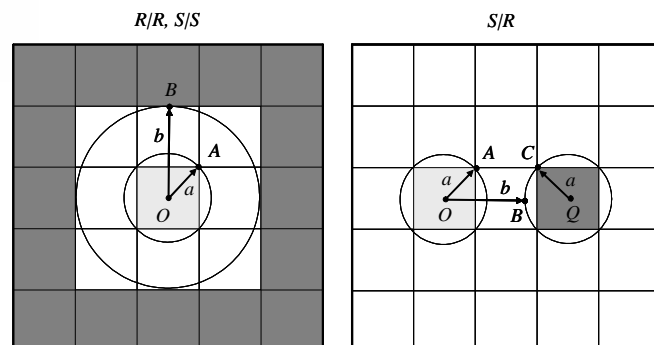
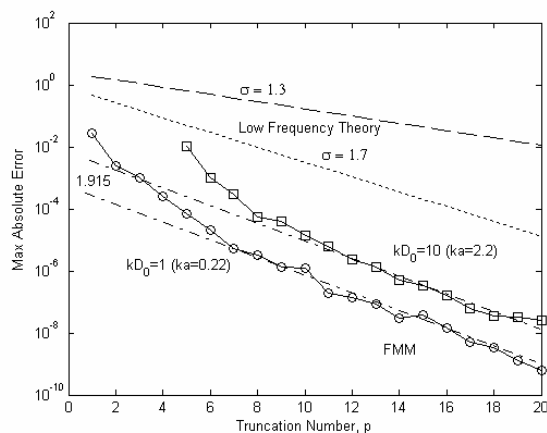
We proved that for source summation problems the truncation numbers can be selected based on the above chart when using translations with rectangularly truncated matrices



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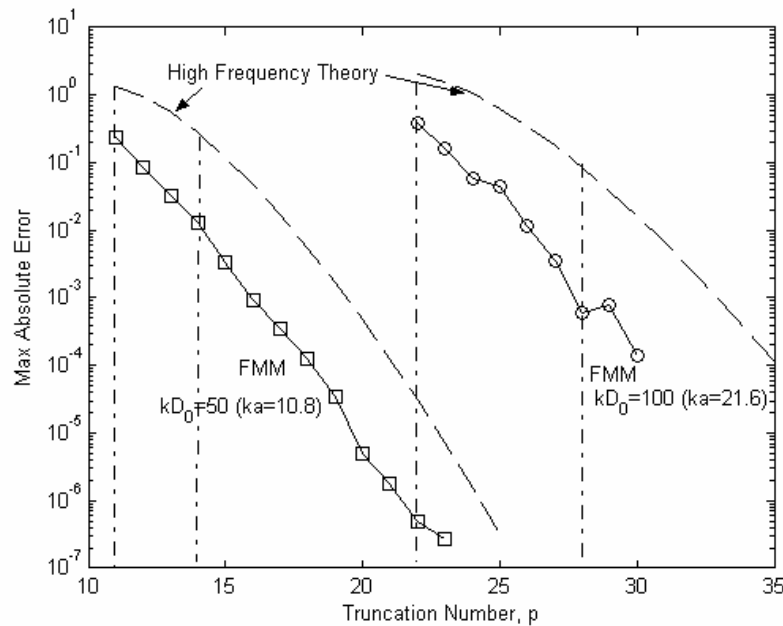
## Low Frequency FMM Error



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# High Frequency FMM Error



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## Multiple Scattering Problem

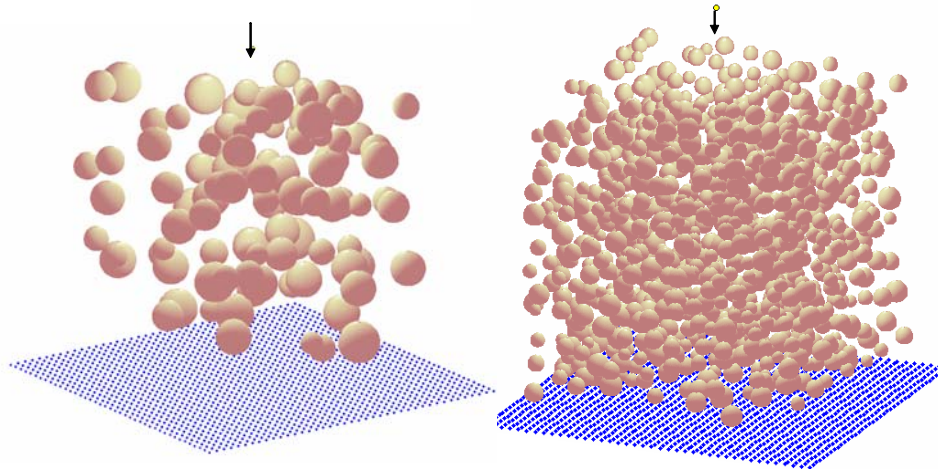
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# Problem

Boundary Conditions:

$$|\mathbf{r} - \mathbf{r}'_q| = a_q : \quad \frac{\partial \psi(\mathbf{r})}{\partial n_q} + i\sigma_q \psi(\mathbf{r}) = 0, \quad q = 1, \dots, N.$$



CSCAMM FAM04: 04/19/2004 100 random spheres

© Duran & Gumerov, 2003-2004 1000 random spheres

## T-Matrix Method

### Scattered Field Decomposition

$$\psi_{scat}(\mathbf{r}) = \sum_{p=1}^N \psi_p(\mathbf{r}), \quad \lim_{r \rightarrow \infty} r \left( \frac{\partial \psi_p}{\partial r} - ik\psi_p \right) = 0, \quad p = 1, \dots, N.$$

$$\psi_p(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \underset{\substack{\uparrow \\ \text{Expansion Coefficients}}}{A_n^{(p)m}} \underset{\substack{\downarrow \\ \text{Singular Basis Functions}}}{S_n^m(\mathbf{r} - \mathbf{r}'_p)}, \quad S_n^m(\mathbf{r}) = \underset{\substack{\downarrow \\ \text{Hankel Functions}}}{h_n(kr)} \underset{\substack{\uparrow \\ \text{Spherical Harmonics}}}{Y_n^m(\theta, \varphi)}.$$

$$\mathbf{A} = (A_0^0, A_1^{-1}, A_1^0, A_1^1, A_2^{-2}, A_2^{-1}, A_2^0, A_2^1, A_2^2, \dots)^T,$$

Vector Form:

$$\psi_p(\mathbf{r}) = \overline{\mathbf{A}^{(p)}} \cdot \mathbf{S}(\mathbf{r} - \mathbf{r}'_p).$$

dot product

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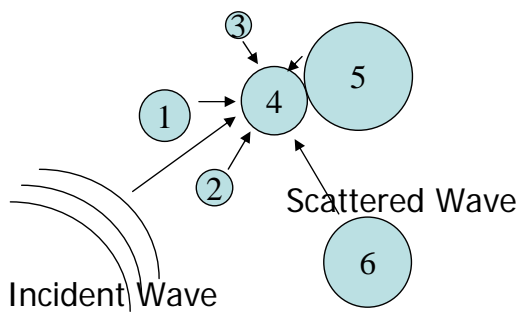
## Solution of Multiple Scattering Problem

"Effective" Incident Field

$$\psi(\mathbf{r}) = \psi_q(\mathbf{r}) + \psi_{in}(\mathbf{r}) + \psi_{other}^{(q)}(\mathbf{r}) = \psi_q(\mathbf{r}) + \psi_{eff}^{(q)(in)}(\mathbf{r}),$$

$$\psi_{other}^{(q)}(\mathbf{r}) = \sum_{p \neq q} \overline{\mathbf{A}^{(p)}} \cdot \mathbf{S}(\mathbf{r}_p) = \overline{\mathbf{B}^{(q)}} \cdot \mathbf{R}(\mathbf{r}_q), \quad \psi_{eff}^{(q)(in)}(\mathbf{r}) = \overline{\mathbf{E}_{eff}^{(q)}} \cdot \mathbf{R}(\mathbf{r}_q).$$

Coupled System of Equations:



$$\mathbf{A}^{(q)} = \mathbf{T}^{(q)} \mathbf{E}_{eff}^{(q)},$$

$$\mathbf{B}^{(q)} = \sum_{p \neq q} (\mathbf{S}|\mathbf{R})(\mathbf{r}'_q - \mathbf{r}'_p) \mathbf{A}^{(p)},$$

$$\mathbf{E}_{eff}^{(q)} = \mathbf{E}^{(in)}(\mathbf{r}'_q) + \mathbf{B}^{(q)}, \quad q = 1, \dots, N$$

(S|R)-Translation Matrix

## Iterative Methods

### Reflection Method & Krylov Subspace Method (GMRES)

Reflection (Simple Iteration) Method:

$$\mathbf{A}_j^{(q)} = \mathbf{T}^{(q)} [\mathbf{E}^{(in)}(\mathbf{r}'_q) + \mathbf{B}_j^{(q)}],$$

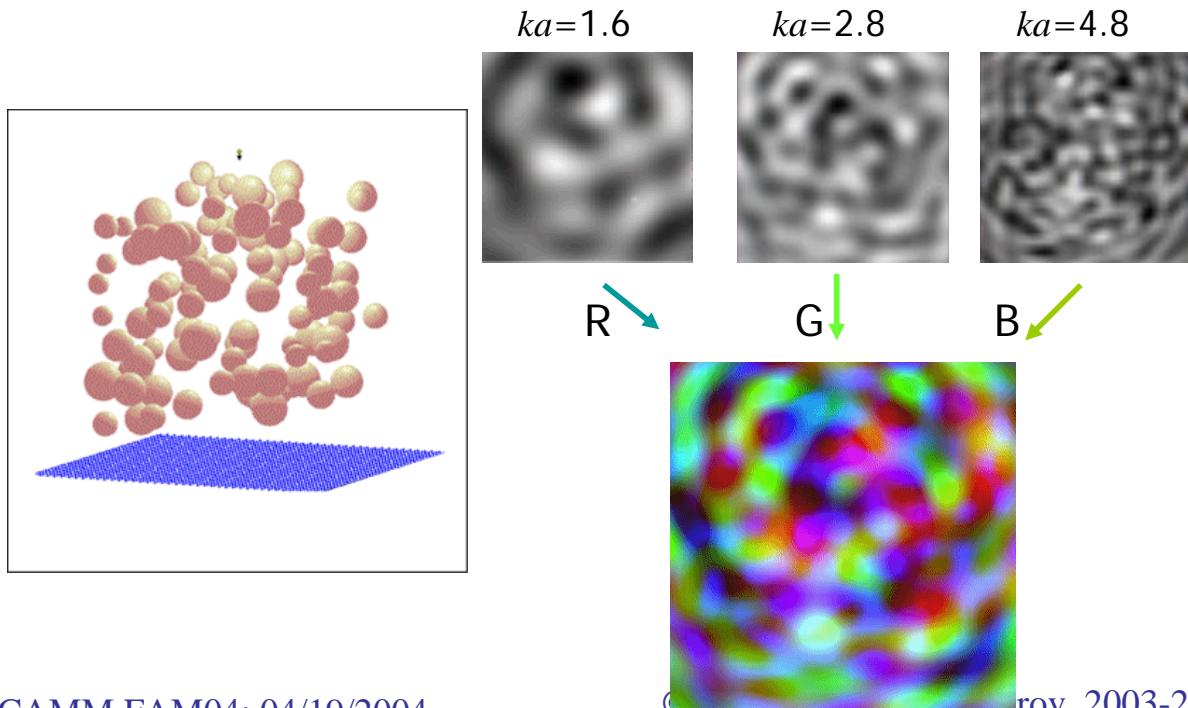
$$\mathbf{B}_{j+1}^{(q)} = \sum_{p \neq q} (\mathbf{S}|\mathbf{R})(\mathbf{r}'_q - \mathbf{r}'_p) \mathbf{A}_j^{(p)},$$

$$|\mathbf{A}_j^{(q)} - \mathbf{A}_{j+1}^{(q)}| < \epsilon, \quad q = 1, \dots, N.$$

General Formulation (used in GMRES)

$$\left[ \mathbf{I} - \mathbf{T}^{(q)} \sum_{p \neq q} (\mathbf{S}|\mathbf{R})(\mathbf{r}'_q - \mathbf{r}'_p) \right] \mathbf{A}^{(q)} = \mathbf{T}^{(q)} \mathbf{E}^{(in)}(\mathbf{r}'_q).$$

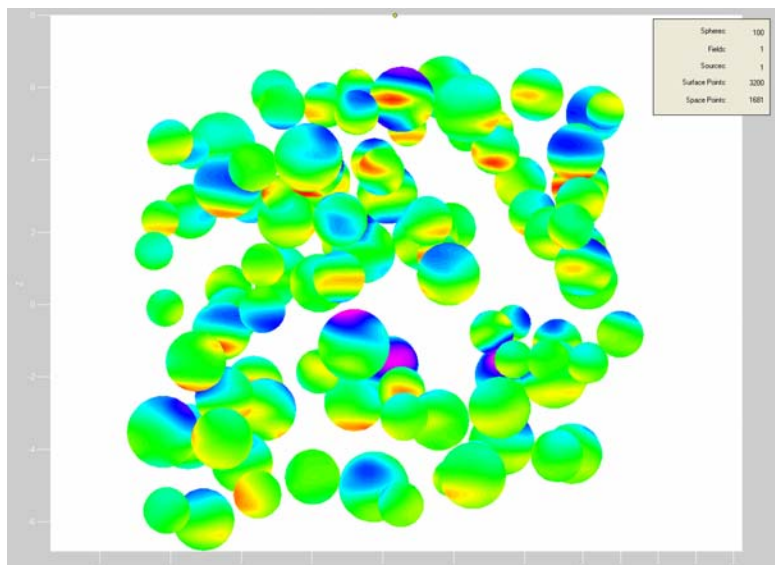
## 100 random spheres (MLFMM)



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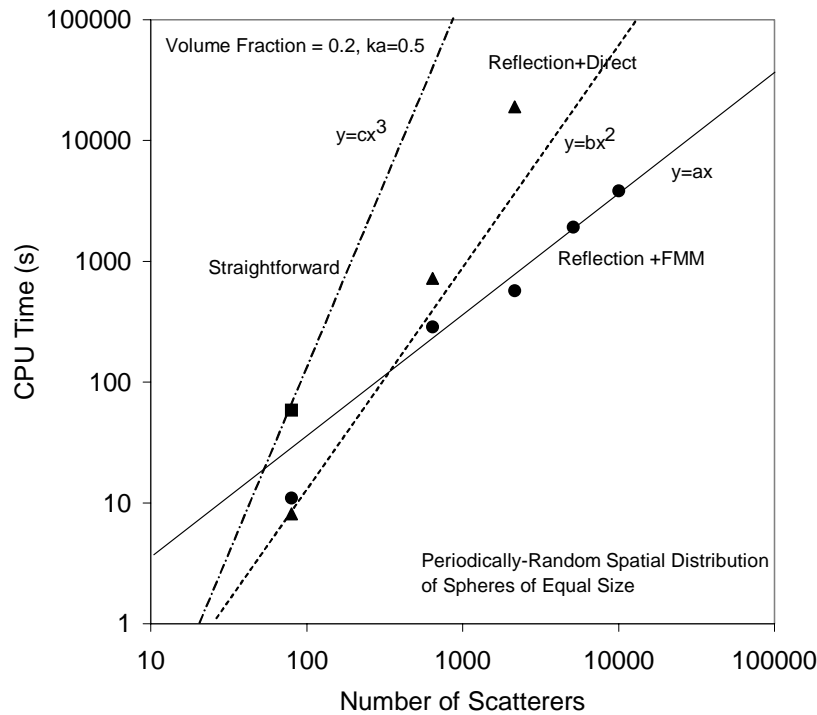
## Surface Potential Imaging



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# Performance Test

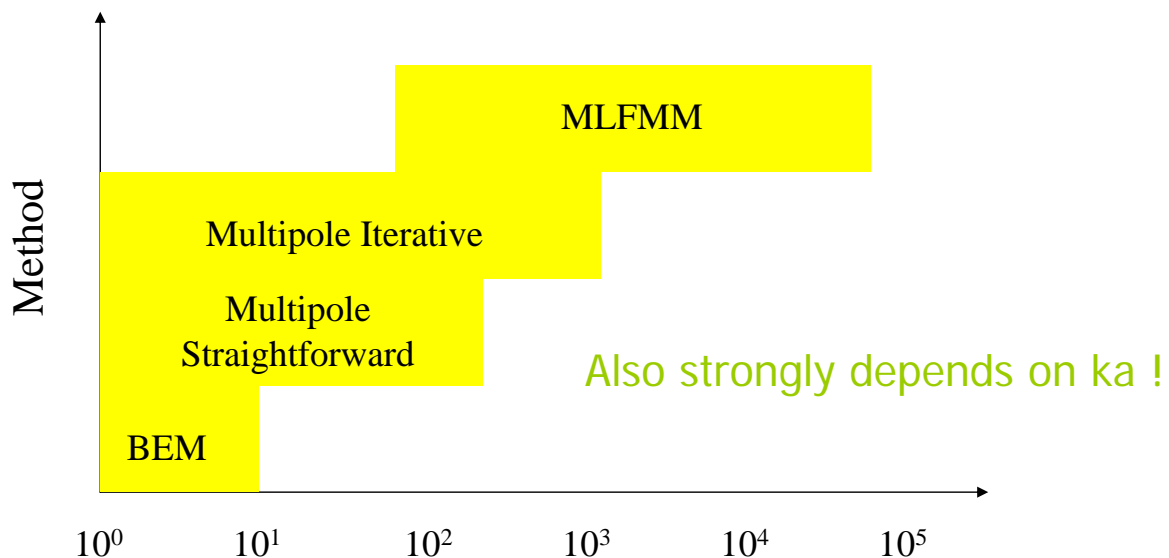


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## MLFMM

# Computable Problems on Desktop PC



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# More About This Problem in Our Talk Next Week