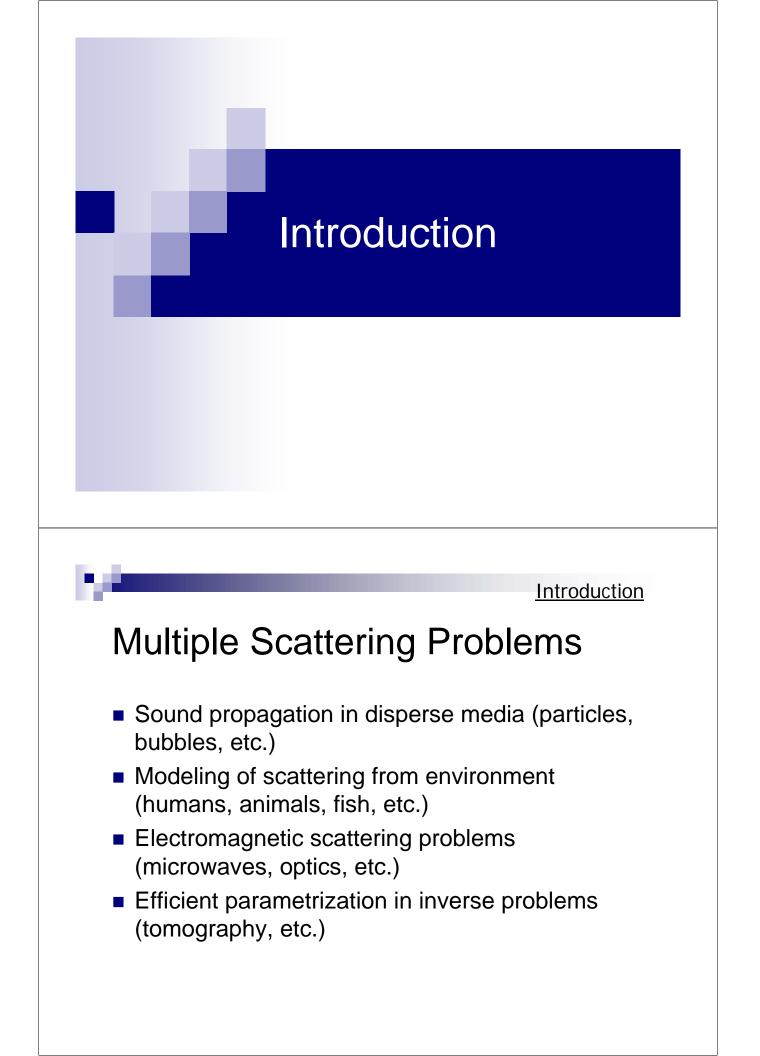
Computation of Scattering Clusters of Spheres Using the Fast Multipole Method

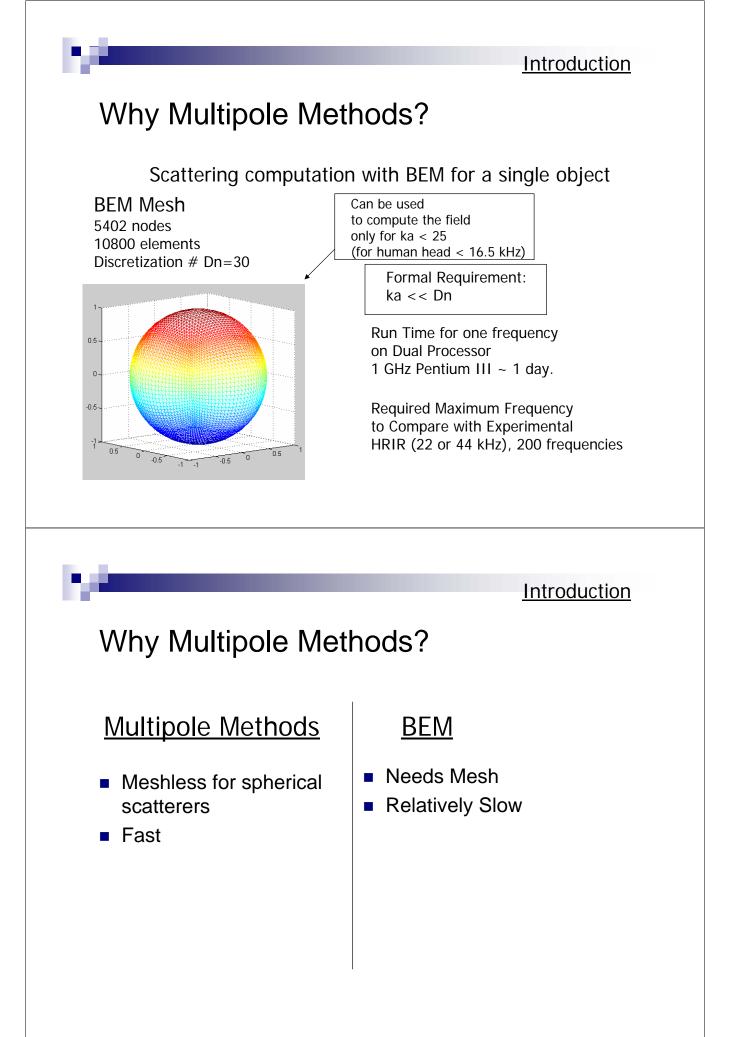
Nail A. Gumerov Ramani Duraiswami

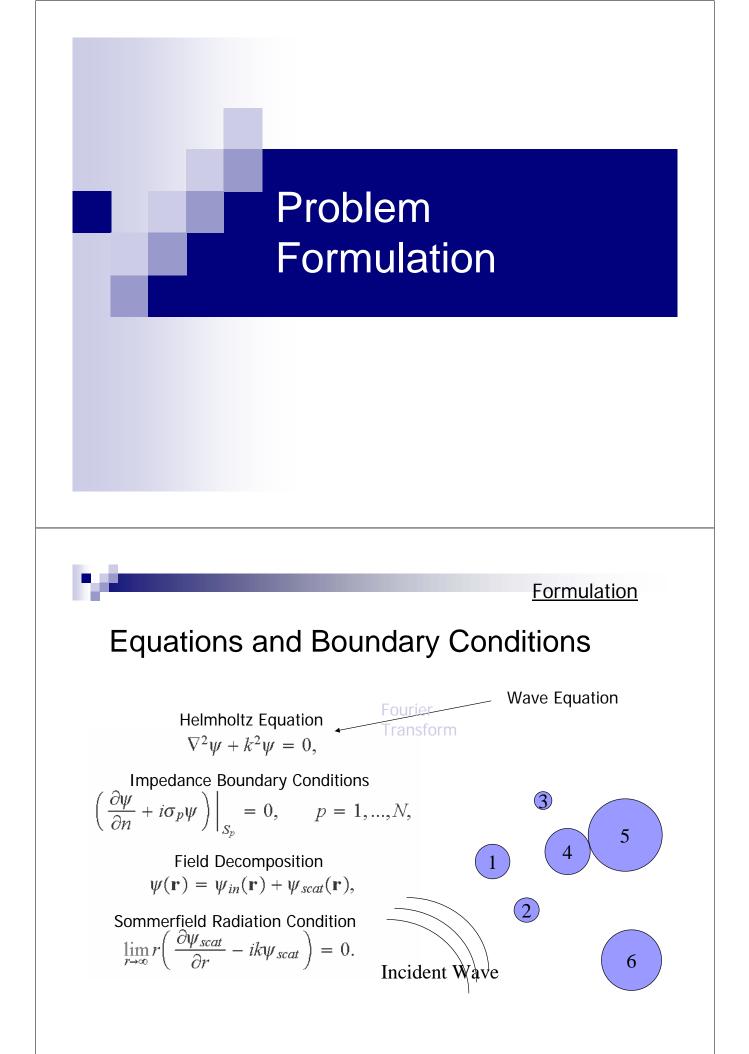
Institute for Advanced Computer Studies University of Maryland at College Park <u>www.umiacs.umd.edu/~gumerov</u> www.umiacs.umd.edu/~ramani This study has been supported by NSF

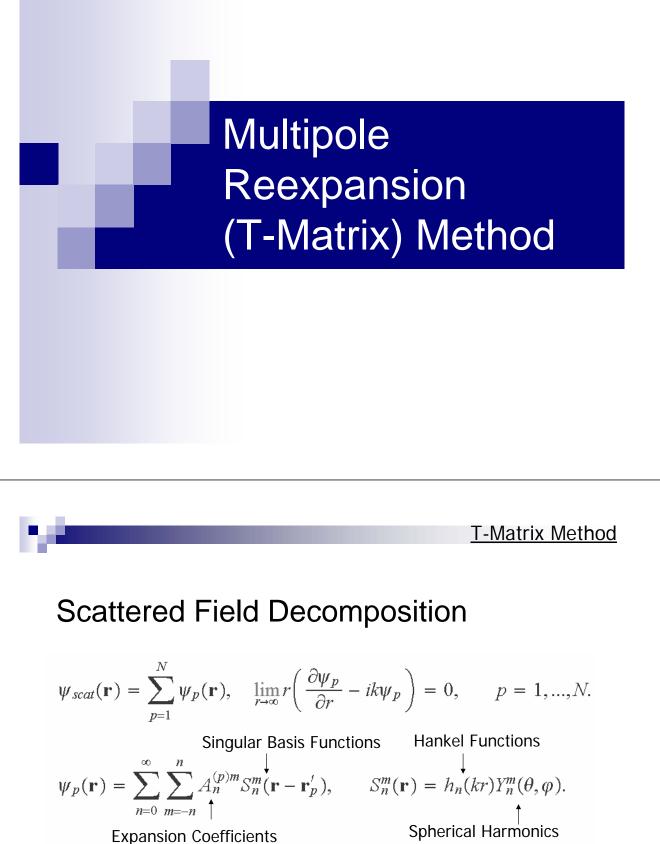
Outline

- Introduction
- Problem Formulation
- Method of Solution
 Multipole Reexpansion (T-matrix) Method
 Iterative Methods
 - □ Fast Multipole Method
- Results of Computations
- Conclusion





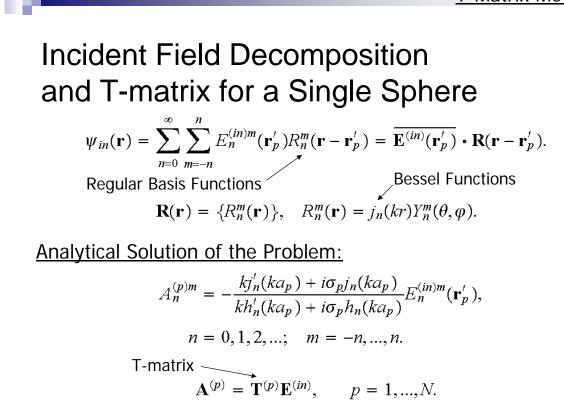


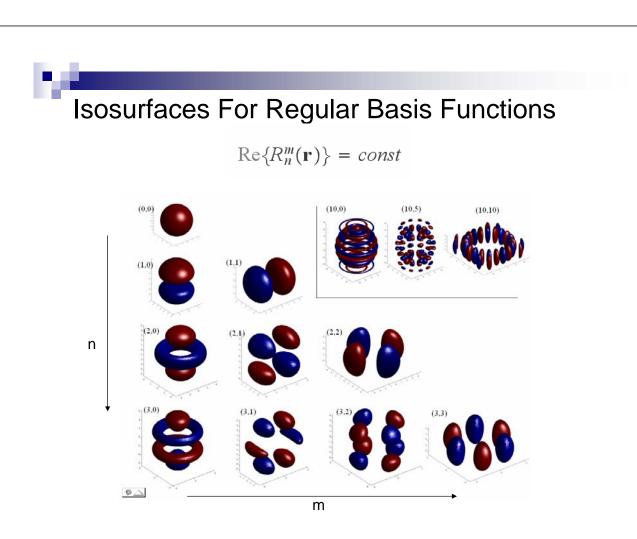


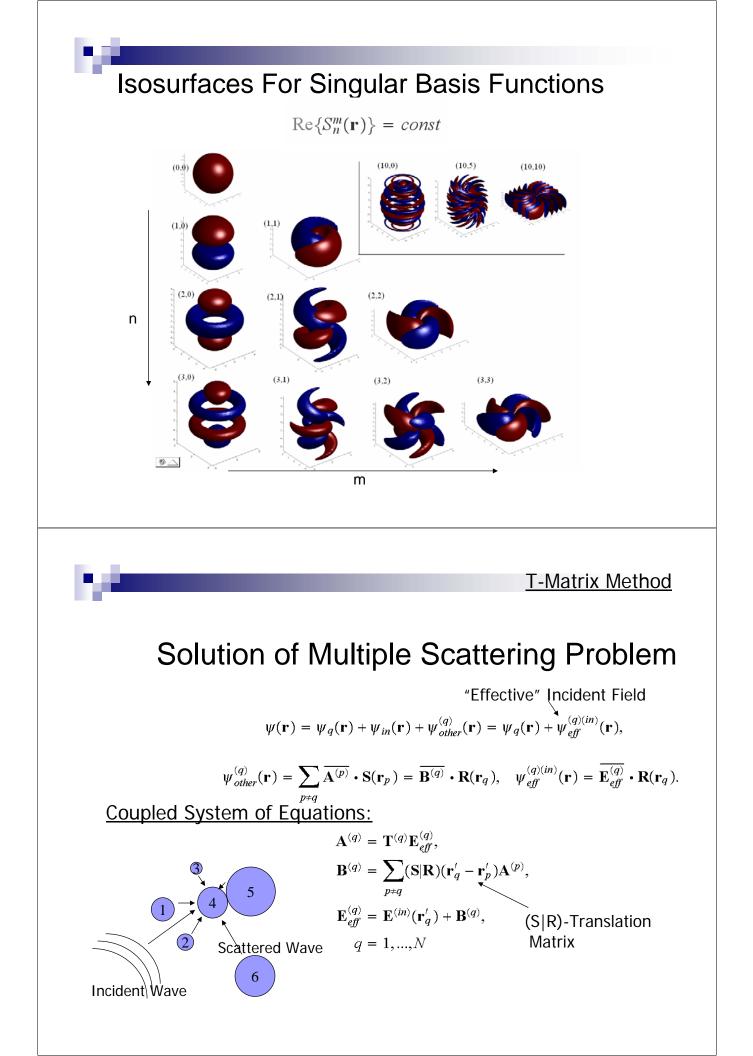
 $\mathbf{A} = \left(A_0^0, A_1^{-1}, A_1^0, A_1^1, A_2^{-2}, A_2^{-1}, A_2^0, A_2^1, A_2^2, \dots\right)^T,$

Vector Form:

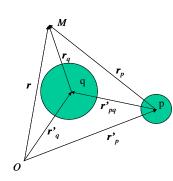
$$\psi_p(\mathbf{r}) = \overline{\mathbf{A}^{(p)}} \cdot \underbrace{\mathbf{S}(\mathbf{r} - \mathbf{r}'_p)}_{\text{dot product}}.$$

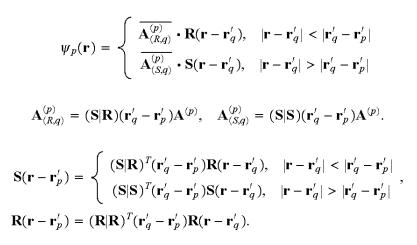






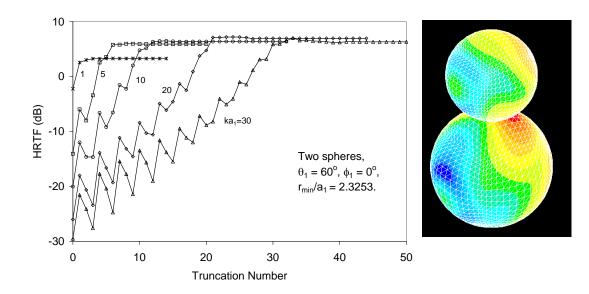
Reexpansions/Translations

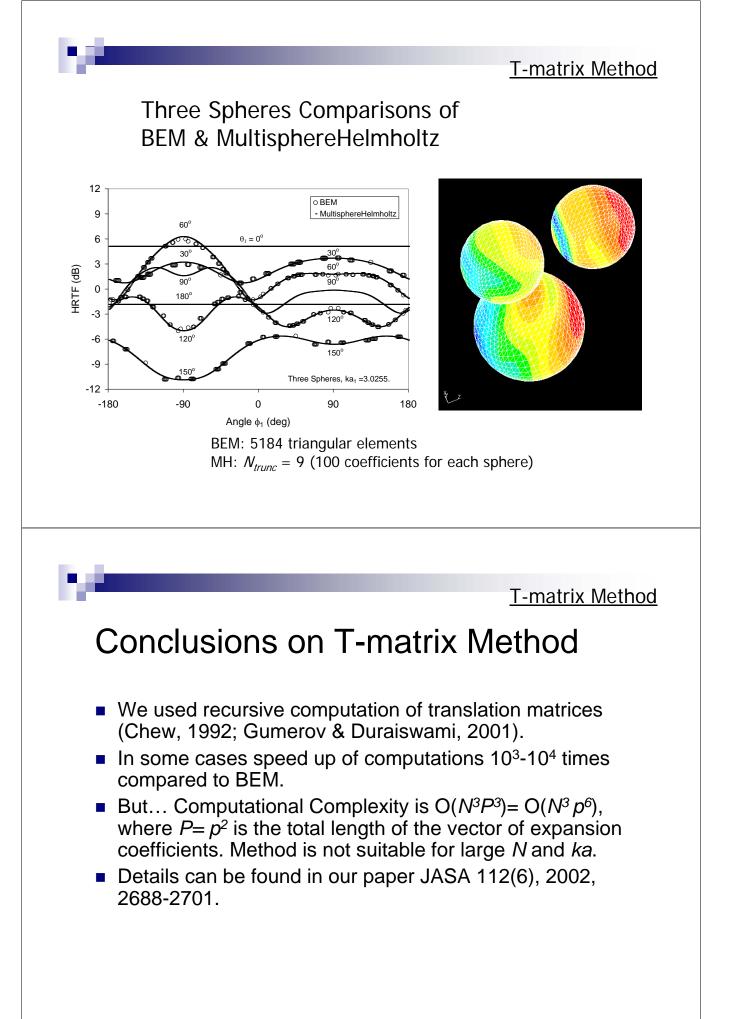


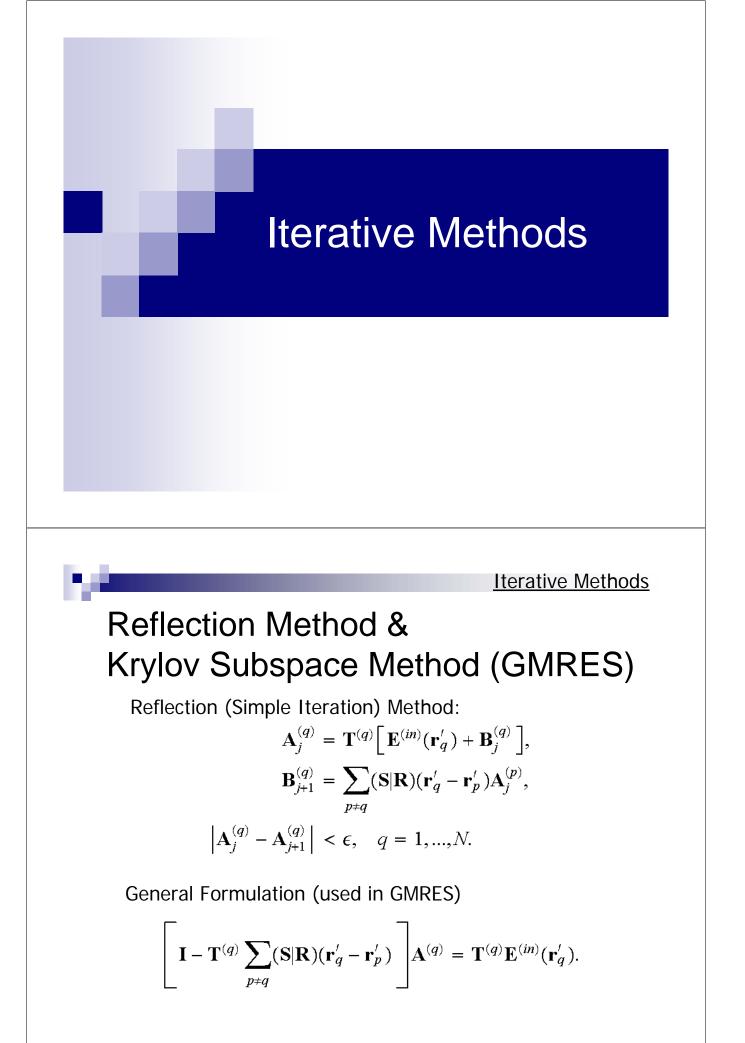


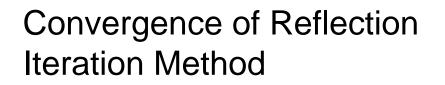
T-matrix Method

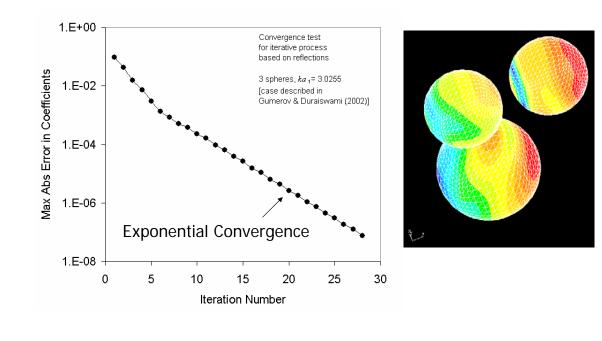
Two Spheres: Convergence with Respect to Truncation Number

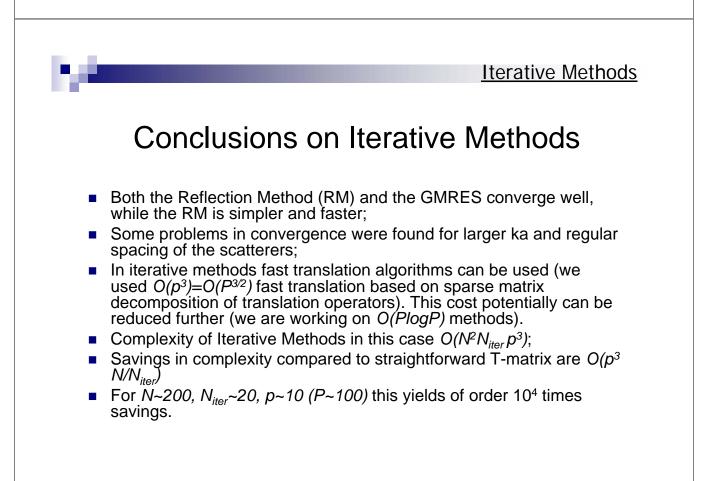










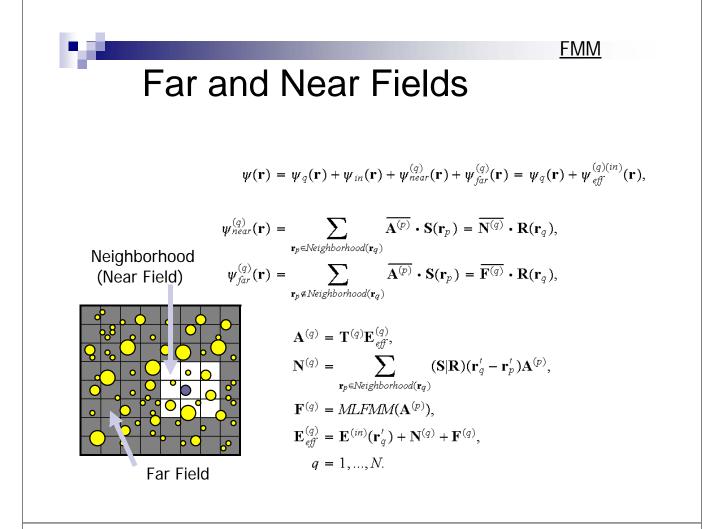


Fast Multipole Method

FMM

Some Facts on the Fast Multipole Methods (FMM)

- Introduced by Rokhlin & Greengard (1987,1988) for computation of 2D and 3D fields for Laplace Equation;
- Reduces complexity of matrix-vector product from O(N²) to O(N) or O(NlogN) (depends on data structure);
- Hundreds of publications for various 1D, 2D, and 3D problems (Laplace, Helmholtz, Maxwell, Yukawa Potentials, etc.);
- Application to acoustical scattering problems (Koc & Chew, 1998; JASA);
- We taught the first in the country course on FMM fundamentals & application at the University of Maryland (2002,2003);
- Some technical reports are available online;
- A book on the FMM for the 3D Helmholtz equation submitted to Academic Press.



Max Level of Space Subdivision

$$D_{l_{\max}} > \frac{4}{3 - \sqrt{3}} a_{\max}, \quad l_{\max} < \log_2 \left(\frac{3 - \sqrt{3}}{4} \frac{D_0}{a_{\max}} \right),$$

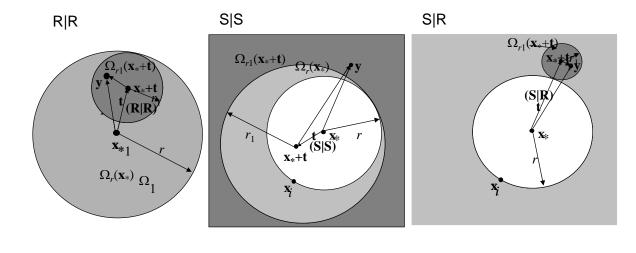
<u>FMM</u>

Translations

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

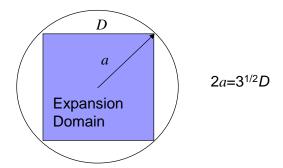
$$C_n^m(\mathbf{x}_{*2}) = \sum_{n'=0}^{\infty} \sum_{m'=-n'}^{n'} (E|F)_{nn'}^{nmn'}(\mathbf{t}) C_{n'}^{m'}(\mathbf{x}_{*1}), \quad \mathbf{t} = \mathbf{x}_{*2} - \mathbf{x}_{*1}$$

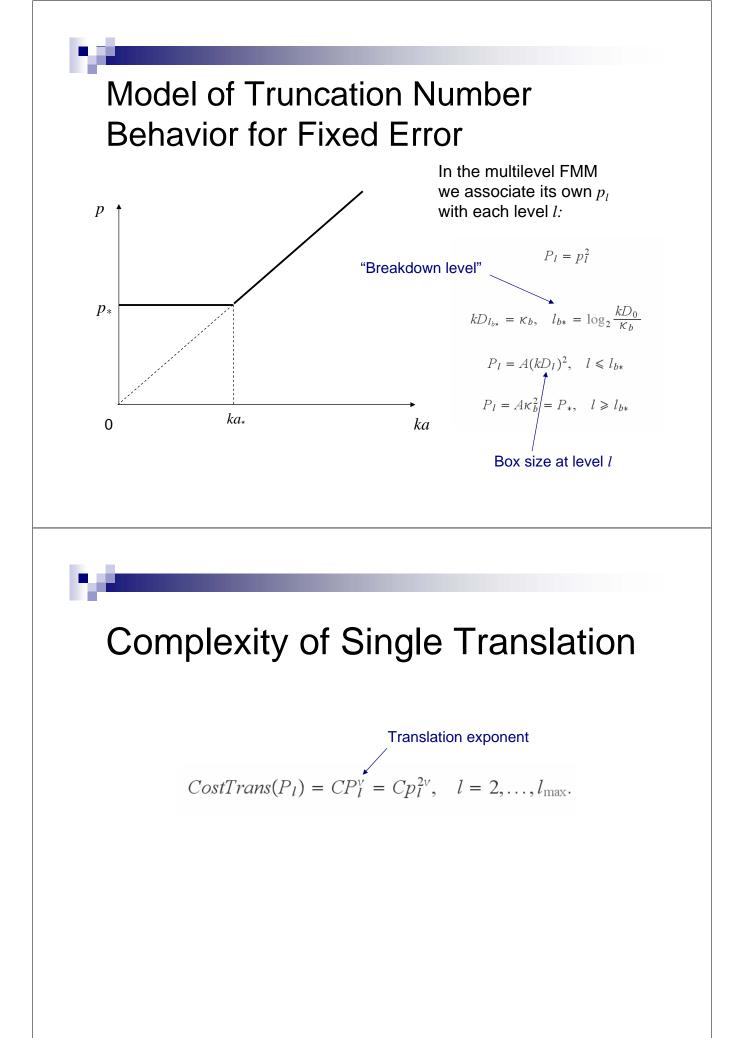
$$E, F = S, R, \quad n = 0, 1, \dots, \quad m = -n, \dots, n.$$

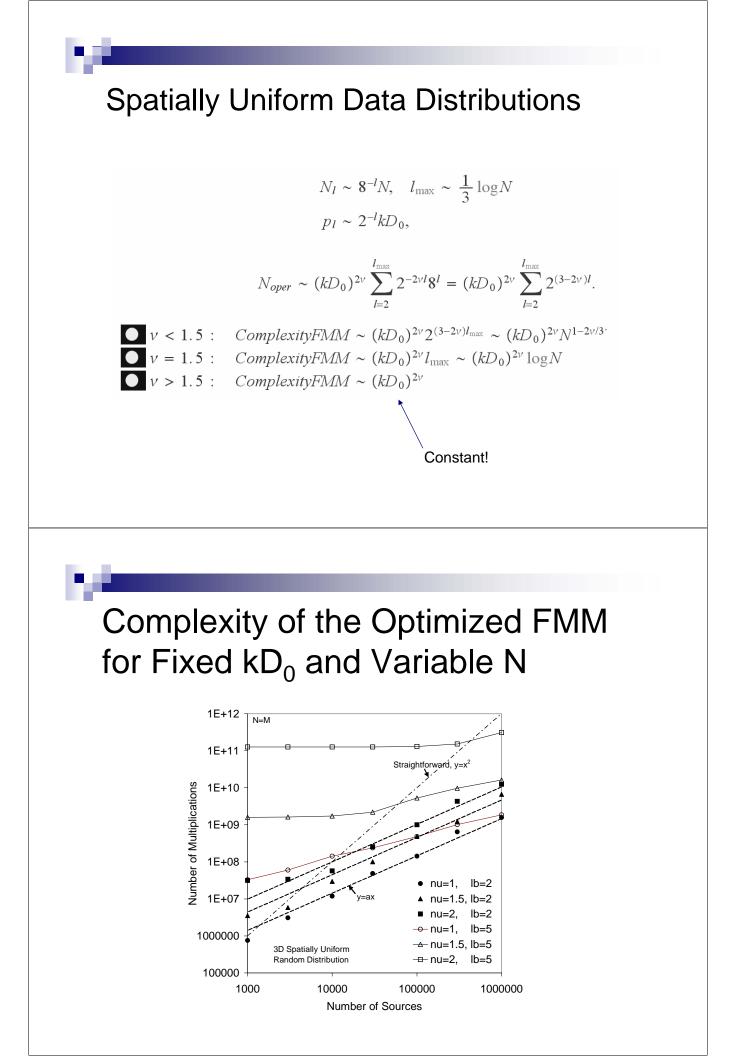


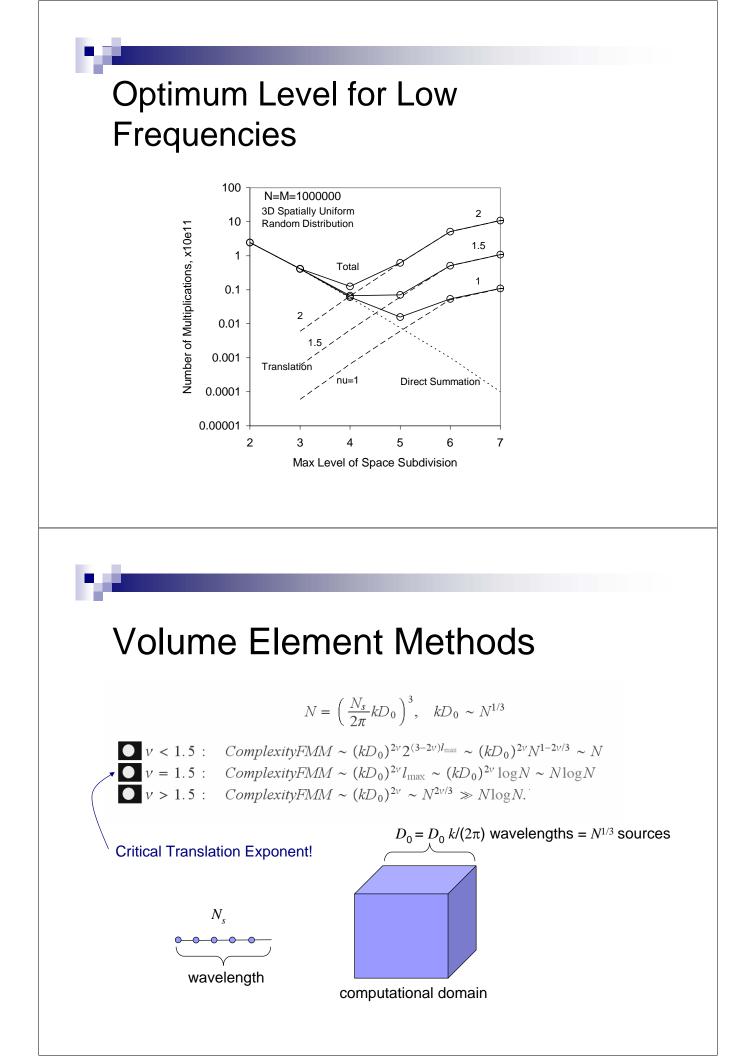
Problem:

- 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).









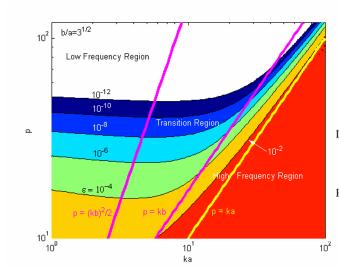
What Happens if Truncation Number is Constant for All Levels?

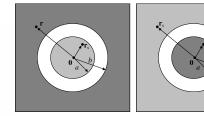
$$N_{oper} \sim (kD_0)^{2\nu} \sum_{l=2}^{l_{max}} 8^l = (kD_0)^{2\nu} \sum_{l=2}^{l_{max}} 2^{3l} \sim (kD_0)^{2\nu} 2^{3l_{max}} \sim (kD_0)^{2\nu} N \sim N^{1+2\nu/3}.$$

 $\begin{array}{l} \bullet v < 1.5: \quad N \ll ComplexityFMM \ll N^2 \\ \bullet v = 1.5: \quad ComplexityFMM \sim N^2 \\ \bullet v > 1.5: \quad ComplexityFMM \sim N^{1+2\nu/3} \gg N^2 \end{array}$

"Catastrophic Disaster of the FMM"

Source Expansion Errors



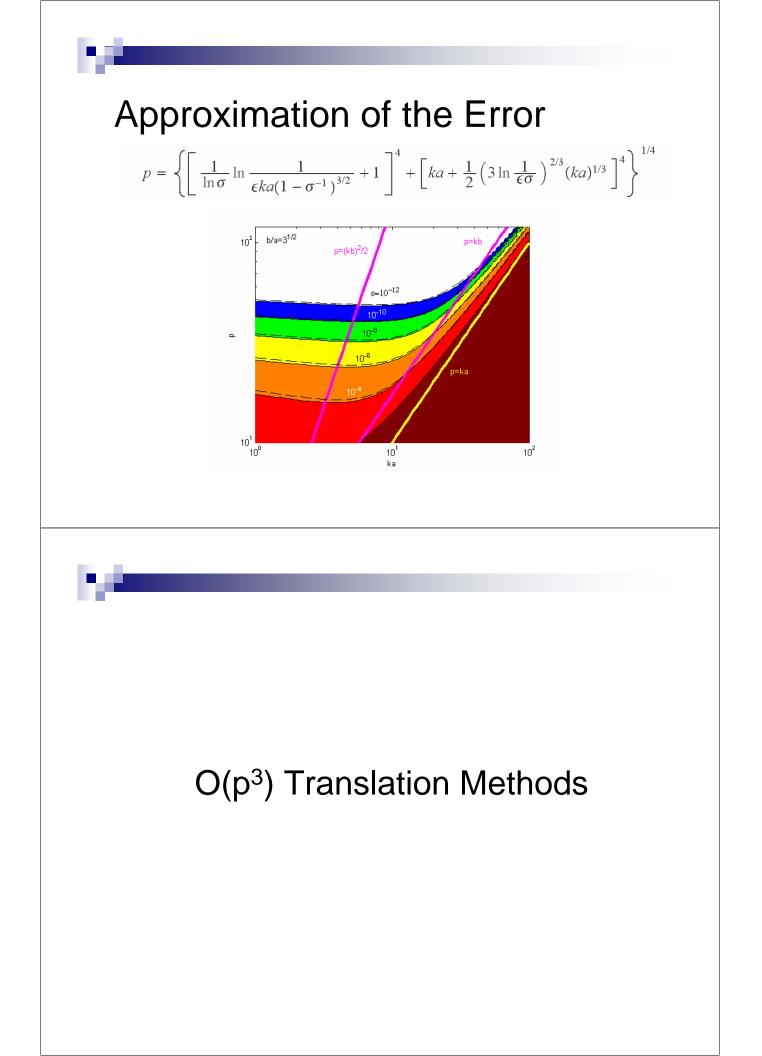


Low frequencies:

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

High frequencies:

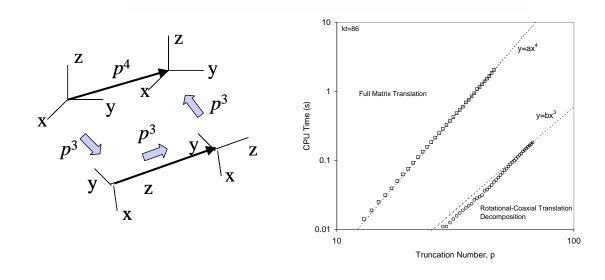
$$b = ka + \frac{1}{2} \left(3 \ln \frac{1}{\epsilon \sigma} \right)^{2/3} (ka)^{1/3}$$



Rotation - Coaxial Translation Decomposition (Complexity O(p³))

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

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



Sparse Matrix Decomposition

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

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

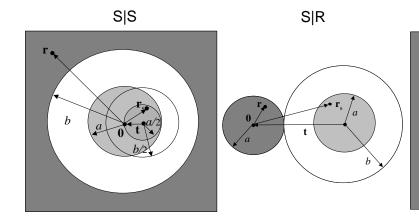
Matrix-vector products with these matrices computed recursively

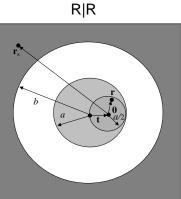
$$\Lambda_r(kt, -i\mathbf{D}_t) = \sum_{n=0}^{\infty} (2n+1)i^n j_n(kt) P_n(-i\mathbf{D}_t)$$

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

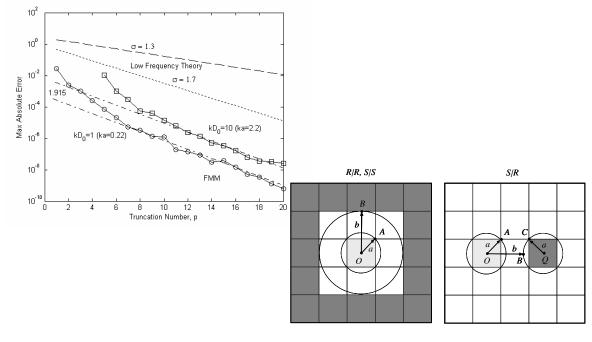
 $\begin{aligned} (\mathbf{D}_{\mathbf{t}}\mathbf{C})_{n}^{m} &= \frac{1}{2t} \Big[(t_{x} + it_{y}) \Big(C_{n-1}^{m+1} b_{n}^{m} - C_{n+1}^{m+1} b_{n+1}^{-m-1} \Big) + (t_{x} - it_{y}) \Big(C_{n-1}^{m-1} b_{n}^{-m} - C_{n+1}^{m-1} b_{n+1}^{m-1} \Big) \Big] \\ &+ \frac{t_{z}}{t} (a_{n}^{m} C_{n+1}^{m} - a_{n-1}^{m} C_{n-1}^{m}), \qquad m = 0, \pm 1, \pm 2, \dots, \quad n = |m|, |m| + 1, \dots \end{aligned}$

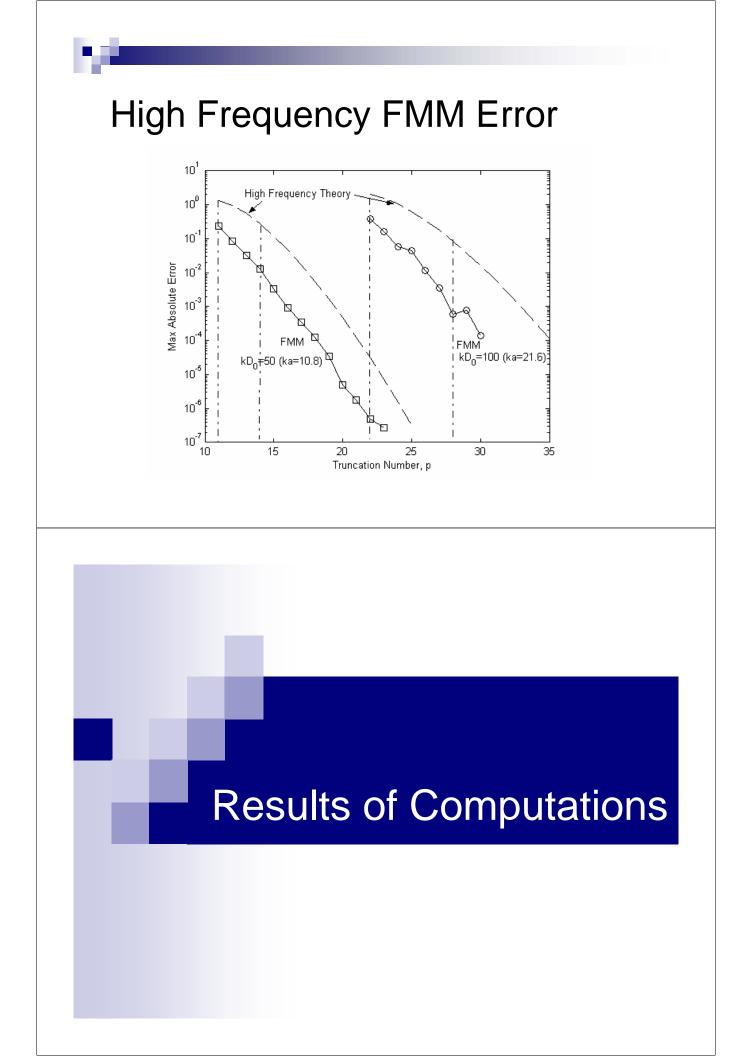
It can be proved that for source summation problems the truncation numbers can be selected based on the above chart when using translations with rectangularly truncated matrices





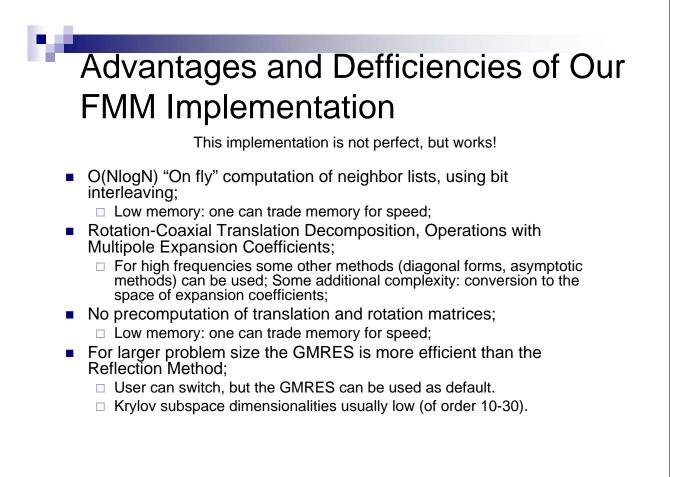


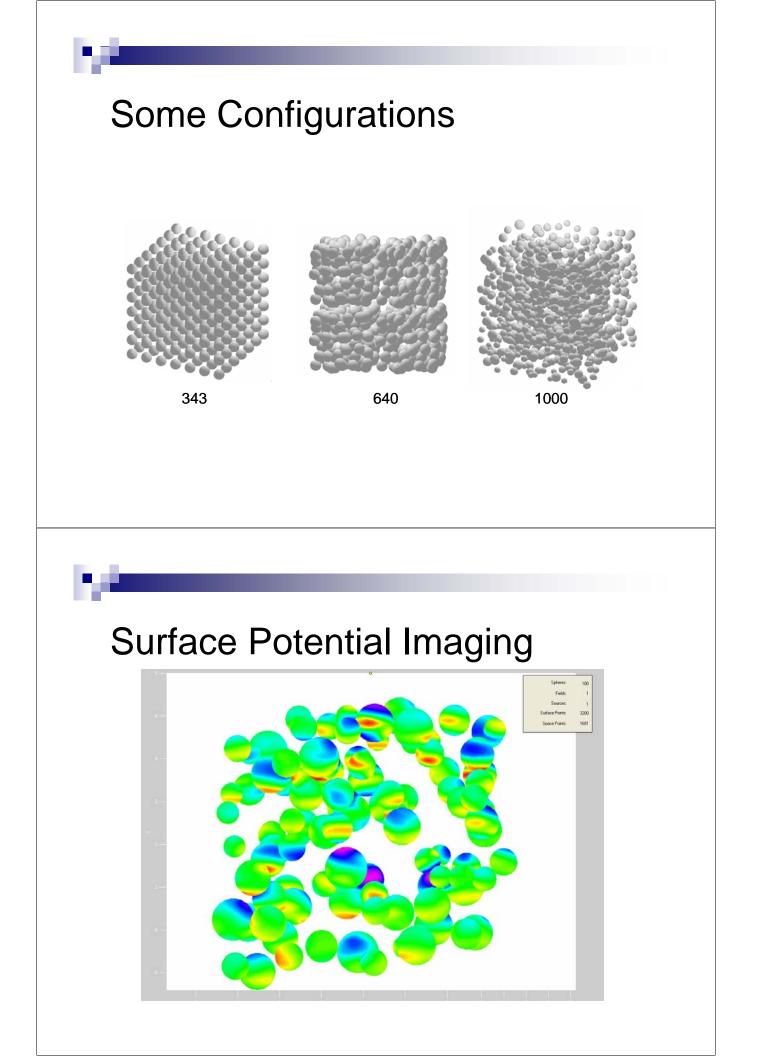


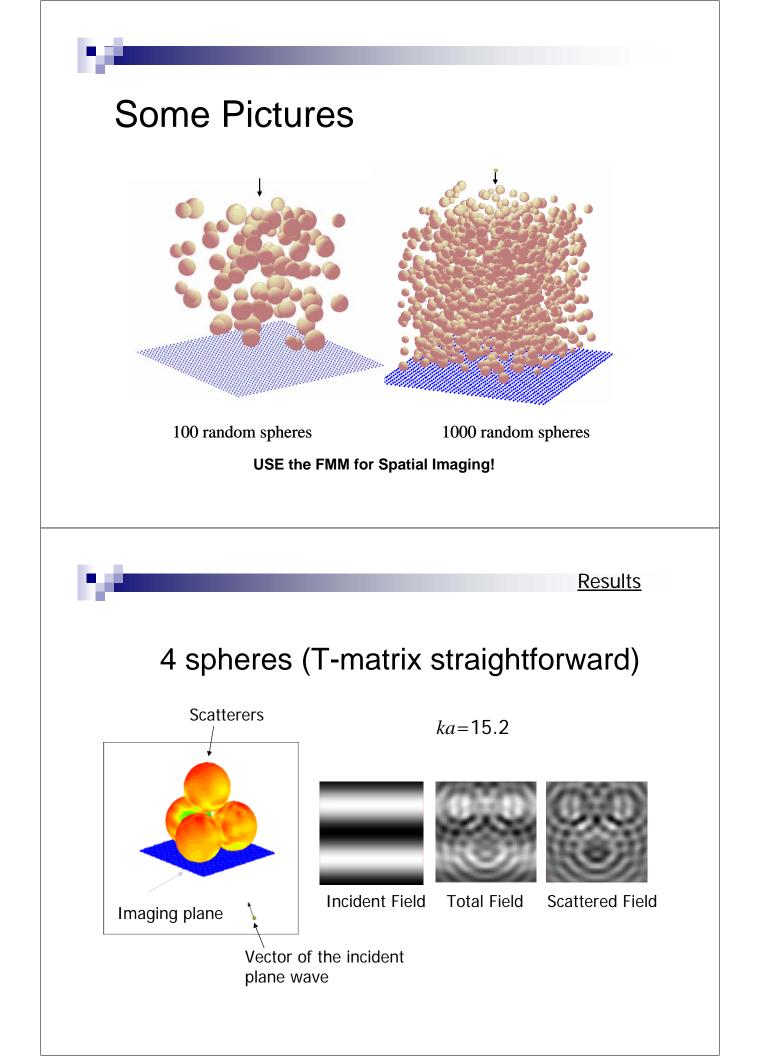


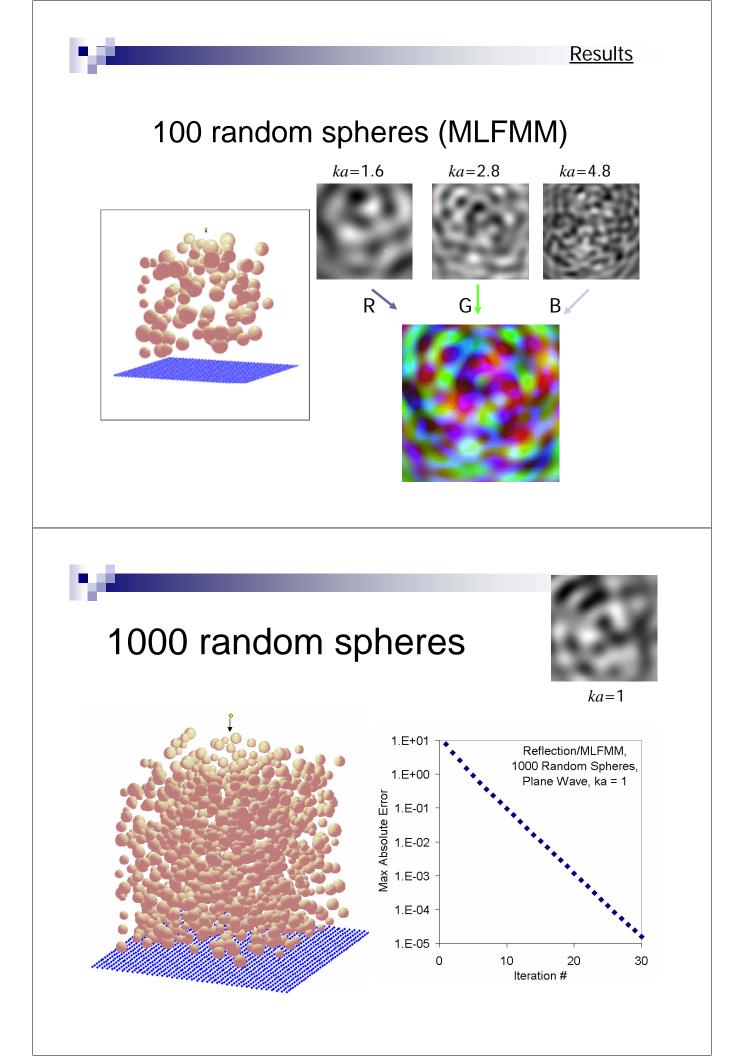


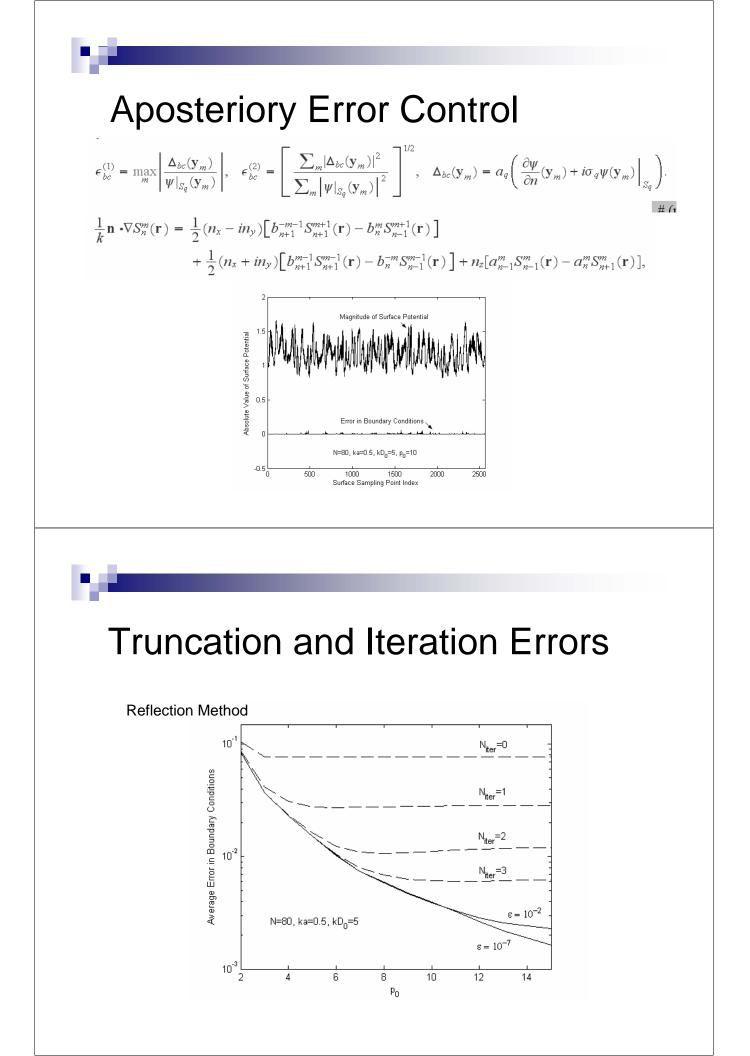
- Number of Spheres: *1-10*⁴;
- *ka: 0.1-10*; *kD*₀: 1-100;
- Random and regularly spaced grids of spheres;
- Polydispersity: 0.5-1.5 (ratio to the mean radius);
- Volume fractions: 0.01-0.2;

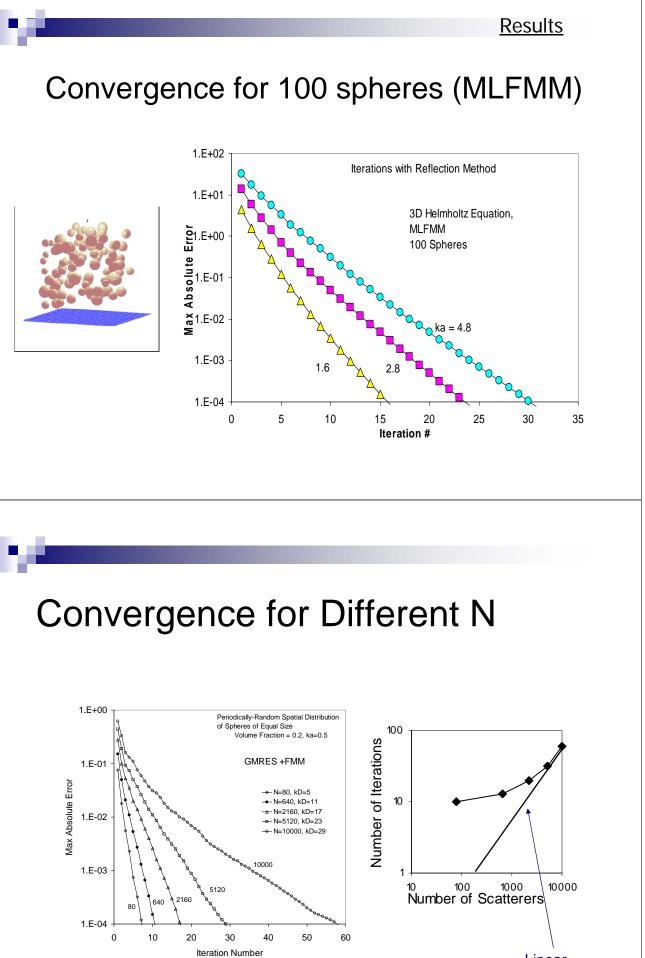




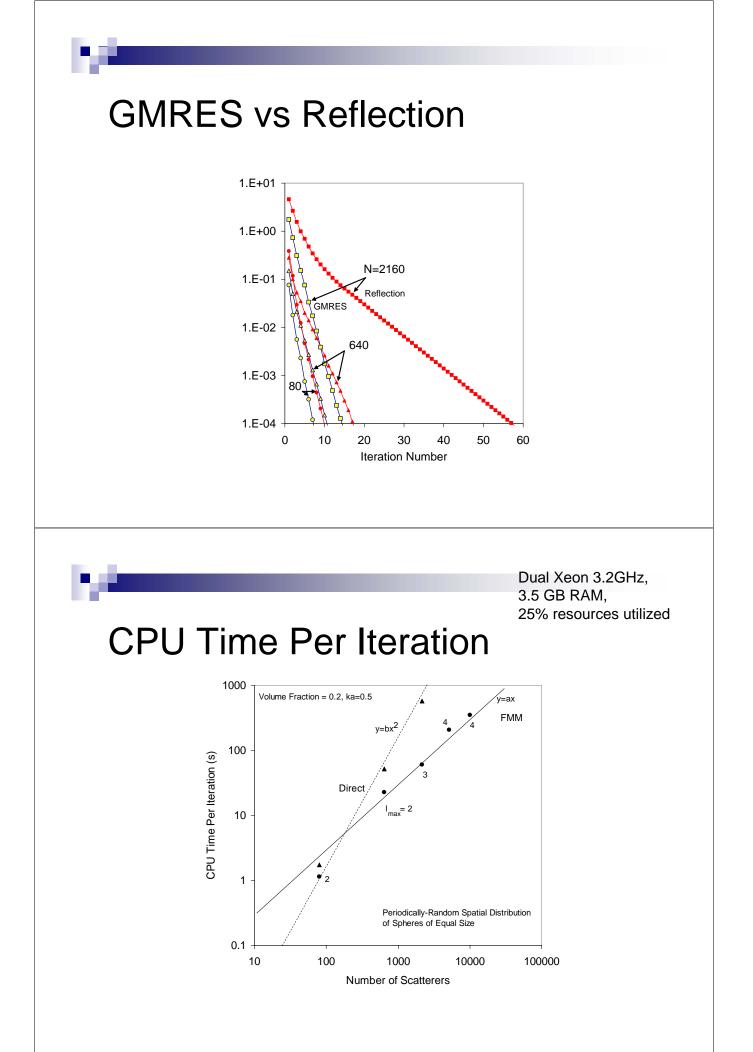


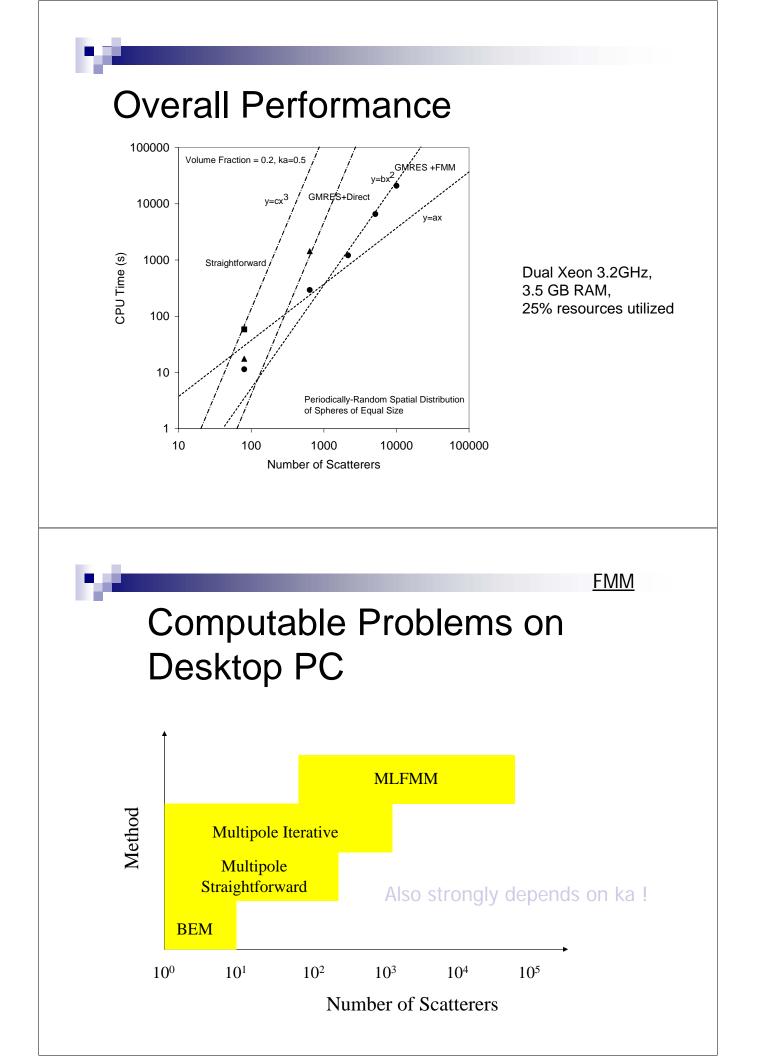


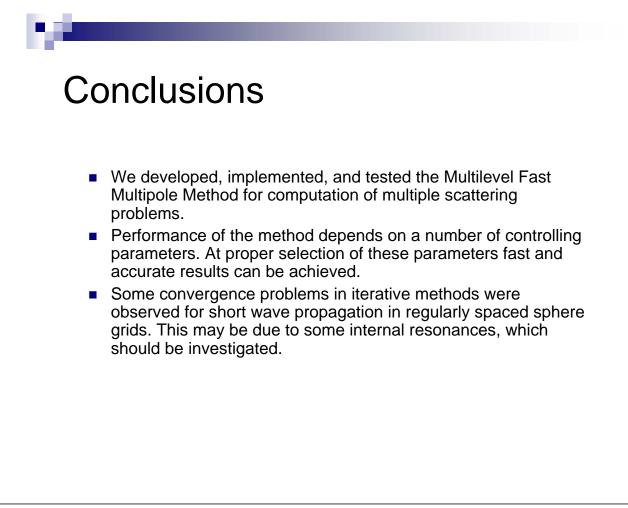




Linear







Future work

- Development of faster translation algorithms, covering higher frequencies;
- Extension for non-spherical scatterrers;
- Comparisons with continuum (averaging) theories and theories of wave propagation in random media;
- Computations of acoustic fields in disperse systems (bubbly liquids, particulate systems);
- Comparisons with experimental data.