Fast Multipole Methods for Incompressible Flow Simulation

Nail A. Gumerov & Ramani Duraiswami
Institute for Advanced Computer Studies
University of Maryland, College Park

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Fast Multipole Methods

- Complex geometric features (e.g., aircraft, submarine, or turbine geometries), physics (high $\mathbb{R}$, wake-structure interactions etc.) all tend to increase problem sizes
  - Many simulations involve several million variables
- Most large problems boil down to solution of linear systems or performing several matrix-vector products
- Regular product requires $O(N^2)$ time and $O(N^2)$ memory
- The FMM is a way to
  - accelerate the products of particular dense matrices with vectors
  - Do this using $O(N)$ memory
- FMM achieves product in $O(N)$ or $O(N \log N)$ time and memory
- Combined with iterative solution methods, can allow solution of problems hitherto unsolvable

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Fast Multipole Methods

• To speed up a matrix vector product $\sum_i \Phi_{ij} u_i = v_j$

• Key idea: Let $\Phi_{ij} = \phi(x_i, y_j)$
  - “Translate” elements corresponding to different $x_i$ to common location, $x_*$
  - $\phi(x_i, y_j) = \sum_{l=1}^p \beta_l \psi_l(x_i - x_*) \Psi_l(y_j - x_*)$
  - Achieves a separation of variables by translation
  - The number of terms retained, $p$, is only related to accuracy

$$v_j = \sum_{j=1}^N u_i \sum_{l=1}^p \beta_l \psi_l(x_i) \Psi_l(y_j) = \sum_{l=1}^p \beta_l \Psi_l(y_j) \sum_{i=1}^N u_i \psi_l(x_i)$$

• Can evaluate $p$ sums over $i$

$$A_i = \sum_{j=1}^N u_i \psi_l(x_i)$$

  - Requires $Np$ operations

• Then evaluate an expression of the type

$$S(x_i) = \sum_{l=1}^p A_l \beta_l \psi_l(x_i) \quad i=1, \ldots, M$$
Outline

- Incompressible Fluid problems where FMM can be used
  - Boundary integral and particle formulations
    - Potential flow
    - Stokes Flow
    - Vortex Element Methods
    - Component of Navier-Stokes Solvers via Generalized Helmholtz decomposition
  - Multi-sphere simulations of multiphase flow
    - Laplace
    - Stokes
    - Helmholtz
- Numerical Analysis issues in developing efficient FMM
- Towards black-box FMM solvers

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FMM & Fluid Mechanics

- **Basic Equations**

  **Incompressibility condition**
  \[ \nabla \cdot \mathbf{u} = 0 \]

  **Momentum Equation**
  \[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla \cdot \mathbf{\tau} + \mathbf{b} \]

  **Incompressible Newtonian fluid**
  \[ \mathbf{\tau} = p \mathbf{I} + \mu (\nabla \mathbf{u} + \mathbf{u} \nabla) \]

  **No body forces and non-dimensionalize**
  \[ \nabla \cdot \mathbf{u} = 0 \]
  \[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla p + \mathcal{R}^{-1} \nabla^2 \mathbf{u} \]

  **Boundary Conditions**

  **Continuity of normal flow**
  \[ \mathbf{n} \cdot \mathbf{u} = \mathbf{U} \cdot \mathbf{n} = 0 \]

  **Continuity of normal and tangential stresses**
  \[ (\tau_{ij}^1 - \tau_{ij}^2) \cdot \mathbf{n} = (\sigma \nabla \cdot \mathbf{n}) \mathbf{n} - \nabla_s \sigma \]

  **No slip assumption**
  \[ \mathbf{t} \cdot \mathbf{u} = \mathbf{U} \cdot \mathbf{t} = 0 \]

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Helmholtz Decomposition

- Key to integral equation and particle methods

Separate velocity vector into dilatational and rotational parts (Batchelor, 1967)

\[ \mathbf{u} = \nabla \phi + \nabla \times \mathbf{A} \]

Incompressibility leads to Laplace’s equation for the scalar potential \( \phi \)

\[ \nabla \cdot \mathbf{u} = \nabla^2 \phi = 0 \]

Vector potential \( \mathbf{A} \) is related to the vorticity \( \omega \)

\[ \omega = \nabla \times \mathbf{u} = \nabla \times \nabla \times \mathbf{A} \]

For irrotational flow \( \omega = 0 \)

\[ \mathbf{u} = \nabla \phi, \quad \nabla^2 \phi = 0 \]
Potential Flow

Inviscid, irrotational flow $\mathcal{R} \rightarrow \infty$

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \nabla p$$

Momentum equation can be integrated as

$$p + \rho \left( \frac{\partial \phi}{\partial t} + \frac{1}{2} \nabla \phi \cdot \nabla \phi + gz \right) = p_\infty$$

- Knowledge of the potential is sufficient to compute velocity and pressure
- Need a fast solver for the Laplace equation
- Applications – panel methods for subsonic flow, water waves, bubble dynamics, …
BEM/FMM Solution Laplace’s Equation

Green’s function for Laplace’s equation $\nabla^2 \phi = 0$

$$G(x, y) = \frac{1}{4\pi |x - y|}, \quad n \cdot \nabla_x G = -\frac{(x - y) \cdot n}{4\pi |x - y|}$$

Green’s identity

$$\frac{1}{2} \phi(y) = \int_{S_x} \frac{\partial \phi}{\partial n_x} G(x, y) dS_x - \int_{S_x} \phi(x) \frac{\partial G}{\partial n_x}(x, y) dS_x$$

Single and double layer functions

$$\phi = L \frac{\partial \phi}{\partial n} - M \phi$$

Discretize by dividing surface into $N$ triangles and collocating

$$\frac{1}{2} \phi(y) = \sum_{i=1}^{N} \int_{S_i} \frac{\partial \phi}{\partial n_x} G(x, y) dS_x - \sum_{i=1}^{N} \int_{S_i} \phi(x) \frac{\partial G}{\partial n_x}(x, y) dS_x$$

Boundary conditions

$$\frac{dx}{dt} = \nabla \phi, \quad p = p_0 - \sigma C = \rho \left( \frac{\partial \phi}{\partial t} + \frac{1}{2} \nabla \phi \cdot \nabla \phi + gz \right)$$

$$n \cdot \nabla \phi = 0$$

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- Jaswon/Symm (60s) Hess & Smith (70s),
- Korsmeyer et al 1993, Epton & Dembart 1998,
- Boschitsch & Epstein 1999

Lohse, 2002
Stokes Flow

\[ \nabla \cdot \mathbf{u} = 0, \quad \nabla p = \nabla^2 \mathbf{u} \]

- Green’s function (Ladyzhenskaya 1969, Pozrikidis 1992)

\[ G_{ij}(x, y) = \frac{1}{8\pi} \left( \delta_{ij} \frac{1}{|x - y|} \mathbf{1} + \frac{(x_i - y_i)(x_j - y_j)}{|x - y|^3} \right) \]

\[ \sigma_{ijk}(x, y) = \frac{3}{4\pi} \frac{(x_i - y_i)(x_j - y_j)(x_k - y_k)}{|x - y|^5} \]

- Integral equation formulation

\[ u_i(y) + \int_S \sigma_{ijk} u_j n_k dS_x = - \int_S G_{ij} f_j dS_x \]

- Stokes flow simulations remain a very important area of research
- MEMS, bio-fluids, emulsions, etc.
- BEM formulations (Tran-Cong & Phan-Thien 1989, Pozrikidis 1992)
- FMM (Kropinski 2000 (2D), Power 2000 (3D))

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Rotational Flows and VEM

- For rotational flows
  - Vorticity released at boundary layer or trailing edge and advected with the flow
    - Simulated with vortex particles
  - Especially useful where flow is mostly irrotational
  - Fast calculation of Biot-Savart integrals

\[
V(x) = \frac{1}{4\pi} \int \Gamma(y) \times \frac{(x - y)}{|x - y|^3} dy
\]

\[
\bar{\omega} = (\Gamma \hat{n})
\]

Evaluation point

Far field

(wher \( y \) is the mid point of the filament)
Vorticity formulations of NSE

Vorticity equation for an incompressible fluid

\[ \frac{\partial \omega}{\partial t} + (u \cdot \nabla) \omega = (\omega \cdot \nabla) u + R^{-1} \nabla^2 \omega \]

- Problems with boundary conditions for this equation (see e.g., Gresho, 1991)
  - Divergence free and curl-free components are linked only by boundary conditions
  - Splitting is invalid unless potentials are consistent on boundary
- Recently resolved by using the generalized Helmholtz decomposition (Kempka et al, 1997; Ingber & Kempka, 2001)
- This formulation uses a kinematically consistent Helmholtz decomposition in terms of boundary integrals
- When widely adopted will need use of boundary integrals, and hence the FMM
  - Preliminary results in Ingber & Kempka, 2001
Generalized Helmholtz Decomposition

• Helmholtz decomposition \( \mathbf{u} = \nabla \phi + \nabla \times \mathbf{A} \) leaves too many degrees of freedom

• Way to achieve decomposition valid on boundary and in domain, with consistent values is to use the GHD

\[
\begin{aligned}
&\begin{cases}
0 & \text{outside } R \text{ and } S \\
\alpha(x_b)2\pi(d-1)[u_b(x_b) - \gamma_c(x_b) \times \hat{n}(x_b)] & \text{on } S \\
2\pi(d-1)u(x) & \text{in } R
\end{cases}
\end{aligned}
\]

\[
\int_R \frac{\varphi(x') \times (x - x')}{|x - x'|^d} \, dR(x') + \int_S \frac{[\gamma_c(x_b) - \hat{n}(x_b') \times u_b(x_b')] \times (x - x')}{|x - x'|^d} \, dS(x_b') +
\int_R \frac{D(x') (x - x')}{|x - x'|^d} \, dR(x') + \int_S \frac{[\hat{n}(x_b') \cdot u_b(x_b')] (x - x')}{|x - x'|^d} \, dS(x_b')
\]

• \( D \) is the domain dilatation (zero for incompressible flow)

• Requires solution of a boundary integral equation as part of the solution => role for the FMM in such formulations
Multi Sphere Problems

- So far we have seen FMM for boundary integral problems
- Can also use the FMM in problems involving many spheres
  - Simulations of multiphase flow, effective media (porous media), dusty gases, slurries, and the like
  - Key is a way to enforce proper boundary/continuity conditions on the spheres
  - Translation theorems provide an ideal way to do this
  - With FMM one can easily simulate $10^4$-$10^5$ particles on desktops and $10^6$-$10^7$ particles on supercomputers
- Stokesian Dynamics (Brady/Bossis 1988; Kim/Karilla 1991)
Fast Multipole Methods

- Matrix-Vector Multiplication
- Middleman and Single Level Methods
- Multilevel FMM (MLFMM)
- Adaptive MLFMM
- Fast Translations
- Some computational results
- Conclusions
Iterative Methods

• To solve linear systems of equations;
• Simple iteration methods;
• Conjugate gradient or similar methods;
• We use Krylov subspace methods (GMRES):
  ■ Preconditioners;
  ■ Research is ongoing.
• Efficiency of these methods depends on efficiency of the matrix-vector multiplication.
Matrix-Vector Multiplication

\[ \mathbf{v} = \Phi \mathbf{u}, \]

\[
\Phi = \begin{pmatrix}
\Phi_{11} & \Phi_{12} & \ldots & \Phi_{1N} \\
\Phi_{21} & \Phi_{22} & \ldots & \Phi_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
\Phi_{M1} & \Phi_{M2} & \ldots & \Phi_{MN}
\end{pmatrix}
\]

\[ v_j = \sum_{i=1}^{N} u_i \Phi_{ji}, \quad j = 1, \ldots, M. \]

Complexity of computation of \( \mathbf{v} \):

\( O(MN) \) operations

\( O(MN) \) memory for \( \Phi \) storage
FMM Works with Influence Matrices

\[ \mathbf{v} = \Phi \mathbf{u}, \]

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

\[ \mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}, \quad \mathbf{x}_i \in \mathbb{R}^d, \quad i = 1, \ldots, N, \]

\[ \mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_M\}, \quad \mathbf{y}_j \in \mathbb{R}^d, \quad j = 1, \ldots, M. \]

\[ \mathbf{v}_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i), \quad j = 1, \ldots, M. \]
Examples of Influence Matrices

- Green’s functions of Laplace and Helmholtz equations
  \[ \Phi(y, x) = \frac{1}{4\pi |y - x|}, \]
  \[ \Phi(y, x) = \frac{\exp \{ik|y - x|\}}{4\pi |y - x|}. \]

- Potential velocity field of a source located at \( x_i \)
  \[ \Phi(y, x_i) = V(y, x_i) = \frac{1}{4\pi} \nabla_y \left( \frac{1}{|y - x_i|} \right). \]

- Normal derivative on the surface
  \[ \Phi(y, x) = \frac{\partial}{\partial n(x)} \frac{1}{4\pi |y - x|} = \mathbf{n}(x) \cdot \nabla_x \frac{1}{4\pi |y - x|}. \]

- Vorticity (vortex element is located at \( x_i \))
  \[ \Phi(y, x_i) = \nabla_y \times V(y, x_i). \]
Complexity of Standard Method

Standard algorithm

Sources \(N\) \(\rightarrow\) Evaluation Points \(M\)

Total number of operations: \(O(NM)\)
Goal of FMM

- Reduce complexity of matrix-vector multiplication (or field evaluation) by trading exactness for speed
- Evaluate to arbitrary accuracy
Five Key Stones of FMM

- Factorization
- Error Bound
- Translation
- Space Partitioning
- Data Structure
Factorization

Degenerate Kernel: 
\[ \Phi(y_j, x_i) = \sum_{m=0}^{p-1} A_m(x_i)F_m(y_j). \]

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{i=1}^{N} u_i \sum_{m=0}^{p-1} A_m(x_i)F_m(y_j) \]

\[ \sum_{m=0}^{p-1} \left( \sum_{i=1}^{N} u_i A_m(x_i) \right) \cdot F_m(y_j) = \sum_{m=0}^{p-1} B_m F_m(y_j). \]

\[ O(pN) \text{ operations:} \quad B_m = \sum_{i=1}^{N} u_i A_m(x_i), \quad m = 0, \ldots, p-1, \]

\[ O(pM) \text{ operations:} \quad v_j = \sum_{m=0}^{p-1} B_m F_m(y_j), \quad j = 1, \ldots, M. \]

Total Complexity: \( O(p(N+M)) \)
Factorization (Example)

Scalar Product in d-dimensional space:

\[ x_i = (x_{1i}, \ldots, x_{di}), \]
\[ y_j = (y_{1j}, \ldots, y_{dj}). \]

\[ \Phi(y_j, x_i) = (y_j \cdot x_i) = \sum_{m=1}^{d} x_{mi} y_{mj}, \]

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{i=1}^{N} u_i \sum_{m=1}^{d} x_{mi} y_{mj} \]

\[ = \sum_{m=1}^{d} \left[ \sum_{i=1}^{N} u_i x_{mi} \right] y_{mj} \]

\( O(dM) \) operations:

\( O(dN) \) operations

Total Complexity: \( O(d(N+M)) \)
Middleman Algorithm

**Standard algorithm**

Sources

\[
N \rightarrow M
\]

Evaluation Points

\[
O(NM)
\]

**Middleman algorithm**

Sources

\[
N \rightarrow M
\]

Evaluation Points

\[
O(N+M)
\]
Factorization

Non-Degenerate Kernel:

\[
\Phi(y_j, x_i) = \sum_{m=0}^{p-1} A_m(x_i) F_m(y_j) + Error(p; x_i, y_j).
\]

\[
v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{i=1}^{N} u_i \sum_{m=0}^{p-1} A_m(x_i) F_m(y_j) + \sum_{i=1}^{N} u_i Error(p; x_i, y_j)
\]

\[
= \sum_{m=0}^{p-1} B_m F_m(y_j) + Error_j(p, N), \quad j = 1, \ldots, M.
\]

Error Bound:

\[
|Error_j(p, N)| < N \max_i |u_i| \max_j |Error(p; x_i, y_j)|.
\]

Middleman Algorithm

Applicability:

\[
p \ll \min(M, N),
\]

\[
|Error_j(p, N)| < \epsilon.
\]
Factorization Problem:

Usually there is no factorization available that provides a uniform approximation of the kernel in the entire computational domain.
Far and Near Field Expansions

Far Field: \[ \Phi(y_j, x_i) = \sum_{m=0}^{p-1} C_m(x_i, x_*) S_m(y_j - x_*) + \text{Error}. \]

Near Field: \[ \Phi(y_j, x_i) = \sum_{m=0}^{p-1} D_m(x_i, x_*) R_m(y_j - x_*) + \text{Error}. \]

S: “Singular”  
(also “Multipole”,  
“Outer”  
“Far Field”),

R: “Regular”  
(also “Local”,  
“Inner”  
“Near Field”)
Example of S and R expansions (3D Laplace)

Spherical Coordinates:
\[ r = r(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \]

Spherical Harmonics:
\[
\Phi(y_j, x_i) = \sum_{n=0}^{p-1} \sum_{m=-n}^{n} C_n^m S_n^m(y_j - x_*) + \text{Error}(p),
\]
\[
\Phi(y_j, x_i) = \sum_{n=0}^{p-1} \sum_{m=-n}^{n} D_n^m R_n^m(y_j - x_*) + \text{Error}(p),
\]
\[
S_n^m(r) = \left(\frac{-1}{i}\right)^{|m|} \frac{4\pi}{\sqrt{2n+1}} \frac{1}{r^{n+1}} Y_n^m(\theta, \varphi),
\]
\[
R_n^m(r) = i^{-|m|} a_n^m \frac{4\pi}{\sqrt{2n+1}} r^n Y_n^m(\theta, \varphi),
\]
\[
a_n^m = a_{-m}^m = \frac{(-1)^n}{\sqrt{(n-m)!(n+m)!}}.
\]

Spherical Harmonics:
\[
Y_n^m(\theta, \varphi) = (-1)^m \frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!} P_n^{|m|}(\cos \theta) e^{i m \varphi}
\]

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S and R Expansions (3D Helmholtz)

\[ \nabla^2 \Phi + k^2 \Phi = 0 \]

\[ \Phi(y_j, x_i) = \sum_{n=0}^{p-1} \sum_{m=-n}^{n} C_n^m S_n^m(y_j - x_*) + \text{Error}(p), \]

\[ \Phi(y_j, x_i) = \sum_{n=0}^{p-1} \sum_{m=-n}^{n} D_n^m R_n^m(y_j - x_*) + \text{Error}(p), \]

Spherical Coordinates:
\[ \mathbf{r} = r(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \]

Spherical Hankel Functions
\[ S_n^m(r) = h_n(kr) Y_n^m(\theta, \varphi), \]

\[ R_n^m(r) = j_n(kr) Y_n^m(\theta, \varphi). \]
Idea of a Single Level FMM

**Standard algorithm**

- Total number of operations: $O(NM)$

**SLFMM**

- Total number of operations: $O(N+M+KL)$

Needs Translation!
Space Partitioning

Potentials due to sources in these spatial domains

\[ \Phi_1^{(n)}(y) = \sum_{x_i \in E_1(n)} u_i \Phi(y, x_i) \]

\[ \Phi_2^{(n)}(y) = \sum_{x_i \in E_2(n)} u_i \Phi(y, x_i) \]

\[ \Phi_3^{(n)}(y) = \sum_{x_i \in E_3(n)} u_i \Phi(y, x_i) \]
Single Level Algorithm

1. For each box build Far Field representation of the potential due to all sources in the box.

2. For each box build Near Field representation of the potential due to all sources outside the neighborhood.

3. Total potential for evaluation points belonging to this box is a direct sum of potentials due to sources in its neighborhood and the Near Field expansion of other sources near the box center.
The SLFMM requires $S|R$-translation:
S|R-translation

Also “Far-to-Local”, “Outer-to-Inner”, “Multipole-to-Local”

\[ R_2 = \min \{ |x_2 - x_1| - R_c |x_i - x_1|, r_c |x_i - x_2| \} \]
S|R-translating Operator

\[
\Phi(y) = \sum_{m=0}^{p-1} C_m S_m (y - x_{1*}) + \text{Error}.
\]

\[
\Phi(y) = \sum_{m=0}^{p-1} D_m R_m (y - x_{2*}) + \text{Error}.
\]

S|R-Translation Coefficients

\[
S_{m1}(y - x_{1*}) = \sum_{m=0}^{p-1} (S|R)_{mm} (x_{2*} - x_{1*}) R_m (y_j - x_{2*}) + \text{Error}.
\]

S|R-Translation Matrix

\[
D_m (y - x_{1*}) = \sum_{m=0}^{p-1} (S|R)_{mm} (x_{2*} - x_{1*}) C_n (y_j - x_{2*}) + \text{Error}.
\]

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S|R-translation Operators
for 3D Laplace and Helmholtz equations

\[ \Phi(y) = \sum_{n=0}^{p-1} \sum_{m=n}^{n} C^{mn}_{n2} S^{mn}_{n2}(y - x_{*1}) + Error. \]

\[ \Phi(y) = \sum_{n=0}^{p-1} \sum_{m=n}^{n} D^{mn}_{n2} R^{mn}_{n2}(y - x_{*2}) + Error. \]

\[ S^{mn}_{n2}(y - x_{*1}) = \sum_{n' = 0}^{p-1} \sum_{m' = -n'}^{n'} (S|R)_{n' n2}^{mn} (x_{*2} - x_{*1}) R^{m'}_{m2} (y_j - x_{*2}) + Error. \]

\[ D^{mn}_{n2}(y - x_{*1}) = \sum_{n' = 0}^{p-1} \sum_{m' = -n'}^{n'} (S|R)_{n' n2}^{mn} (x_{*2} - x_{*1}) C^{m'}_{m2} (y_j - x_{*2}) + Error. \]

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Complexity of SLFMM

We have $p^2$ terms and $P(p)$ translation cost:

\[
Complexity = O(F(K))
\]

\[
F(K) = Np^2 + PK^2 + Mp^2 + 27MN/K
\]

\[
F'(K) = 2PK - 27MN/K^2 = 0
\]

\[
K_{opt} = 3 \left( \frac{MN}{2P} \right)^{1/3}
\]

\[
F(K_{opt}) = (N + M)p^2 + 21 \left( \frac{MN}{2} \right)^{2/3} p^{1/3}
\]

For $M \sim N$:

\[
Complexity = O(N^{4/3})
\]

"Middleman" complexity

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Idea of Multilevel FMM

Source Data Hierarchy

Evaluation Data Hierarchy

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Complexity of MLFMM

Definitions:
Upward Pass: Going Up on SOURCE Hierarchy
Downward Pass: Going Down on EVALUATION Hierarchy

We have $N$ sources. Let us group them hierarchically. At level $l$ we have $N_l$ source groups. Each group at level $l+1$ contains $N_lS$ sources, so

$$N_{l+1} = N_lS, \quad l = 2, 3, ..., L,$$

and

$$N_L = N.$$

Then the number of operations for the Upward Pass is of order

$$N_L + N_{L-1} + ... + N_2 = N + \frac{N}{S} + \frac{N}{S^2} + ... + \frac{N}{S^{L-2}}$$

$$= N \left( 1 + \frac{1}{S} + ... + \frac{1}{S^{L-2}} \right) = N \frac{1 - 1/S^{L-1}}{1 - 1/S} = O(N).$$

Similarly, the number of operations for the Downward Pass is of order $O(M)$.

**MLFMM Complexity** = $O(M+N)$!

Not factorial!
Hierarchical Spatial Domains

$E_1$  $E_2$

$E_3$  $E_4$
Upward Pass. Step 1.

S-expansion valid in $\Omega$

S-expansion valid in $E_3(n,L)$
Upward Pass. Step 2.

S|S-translation.
Build potential for the parent box (find its S-expansion).
Downward Pass. Step 1.

S|R-translation

Level 2:

Level 3:
Figure shows that local-to-local translation is applicable in this case (smaller sphere is located completely inside the larger sphere), and junction of structures $E_3(n, l)$ and $E_4(n, l + 1)$ produces $E_3(n, l + 1)$:

$$E_3(n, l + 1) = E_3(n, l) \cup E_4(n, l + 1).$$
Final Summation

Contribution of \textit{near sources} (calculated directly)

Contribution of \textit{far sources} (represented by R-expansion)
Adaptive MLFMM

Goal of computations:

We want to evaluate $\Phi(y_j), j = 1, \ldots, M$ only for $y_j \in Y$. This goal is different from the outcome of the regular multilevel method which results in ability to evaluate $\Phi(y)$ for any $y \in E_1(0,0)$.
Idea of Adaptation

Each evaluation box in this picture contains not more than 3 sources in the neighborhood.
Very important for particle methods with concentrations of particles.
We have implemented MLFMM

• General “MLFMM shell” software:
  - Arbitrary dimensionality;
  - Variable sizes of neighborhoods;
  - Variable clustering parameter;
  - Regular and Adaptive versions;
  - User Specified basis functions, and translation operators;
  - Efficient data structures using bit interleaving;
  - Technical Report #1 is available online (visit the authors’ home pages).

Optimal choice of the clustering parameter is important
Speed of computation

- Straightforward
- \( y = cx^2 \)
- FMM (s=4)
- FMM/(a*\log(N))
- Setting FMM
- Middleman
- Regular Mesh, \( d=2, k=1, \) Reduced S|R
Error analysis

![Graph showing error analysis with theoretical error bounds for different truncation numbers and indices.](image)

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Complexity of Translation

- For 3D Laplace and Helmholtz series have $p^2$ terms;
- Translation matrices have $p^4$ elements;
- Translation performed by direct matrix-vector multiplication has complexity $O(p^4)$;
- Can be reduced to $O(p^3)$;
- Can be reduced to $O(p^2 \log^2 p)$;
- Can be reduced to $O(p^2)$ (?).
Rotation-Coaxial Translation Decomposition Yields $O(p^3)$ Method

Coaxial Translation

\[
\mathcal{F}_n^m (\mathbf{\hat{r}} + i_z d) = \sum_{|n|} (S|R)_n^m (d) R_n^m (\mathbf{\hat{r}}), \quad |\mathbf{\hat{r}}| < d,
\]

\[
\mathcal{F}_n^m (\mathbf{\hat{r}} + i_z d) = \sum_{|n|} (S|S)_n^m (d) S_n^m (\mathbf{\hat{r}}), \quad |\mathbf{\hat{r}}| > d,
\]

\[
\mathcal{F}_n^m (\mathbf{\hat{r}} + i_z d) = \sum_{|n|} (R|R)_n^m (d) R_n^m (\mathbf{\hat{r}}).
\]

\[
(E|F)_n^m (d) = \langle (E|F)_{\delta \phi}^m (d) \rangle |q_{\phi} = 0, \quad E, F = S, R.
\]

\[
Y_n^m (\theta, \varphi) = \sum_{\nu = -n}^{n} T_{n}^{m} (Q) Y_{\nu}^n (\tilde{\theta}, \tilde{\varphi}),
\]

\[
Q = \begin{pmatrix}
    i_{\tilde{x}} \cdot i_{\tilde{x}} & i_{\tilde{x}} \cdot i_{\tilde{y}} & i_{\tilde{x}} \cdot i_{\tilde{z}} \\
    i_{\tilde{y}} \cdot i_{\tilde{x}} & i_{\tilde{y}} \cdot i_{\tilde{y}} & i_{\tilde{y}} \cdot i_{\tilde{z}} \\
    i_{\tilde{z}} \cdot i_{\tilde{x}} & i_{\tilde{z}} \cdot i_{\tilde{y}} & i_{\tilde{z}} \cdot i_{\tilde{z}}
\end{pmatrix}.
\]

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FFT-based Translation for 3D Laplace Equation Yields $O(p^2 \log^2 p)$ Method

Translation Matrices are Toeplitz and Hankel

$$(S|R)_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t) = S_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t),$$

$$(S|S)_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t) = R_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t),$$

$$(R|R)_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t) = R_{\mathbb{R}^2 \times \mathbb{R}^2}^{n \times m} (t).$$

Multiplication can be performed using FFT (Elliot & Board 1996; Tang et al 2003)
Sparse Matrix Decompositions Can Result in $O(p^2)$ Methods

Laplace and Helmholtz:

\[
(S|S)(t) = \left\{ tD\left(\frac{t}{|t|}\right) \right\} = \sum_{n=0}^{q(\varepsilon)} \frac{t^n}{n!} D^n\left(\frac{t}{|t|}\right) + \text{Error},
\]

\[
(R|R)(t) = \left\{ tD\left(\frac{t}{|t|}\right) \right\} = \sum_{n=0}^{q(\varepsilon)} \frac{t^n}{n!} D^n\left(\frac{t}{|t|}\right) + \text{Error},
\]

Helmholtz 3D:

\[
(S|R)(t) = \sum_{n=0}^{q(\varepsilon)} (2n+1)i^n h_n(t) P_n\left(iD\left(\frac{t}{|t|}\right)\right) + \text{Error}.
\]

D is a sparse matrix
Interaction of Multiple Spherical Particles

Helmholtz (acoustical scattering)

\[ \nabla^2 \psi + k^2 \psi = 0, \]

\[ \left( \frac{\partial \psi}{\partial n} + i k \sigma_p \psi \right) \bigg|_{s_p} = 0, \quad p = 1, \ldots, N, \]

\[ \psi(\mathbf{r}) = \psi_{\text{in}}(\mathbf{r}) + \psi_{\text{scat}}(\mathbf{r}), \]

\[ \lim_{r \to \infty} r \left( \frac{\partial \psi_{\text{scat}}}{\partial r} - i k \psi_{\text{scat}} \right) = 0. \]

Laplace (potential incompressible flow)

\[ \nabla^2 \phi = 0, \]

\[ \frac{\partial \phi}{\partial n} \bigg|_{s_p} = 0, \quad p = 1, \ldots, N, \]

\[ \phi(\mathbf{r}) = \phi_{\infty}(\mathbf{r}) + \phi_{\text{ind}}(\mathbf{r}), \]

\[ \lim_{r \to \infty} \phi_{\text{ind}}(\mathbf{r}) = 0. \]

\[ k \to 0 \]
Multipole Solution

\[ \psi_{\text{scal}}(\mathbf{r}) = \sum_{q=1}^{N} \psi_{q}(\mathbf{r}), \]

\[ \psi_{q}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{\mathbf{r}_{q}} A_{q}^{(q)n} S_{q,n}^{|q|} (\mathbf{r} - \mathbf{r}_{q}'), \quad q = 1, \ldots, N. \]

\[ \psi_{\text{int}}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{\mathbf{r}_{q}} E_{q}^{(\text{int})n} (\mathbf{r}_{q}) R_{q,n}^{|q|} (\mathbf{r} - \mathbf{r}_{q}'). \]

1) Reexpand solution near the center of each sphere, and satisfy boundary conditions
2) Solve linear system to determine the expansion coefficients
Computational Methods Used

Computable on 1 GHz, 1 GB RAM Desktop PC

- BEM
- Multipole Straightforward
- Multipole Iterative
- MLFMM

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Comparisons with BEM

BEM discretization with 5400 elements
Convergence of the Iterative Procedure

For Laplace equation convergence is much faster

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Multiple Scattering from 100 spheres

FMM also used here for visualization
Various Configurations

343 spheres in a regular grid

1000 randomly placed spheres

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Truncation Errors

1000 Spheres, $ka=0.001$

max relative error $< 0.7\%$

Sphere #1
(near the cluster center)

Sphere #958
(far from the cluster center)
Some Observations for Laplace Equation (limit at small $k$)

- Relative errors below 1% can be achieved even for $p \sim 1$;
- Reflection method converges very fast; Number of iterations can be 2-10 for very high accuracy.
- CPU time on 1GHz, 1GB RAM PC for 1000 spheres $\sim 1$ min.

\[
\text{Straightforward: } O(N^3 p^6) \\
\text{MLFMM: } O(N_{\text{iteration}} N p^2 \log N)
\]

For $p \sim 10$, $N_{\text{iteration}} \sim 10$, $N \sim 10^4$ savings

\[
\text{In speed } \sim \frac{N^3 p^6}{N_{\text{iteration}} N p^2 \log N} \sim 10^{10} \text{ times (!)}
\]

\[
\text{In memory } \sim \frac{N^2 p^4}{N p^2} \sim 10^6 \text{ times (!)}
\]

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Some projects of students in our course related to incompressible flow

1). Jun Shen (Mechanical Engineering, UMD):
2D simulation of vortex flow (particle method + MLFMM)
Project 2- Calculate vortex induced forces

2). Jayanarayanan Sitaraman (Alfred Gessow Rotorcraft Center, UMD): Fast Multipole Methods For 3-D Biot-Savart Law Calculations (free vortex methods)

Break-even point: MLFMM is faster than straightforward for N=M>1300
Conclusions

- We developed a shell and framework for MLFMM which can be used for many problems, including simulations of potential and vortex flows and multiparticle motion.
- MLFMM shows itself as very efficient method for solution of fluid dynamics problems;
- MLFMM enables computation of large problems (sometimes even on desktop PC);
- Research is ongoing.
- Problems:
  - Efficient choice of parameters for MLFMM;
  - Efficient translation algorithms;
  - Efficient iterative procedures;
  - More work on error bounds is needed;
  - Etc.
- **CSCAMM Meeting on FMM in November 2003**
Thank You!