CMSC 858M/AMSC 698R

Fast Multipole Methods

Nail A. Gumerov & Ramani Duraiswami

Lecture 22

Outline

- Problems related to the Laplace and Helmholtz equations
- Direct factorization of Green's functions
  - Biharmonic equation
  - Stokes equations
- Representations via multiple scalar functions
- Conversion operators
- Examples
  - Biharmonic equation
  - Polyharmonic equations
  - Constrained vector Laplace equation
  - Maxwell equations
  - Stokes equations

Problems related to the Laplace and Helmholtz equations

Biharmonic equation (elasticity, Stokes flows, RBF interpolation)

$$\nabla^4 \psi = 0$$

Polyharmonic equation (RBF interpolation, function approximation)

$$\nabla^{2n} \psi = 0$$

Constrained vector Laplace equation (vortical flows, vector potentials)

$$\nabla^2 \mathbf{u} = \mathbf{0}, \quad \nabla \cdot \mathbf{u} = 0$$

Stokes equations (incompressible fluid dynamics at low Reynolds numbers)

$$\nabla^2 \mathbf{v} = \nabla p, \quad \nabla \cdot \mathbf{v} = 0$$

Time harmonic Maxwell equations (electromagnetism)

$$\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\epsilon\mathbf{E}, \quad \nabla \cdot \mathbf{E} = 0, \quad \nabla \cdot \mathbf{H} = 0$$

Direct factorization of Green’s functions

- Many problems can be reduced to summation of singularities, such as Green’s functions (monopoles) and their derivatives (multipoles)
- Examples: Boundary element methods, singularity methods, RBF interpolation
- Green’s functions for some complex equations can be factored, so the problem may reduce to several summations with Laplacian or other known kernels.

Example 1: Biharmonic equation

Fu & Rodin (2000)

$$\begin{aligned}\nabla^4 G^{(b)}(\mathbf{y},\mathbf{x}) &= -\delta(\mathbf{y}-\mathbf{x}),\\ G^{(b)}(\mathbf{y},\mathbf{x}) &= \frac{1}{8\pi}|\mathbf{y}-\mathbf{x}|.\end{aligned}$$

Complexity = 5 runs of the FMM for the Laplace equation

$$\begin{aligned}v_j &= \sum_{i=1}^{N} u_i G\left(\mathbf{y}_j,\mathbf{x}_i\right) = \frac{1}{8\pi}\sum_{i=1}^{N} u_i\left|\mathbf{y}_j-\mathbf{x}_i\right|\\ &= \frac{1}{8\pi}\sum_{i=1}^{N} u_i \frac{\left|\mathbf{y}_j-\mathbf{x}_i\right|^2}{\left|\mathbf{y}_j-\mathbf{x}_i\right|} = \frac{1}{8\pi}\sum_{i=1}^{N} u_i \frac{\left(\mathbf{y}_j-\mathbf{x}_i\right)\cdot\left(\mathbf{y}_j-\mathbf{x}_i\right)}{\left|\mathbf{y}_j-\mathbf{x}_i\right|}\\ &= \frac{\left|\mathbf{y}_j\right|^2}{2}\sum_{i=1}^{N}\frac{u_i}{4\pi\left|\mathbf{y}_j-\mathbf{x}_i\right|} - \mathbf{y}_j\cdot\sum_{i=1}^{N}\frac{\mathbf{x}_i u_i}{4\pi\left|\mathbf{y}_j-\mathbf{x}_i\right|} + \frac{1}{2}\sum_{i=1}^{N}\frac{|\mathbf{x}_i|^2 u_i}{4\pi\left|\mathbf{y}_j-\mathbf{x}_i\right|}\end{aligned}$$

1 FMM

3 FMMs

1 FMM

$$\begin{aligned}\nabla^2 G^{(h)}(\mathbf{y},\mathbf{x}) &= -\delta(\mathbf{y}-\mathbf{x}),\\ G^{(h)}(\mathbf{y},\mathbf{x}) &= \frac{1}{4\pi|\mathbf{y}-\mathbf{x}|}.\end{aligned}$$

Example 1: Biharmonic equation

In fact, complexity
< 5 FMMs, since
direct summation
Can be performed
just one time

Assume well balanced FMM for the Laplace kernel:

Cost of dense matrix-vector product = Cost of sparse matrix vector product = ½ of total FMM cost.

Then the total cost is 5 Dense products + 1 Sparse product = 3 FMMs

Example 2: Stokes equations

Stokeslets

$$S_{ij}(\mathbf{y},\mathbf{x}) = \frac{\delta_{ij}}{|\mathbf{y}-\mathbf{x}|} + \frac{(y_i - x_i)(y_j - x_j)}{|\mathbf{y}-\mathbf{x}|^3}, \quad i,j = 1,2,3$$

$$F_{i,m} = \sum_{n=1}^{N}\sum_{j=1}^{3} S_{ij}(\mathbf{y}_m, \mathbf{x}_n) f_{j,n}, \quad i = 1,2,3, \quad m = 1,\ldots,M$$

Stresslets

$$D_{ij}(\mathbf{y},\mathbf{x};\mathbf{n}) = -\sum_{k=1}^{3} \frac{(y_i - x_i)(y_j - x_j)(y_k - x_k)n_k}{|\mathbf{y}-\mathbf{x}|^5}, \quad i,j = 1,2,3$$

$$U_{i,m} = \sum_{n=1}^{N}\sum_{j=1}^{3} D_{ij}(\mathbf{y}_m, \mathbf{x}_n; \mathbf{n}_n) u_{j,n}, \quad i = 1,2,3, \quad m = 1,\ldots,M$$

Example 2: Stokes equations

Tornberg, Greengard (2008)

Stokeslet summation (Similarly, stresslet summation, see the paper)

$$S_{ij}(\mathbf{y},\mathbf{x}) = \left[\delta_{ij} - (y_j - x_j)\frac{\partial}{\partial y_i}\right]\frac{1}{|\mathbf{y}-\mathbf{x}|}$$

$$\begin{aligned}
F_{i,m} &= \sum_{n=1}^{N}\sum_{j=1}^{3} S_{ij}(\mathbf{y}_m, \mathbf{x}_n) f_{j,n} \\
&= \sum_{n=1}^{N}\sum_{j=1}^{3}\left[\delta_{ij} - y_{j,m}\frac{\partial}{\partial y_{i,m}}\right]\frac{f_{j,n}}{|\mathbf{y}_m - \mathbf{x}_n|} + \sum_{n=1}^{N}\sum_{j=1}^{3} x_{j,n}\frac{\partial}{\partial y_{i,m}}\frac{f_{j,n}}{|\mathbf{y}_m - \mathbf{x}_n|} \\
&= \sum_{j=1}^{3}\left[\delta_{ij} - y_{j,m}\frac{\partial}{\partial y_{i,m}}\right]\underbrace{\sum_{n=1}^{N}\frac{f_{j,n}}{|\mathbf{y}_m - \mathbf{x}_n|}}_{\text{3 FMMs}} + \frac{\partial}{\partial y_{i,m}}\underbrace{\sum_{n=1}^{N}\frac{\mathbf{x}_n \cdot \mathbf{f}_n}{|\mathbf{y}_m - \mathbf{x}_n|}}_{\text{1 FMM}}.
\end{aligned}$$

Representations via multiple scalar functions

Scalar function $$\phi(\mathbf{y}) \to (\phi_1(\mathbf{y}), \phi_2(\mathbf{y}), \ldots, \phi_K(\mathbf{y}); \mathbf{y}; \nabla_{\mathbf{y}})$$

Vector function $$\mathbf{v}(\mathbf{y}) \to (\phi_1(\mathbf{y}), \phi_2(\mathbf{y}), \ldots, \phi_K(\mathbf{y}); \mathbf{y}; \nabla_{\mathbf{y}})$$

Representations in the reference frame centered at 0.

Independent solution of Laplace, Helmholtz, or other equation, for which FMM is available

Translation
$$\begin{aligned}\tilde{\phi}(\mathbf{y}) &= \mathcal{T}(\mathbf{t})[\phi(\mathbf{y})] = \phi(\mathbf{y}+\mathbf{t}) \\ &\to (\phi_1(\mathbf{y}+\mathbf{t}), \phi_2(\mathbf{y}+\mathbf{t}), \ldots, \phi_K(\mathbf{y}+\mathbf{t}); \mathbf{y}+\mathbf{t}; \nabla_{\mathbf{y+t}}) \\ &\to (\hat{\phi}_1(\mathbf{y}), \hat{\phi}_2(\mathbf{y}), \ldots, \hat{\phi}_K(\mathbf{y}); \mathbf{y}+\mathbf{t}; \nabla_{\mathbf{y}})\end{aligned}$$

Look for representation in the form
$$\tilde{\phi}(\mathbf{y}) \to (\tilde{\phi}_1(\mathbf{y}), \tilde{\phi}_2(\mathbf{y}), \ldots, \tilde{\phi}_K(\mathbf{y}); \mathbf{y}; \nabla_{\mathbf{y}})$$

$$(\tilde{\phi}_1(\mathbf{y}), \tilde{\phi}_2(\mathbf{y}), \ldots, \tilde{\phi}_K(\mathbf{y}))^T = \boxed{\mathcal{C}(\mathbf{t})}(\hat{\phi}_1(\mathbf{y}), \hat{\phi}_2(\mathbf{y}), \ldots, \hat{\phi}_K(\mathbf{y}))^T$$

Conversion operator (linear!)

Example 1: Biharmonic equation

$$\nabla^4\phi = 0,$$
$$\phi(\mathbf{r}) = \phi_1(\mathbf{r}) + r^2\phi_2(\mathbf{r}), \quad \nabla^2\phi_1 = 0, \quad \nabla^2\phi_2 = 0.$$

$$\begin{aligned}\tilde{\phi}(\mathbf{r}) &= \phi(\mathbf{r}+\mathbf{t}) = \phi_1(\mathbf{r}+\mathbf{t}) + |\mathbf{r}+\mathbf{t}|^2\phi_2(\mathbf{r}+\mathbf{t}) \\ &= \hat{\phi}_1(\mathbf{r}) + (\mathbf{r}+\mathbf{t})\cdot(\mathbf{r}+\mathbf{t})\hat{\phi}_2(\mathbf{r}) \\ &= [\hat{\phi}_1(\mathbf{r}) + t^2\hat{\phi}_2(\mathbf{r})] + 2(\mathbf{r}\cdot\mathbf{t})\hat{\phi}_2(\mathbf{r}) + r^2\hat{\phi}_2(\mathbf{r}) \\ &= \tilde{\phi}_1(\mathbf{r}) + r^2\tilde{\phi}_2(\mathbf{r}).\end{aligned}$$

It is very convenient to consider the RCR-decomposition: Rotation does not affect basic decomposition, translation should be only along the z-axis

Example 1: Biharmonic equation

$$zR_n^m(\mathbf{r}) = -\frac{1}{2n+1}[(n+m+1)(n-m+1)R_{n+1}^m(\mathbf{r}) + r^2R_{n-1}^m(\mathbf{r})]$$
$$= \gamma_n^m R_{n+1}^m + \delta_n r^2 R_{n-1}^m$$

$$\breve{\phi}_2(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \breve{\phi}_{2,n}^m R_n^m,$$

$$z\breve{\phi}_2(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \breve{\phi}_{2,n}^m zR_n^m = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \breve{\phi}_{2,n}^m(\gamma_n^m R_{n+1}^m + \delta_n r^2 R_{n-1}^m)$$
$$= \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \breve{\phi}_{2,n-1}^m \gamma_{n-1}^m R_n^m + r^2 \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \delta_{n+1} \breve{\phi}_{2,n+1}^m R_n^m$$

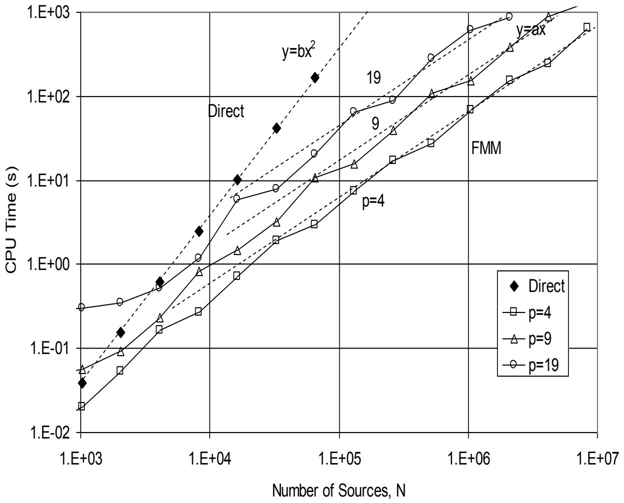
Representation of the conversion operator in the space of R-expansion coefficients

$$\boxed{\begin{aligned}\breve{\phi}_{1,n}^m &= \phi_{1,n}^m + t^2\phi_{2,n}^m - 2t\frac{(n+m)(n-m)}{2n-1}\breve{\phi}_{2,n-1}^m,\\ \breve{\phi}_{2,n}^m &= \phi_{2,n}^m - \frac{2t}{2n+3}\phi_{2,n+1}^m.\end{aligned}}$$

Very sparse matrix!
Only 2 FMMs are needed!

Similarly for S-expansions. See Gumerov, Duraiswami (2006).

Performance of 3D FMM for biharmonic kernel



(3.2 GHz Intel Xeon, 3.5 GB RAM)

Example 2: Polyharmonic equation

$$\nabla^{2k}\phi = 0$$

$$\phi(\mathbf{r}) = \phi_1(\mathbf{r}) + r^2\phi_2(\mathbf{r}) + \ldots + r^{2k-2}\phi_k(\mathbf{r}), \quad \nabla^2\phi_j = 0.$$

$$\begin{aligned}\hat{\phi}(\mathbf{r}) = \phi(\mathbf{r}+\mathbf{t}) &= \mathcal{T}(\mathbf{t})\sum_{j=1}^{k}(\mathbf{r}\cdot\mathbf{r})^{2j-2}\phi_j(\mathbf{r}) \\ &= \sum_{j=1}^{k}[(\mathbf{r}+\mathbf{t})\cdot(\mathbf{r}+\mathbf{t})]^{2j-2}\hat{\phi}_j(\mathbf{r}) \\ &= \sum_{j=1}^{k}[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2]^{j-1}\hat{\phi}_j(\mathbf{r}).\end{aligned}$$

Recursive reduction to the biharmonic case.

Example 3: Constrained vector Laplace equation

$$\nabla^2\boldsymbol{\omega} = \mathbf{0}, \quad \nabla\cdot\boldsymbol{\omega} = 0.$$

$$\boldsymbol{\omega} = \nabla\psi + \nabla\times(\mathbf{r}\varpi), \quad \nabla^2\psi = 0, \quad \nabla^2\varpi = 0$$

$$\begin{aligned}\hat{\boldsymbol{\omega}}(\mathbf{r}) &= \boldsymbol{\omega}(\mathbf{r}+\mathbf{t}) = \nabla\psi(\mathbf{r}+\mathbf{t}) + \nabla\times((\mathbf{r}+\mathbf{t})\varpi(\mathbf{r}+\mathbf{t})) \\ &= \nabla\hat{\psi}(\mathbf{r}) + \nabla\times\left((\mathbf{r}+\mathbf{t})\hat{\varpi}(\mathbf{r})\right) = \nabla\hat{\psi}(\mathbf{r}) + \nabla\times\left(\mathbf{r}\hat{\varpi}(\mathbf{r})\right) + \nabla\times\left(\mathbf{t}\hat{\varpi}(\mathbf{r})\right),\end{aligned}$$

$$\hat{\boldsymbol{\omega}} = \mathcal{T}_{\mathbf{t}}\boldsymbol{\omega}, \quad \hat{\psi} = \mathcal{T}_{\mathbf{t}}\psi, \quad \hat{\varpi} = \mathcal{T}_{\mathbf{t}}\varpi.$$

$$\hat{\boldsymbol{\omega}}(\mathbf{r}) = \nabla\tilde{\hat{\psi}} + \nabla\times(\mathbf{r}\tilde{\hat{\varpi}}),$$

$$\tilde{\hat{\psi}} = \mathcal{C}_{11}\hat{\psi} + \mathcal{C}_{12}\hat{\varpi}, \quad \tilde{\hat{\varpi}} = \mathcal{C}_{21}\hat{\psi} + \mathcal{C}_{22}\hat{\varpi},$$

$$\mathcal{C}_{11} = \mathcal{I}, \quad \mathcal{C}_{21} = 0.$$

Example 3: Constrained vector Laplace equation

$$\begin{aligned}\widetilde{\psi} &= \widehat{\psi} + \mathcal{C}_{12}\widehat{\varpi} = \widehat{\psi} + \psi', \\ \widetilde{\varpi} &= \mathcal{C}_{22}\widehat{\varpi} = \widehat{\varpi} + \varpi'.\end{aligned}$$

$$\nabla\psi' + \nabla\times(\mathbf{r}\varpi') = \nabla\times\left(\mathbf{t}\widehat{\varpi}\right).$$

$$\mathbf{r}\cdot\nabla\psi' = \mathbf{r}\cdot\nabla\times\left(\mathbf{t}\widehat{\varpi}\right) = \mathbf{r}\cdot\left(\nabla\widehat{\varpi}\times\mathbf{t}\right) = -(\mathbf{r}\times\mathbf{t})\cdot\nabla\widehat{\varpi}.$$

$$\nabla\times\nabla\times(\mathbf{r}\varpi') = \nabla\times\nabla\times\left(\mathbf{t}\widehat{\varpi}\right).$$

Generic vector identities for harmonic functions

$$\begin{aligned}\nabla\times\nabla\times(\mathbf{r}\varpi') &= \nabla(\varpi' + \mathbf{r}\cdot\nabla\varpi'), \\ \nabla\times\nabla\times\left(\mathbf{t}\widehat{\varpi}\right) &= \nabla\left(\mathbf{t}\cdot\nabla\widehat{\varpi}\right),\end{aligned}$$

$$\varpi' + \mathbf{r}\cdot\nabla\varpi' = \mathbf{t}\cdot\nabla\widehat{\varpi}.$$

Since an arbitrary constant can be added to potential

Example 3: Constrained vector Laplace equation

These operators can be represented via sparse matrices in the space of expansion coefficients

$$\mathcal{D}_{\mathbf{r}} = \mathbf{r}\cdot\nabla, \quad \mathcal{D}_{\mathbf{t}} = \mathbf{t}\cdot\nabla, \quad \mathcal{D}_{\mathbf{r}\times\mathbf{t}} = (\mathbf{r}\times\mathbf{t})\cdot\nabla.$$

$$\mathcal{D}_{\mathbf{r}}\psi' = -\mathcal{D}_{\mathbf{r}\times\mathbf{t}}\widehat{\varpi}, \quad (\mathcal{I}+\mathcal{D}_{\mathbf{r}})\varpi' = \mathcal{D}_{\mathbf{t}}\widehat{\varpi}.$$

Finally

Invertable (diagonal) operators

$$\begin{aligned}\widetilde{\psi} &= \widehat{\psi} - \mathcal{D}_{\mathbf{r}}^{-1}\mathcal{D}_{\mathbf{r}\times\mathbf{t}}\widehat{\varpi}, \\ \widetilde{\varpi} &= \widehat{\varpi} + (\mathcal{I}+\mathcal{D}_{\mathbf{r}})^{-1}\mathcal{D}_{\mathbf{t}}\widehat{\varpi}.\end{aligned}$$

$$\mathcal{C}_{12} = -\mathcal{D}_{\mathbf{r}}^{-1}\mathcal{D}_{\mathbf{r}\times\mathbf{t}}, \quad \mathcal{C}_{22} = \mathcal{I} + (\mathcal{I}+\mathcal{D}_{\mathbf{r}})^{-1}\mathcal{D}_{\mathbf{t}}.$$

2 FMMs are needed for this equation!

Example 4: Time harmonic Maxwell equations

$$\mathbf{E} = \nabla\phi \times \mathbf{r} + \nabla \times (\nabla\psi \times \mathbf{r}), \quad \mathbf{H} = \frac{1}{i\omega\mu}(k^2\nabla\psi \times \mathbf{r} + \nabla \times (\nabla\phi \times \mathbf{r})),$$

$$(\nabla^2 + k^2)\phi = 0, \quad (\nabla^2 + k^2)\psi = 0.$$

$$\widehat{\mathbf{E}}(\mathbf{r}) = \mathbf{E}(\mathbf{r}+\mathbf{t}) = \nabla \times (\mathbf{r}\widehat{\phi}) + \nabla \times \nabla \times \left(\mathbf{r}\widehat{\psi}\right) + \nabla \times (\mathbf{t}\widehat{\phi}) + \nabla \times \nabla \times \left(\mathbf{t}\widehat{\psi}\right),$$

$$\widehat{\mathbf{E}} = \mathcal{T}(\mathbf{t})[\mathbf{E}], \quad \widehat{\phi} = \mathcal{T}(\mathbf{t})[\phi], \quad \widehat{\psi} = \mathcal{T}(\mathbf{t})[\psi],$$

$$\widehat{\mathbf{E}}(\mathbf{r}) = \nabla \times (\mathbf{r}\widetilde{\phi}) + \nabla \times \nabla \times (\mathbf{r}\widetilde{\psi}),$$

Gumerov & Duraiswami (2007)

$$\widetilde{\phi} = \mathcal{C}_{11}[\widehat{\phi}] + \mathcal{C}_{12}\left[\widehat{\psi}\right],$$
$$\widetilde{\psi} = \mathcal{C}_{21}[\widehat{\phi}] + \mathcal{C}_{22}\left[\widehat{\psi}\right].$$

2 FMMs are needed for these equations!

Example 5: Stokes equations

- Paper under preparation, but idea is similar (3 FMMs are needed)