The Fast Multipole Method (For BIE's) Leslie Greengard and Rokhlin (1980s).

Disclaimer: These notes are derived from the work of Greengard and Rokhlin.

Motivation

What are we interested in?

⇒ Solution at one point is determined by forces acting over distances on that point
(Force potentials (N body problem), Magnetic Fields, Singularity solutions, ...)
$O(N^2)$!

⇒ BIEs! $u(x) = \int_{\partial\Omega} \underbrace{G(x-y) f(y)}_{\substack{\text{single layer} \\ \text{(point forces)}}} + \underbrace{\frac{\partial G(x-y)}{\partial \nu} h(y)}_{\substack{\text{double layer} \\ \text{(force dipoles)}}} \, dS(y)$

(This is just saying that the sol. at x is due to forces originating on the boundary, dependent on x's distance to the boundary).

(After discretizing the boundary, a BIE turns into computing interaction between pts in the domain and the points that make up the boundary)

Canonical FMM: Computing potential fields in N-particle systems

** Key Idea: For particles well separated, potential field is smooth and can be approximated arbitrarily well by a multipole expansion.

ONly take-away from this talk! ⇒ FMM: $O(N^2) \to O(N)$!

Name of The Game: Modifying multipole expansions.

Problem: N charged particles in 2D (N body problem)

⇒ Start with pot. induced by particle with charge q at z_0,

$$\phi(z) = q \log(z - z_0)$$

$$\nabla(z) = \frac{q}{z - z_0}$$

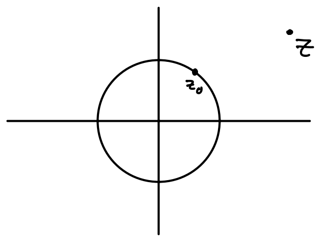
Remember that if we want the force field, just take a derivative!
$u = \mathrm{Re}(w)$ potential ⇒ $\nabla u = (u_x, u_y) = (\mathrm{Re}(w'), -\mathrm{Im}(w'))$

⇒ Goal is to get a p-term expansion for pot. field felt by each particle in $O(N)$ time

Def 1: Particle with charge q at z_0, $\forall\ |z| > |z_0|$

Gravitational Potential: $\phi_{z_0}(z) = q\log(z - z_0) = q\left(\log(z) - \sum_{k=1}^{\infty} \frac{1}{k}\left(\frac{z_0}{z}\right)^k\right)$

Taylor expand $\log(z - z_0)$ about $z_0 = 0$ $\Rightarrow \log(z) - z_0/z - (\tfrac{1}{2})(z_0/z)^2 - \ldots$



Lemma 1: N particles w/ charges q_i $(1 \le i \le n)$ located at z_i with $|z_i| < r$ $\forall i$. Then for any $|z| > r$, the potential $\phi(z)$ induced by the particles is:

$$\phi(z) = Q\log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z_k}, \quad Q = \sum_{i=1}^{N} q_i \quad \text{and} \quad a_k = \sum_{i=1}^{N} \frac{-q_i z_i^k}{k}$$

Error: $p \ge 2$: $\underbrace{\left|\phi(z) - Q\log(z) - \sum_{k=1}^{\infty} \frac{a_k}{z_k}\right|}_{E} \le \frac{\alpha}{(p+1)}\left|\frac{r}{z}\right|^{p+1}$ $\rightarrow$ Error depends on distance from z to circle.

$$\le \left(\frac{A}{p+1}\right)\left(\frac{1}{c-1}\right)\left(\frac{1}{c}\right)^p$$

Where $c = \left|\frac{z}{r}\right|$, $A = \sum_{i=1}^{N} |q_i|$, $\alpha = \frac{A}{1 - |r/z|}$ $\rightarrow A$

c $\downarrow$ >1

A $\downarrow$ possibly large? Known at start.

Proof: $E \le \left|\sum_{k=p+1}^{\infty} \frac{a_k}{z^k}\right| = \left|\sum_{k=p+1}^{\infty} \frac{1}{z^k} \sum_{i=1}^{N} \frac{-q_i z_i^k}{k}\right| \le A \sum_{k=p+1}^{\infty} \frac{r^k}{k|z|^k} \le \frac{A}{p+1} \sum_{k=p+1}^{\infty} \left|\frac{r}{z}\right|^k$

Sum of first p terms

$$= \left(\frac{A}{p+1}\right)\left(\frac{1}{1 - |r/z|} - \frac{1 - |r/z|^{p+1}}{1 - |r/z|}\right)$$

$$= \frac{A}{(p+1)(1 - |r/z|)}\left|\frac{r}{z}\right|^{p+1}$$

$$= \left(\frac{A}{p+1}\right)\left(\frac{1}{c-1}\right)\left(\frac{1}{c}\right)^p$$

$\Rightarrow$ Work done to compute p-term expansion for one particle: $O(p)$.

$\Rightarrow$ Work done to form p-term expansion for box with s particles: $O(sp)$

$\Rightarrow$ Cost to evaluate: $O(p)$ for any $|z| > r$.

Precision? If $C = |z/r| \geq 2$ then $E \leq A\left(\frac{1}{2}\right)^p$ 10 digits? $\Rightarrow p \approx 37$

$\Rightarrow$ The amount of compression depends on distance and precision.

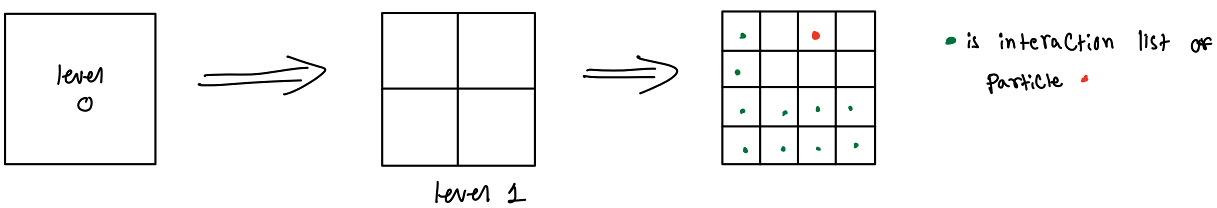
$\divideontimes$ Want $O(\varepsilon)$ $\Rightarrow$ Take $p \approx \log_2(1/\varepsilon)$ then $(1/2)^p \sim (1/2)^{\log_2(1/2)} = \varepsilon$ Nice!

Tree Structure and Recursion

What are the driving ideas behind FMM Lemmas? $\Rightarrow$ Want one p-term expansion for each particle.

$\Rightarrow$ Refine domain into levels of boxes (parent—child $\Rightarrow$ /4)

$\Rightarrow$ Compute interactions between distant boxes of particles by multipole expansions at successive levels of refinement



$\divideontimes \Rightarrow$ Interaction list: Boxes at same level that are children of parent's neighbors and do not share vertex.

$\Rightarrow$ At every level (recursion), the multipole expansion is formed for each box due to the particles it contains. The resulting expansion is evaluated for each particle sufficiently separated (interaction list). This is required for taking $C=2$ and truncation error to be bounded by 2^{-p}

Lemma 2: (Translation of a Multipole expansion) (To parent level) p^2 work

If $\phi(z) = a_0 \log(z-z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z-z_0)^k}$ is m. expansion due N particles with charges $q_1, \dots, q_N$ all inside circle D centered at z_0 w/ radius R, then for z outside of the circle D_1 of radius $(R + |z_0|)$ and centered at the origin,

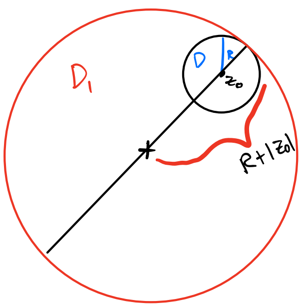
$$\phi(z) = a_0 \log(z) + \sum_{l=1}^{\infty} \frac{b_l}{z^l}, \quad b_l = \frac{-a_0 z_0^l}{l} + \sum_{k=1}^{\infty} a_k z_0^{l-k} \binom{l-1}{k-1}$$

↳ binomial coeffs

For all $p \geq 1$,

$$\left| \phi(z) - a_0 \log(z) - \sum_{l=1}^{p} \frac{b_l}{z^l} \right| \leq \left(\frac{\overset{\text{same } A}{A}}{1 - \left| \frac{|z_0| + R}{z} \right|} \right) \left| \frac{\overset{r/z}{|z_0| + R}}{z} \right|^{p+1}$$

B



$|z| > |R + |z_0||$

* Lets us build expansions for boxes from finest to coarsest levels

* Want one p-term expansion for all charges in a box and its children

Proof: Consider $\log(z-z_0) = \log(z(1-z_0/z)) = \log(z) - \sum_{l=1}^{\infty} \frac{1}{l} \left(\frac{z_0}{z}\right)^l$

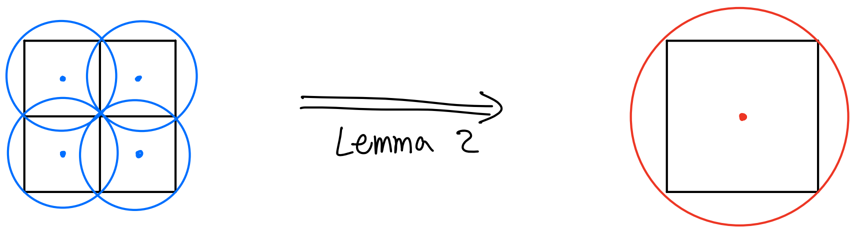
Taylor $\log(z-z_0)$ about $z_0 = 0 \Rightarrow \log(z(1-z_0/z)) = \log(z) - \frac{z_0}{z} - \frac{1}{2}\left(\frac{z_0}{z}\right)^2 - \frac{1}{3}\left(\frac{z_0}{z}\right)^3 - \dots$

And $(z-z_0)^{-k} = \sum_{l=k}^{\infty} \binom{l-1}{k-1} \frac{z_0^{l-k}}{z^l}$

⇒ Error bounds follow from uniqueness of the expansion.

⇒ Shifting without loss of precision since we are obtaining b_l from a_k exactly.

⇒ We want to form multipole expansions for pot. induced by all particles in a box from finest to coarsest level. Thus we need a mechanism to shift expansions centered at child box to one centered at the parent's box.



Lemma 3: (Conversion to local expansion)

N particles w/ Charges $q_1, \dots, {}_N$ located inside Circle D_1 w/ radius R and Center z_0 where $|z_0| > (c+1)R$ and $c > 1$. Then the Corresponding multipole expansion given by Lemma 1 Converges inside Circle D_2 of radius R centered at the origin.

Inside D_2, the pot. due to particles is given by

$$\phi(z) = \sum_{l=0}^{\infty} b_l z^l \quad \text{where}$$

$$b_0 = a\log(-z_0) + \sum_{k=1}^{\infty} \frac{a_k}{z_0^k}(-1)^k \quad \text{and} \quad b_l = \frac{-a_0}{l \cdot z_0^l} + \frac{1}{z_0^l}\sum_{k=1}^{\infty}\frac{a_k}{z_0^k}\binom{l+k-1}{k-1}(-1)^k, \quad l \geq 1.$$

Error: $$E \leq \underbrace{\frac{A(4e(p+c)(c+1)+c^2)}{c(c-1)}}_{D}\left(\frac{1}{c}\right)^{p+1}$$

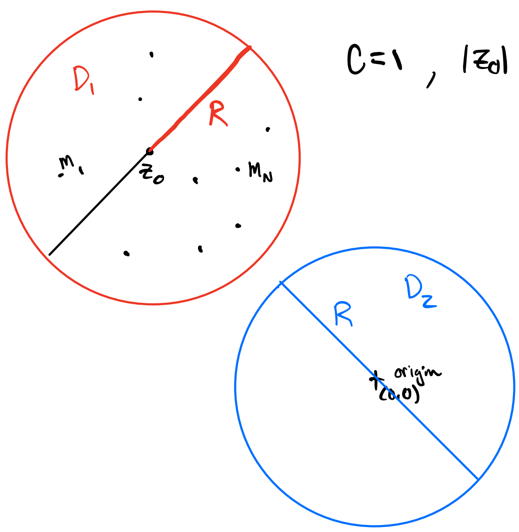
For the proof, note that $\log(z-z_0) = \log\left(-z_0\left(1-\frac{z}{z_0}\right)\right)$

$$= \log(-z_0) + \log(1 - z/z_0) \qquad \text{Taylor about } z=0.$$

$$= \log(-z_0) - \sum_{l=1}^{\infty}\frac{1}{l}\left(\frac{z}{z_0}\right)^l$$

and $$(z-z_0)^{-k} = \left(\frac{1}{-z_0}\right)^k\left(\frac{1}{1-z/z_0}\right)^k$$

$$= \left(\frac{1}{-z_0}\right)^k \sum_{l=0}^{\infty}\binom{l+k-1}{k-1}\left(\frac{z}{z_0}\right)^l$$



$c=1$, $|z_0| > 2R$

* Converges in D_2 for m_i in D_1

⇒ For each box at a level, we use this lemma to Compute the pot. field felt by each particle in a box due to all boxes in the interaction list

Lemma 4: (Translation of a local expansion) (To Child level)

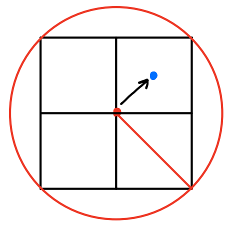
We can translate a ME centered at the center of a parent box to one centered at the center of a child box in $O(p^2)$. (Horner's Method)

The translation of a complex polynomial centered at z_0

$$\sum_{k=0}^{p} a_k (z - z_0)^k \quad \text{into one centered about zero:} \quad \sum_{k=0}^{n} b_k z^k$$

is given by (Horner Scheme):

For j from 0 to $p-1$:
  For k from $p-j-1$ to $p-1$:
    $b_k := a_k - z_0 a_{k+1}$



This is just nested multiplication from the relation:

$$\left(a_m z^j + a_{m-1} z^{j-1} + \dots + a_{m-j}\right)(z - z_0) + a_{m-j-1}$$
$$= a_m z^{j+1} + \tilde{a}_{m-1} z^j + \dots + \tilde{a}_{m-j-1}$$

degree of poly.

$\Rightarrow$ Horner's method is $O(p^2)$, used to find roots of polynomials and evaluate in $O(n)$.

Observations

1) If we have the multipole expansion for each of the 4 children of a box. To form a single expansion for the parent box without re-examining each particle. Lemma 2 provides us the mechanism to do that at $4p^2$ work.

2) If we have the local expansion for a box b which describes the field induced by all particles outside b's nearest neighbors. To transmit this information to b's children, use Lemma 4, $4p^2$ operations.

$\Rightarrow$ Everything so far is analytical, no numerics (even for differentiation, same type error bounds for force)

$\Rightarrow$ These Lemmas allow us to not have to examine <u>every</u> particle at each level of refinement (that is $N \log N$)

FMM Outline   Select $p \sim \log_2(1/\varepsilon)$, # levels $\sim \log_4(N)$ $(4^\ell \le N)$ $\log_4(N)4^\ell p^2$

(upward) ⇒ From finest level up, create expansions for each box due to particles inside it. Pass to parent in $4p^2$.
(Lemma 2) $O(Np^2)$ (ℓth level $4^\ell \le N$ shifts of p^2 work)

(downward) ⇒ From coarsest to finest level, form local exp. about center of each box describing the pot field induced by all particles that are not contained in that box or its nearest neighbors. Use (Lemma 3).
Use (Lemma 4) to shift to children.

$O(28Np^2)$ (At most 27 boxes in an interaction list. Another p^2 to shift to children)

⇒ Finest Level: Add together far field expansion + pot. induced by particles in same box and nearest neighbors. Evaluate.

in same box is $O(1)$.

$\approx s$ particles per box at finest level (N/s boxes)

Runtime: $Np + 29\left(\frac{N}{s}\right)p^2 + Np + 9Ns$

Forming expansions   Shifting   Evaluating local expansions   Near neighbor interactions

$s \approx p^2 \Rightarrow 40Np \sim O(Np)$

3D ⇒ Spherical harmonics, Legendre functions   Still $O(N)$!

Resources ⇒ Greengard, Alex Barnett, David Stein
Code   BIEs / CODE   Code

N-body Example:

1000 particles, 1000 timesteps

Direct: ~15 min $\quad 1000 \cdot N^2 \sim N^3$

FMM: 5 seconds $\quad 1000 \cdot N \sim N^2$

(FMM overhead)

BIE Example

Unknown: $\phi(x) \Rightarrow \begin{cases} \nabla^2 \phi = 0 & \text{in } \Omega \\ \frac{\partial \phi}{\partial n} = q & \text{on } \partial\Omega \end{cases}$ $\quad (\phi \to 0 \text{ at } \infty)$

$$\frac{\phi(x)}{2} = \int_{\partial\Omega} \left[G(x,y)\, q(y) - \frac{\partial G}{\partial \nu}(x,y)\, \phi(y) \right] ds(y), \quad x \in \partial\Omega$$

$G = \frac{1}{2\pi} \log|x-y|$

$\frac{\partial G}{\partial \nu} = \frac{1}{2\pi} \nu(y) \cdot \frac{(x-y)}{|x-y|^2}$

$\Rightarrow$ Discretize boundary N, quadrature weights w_j (Pick quadrature scheme to handle singularity)

$$\underbrace{\left[\tfrac{1}{2}\delta_{ij} - G'_{ij} \right]}_{L_{ij}} \phi_j = G_{ij} q_i \quad \Rightarrow \text{Linear system (GMRES } O(N^2) \text{ dense)}$$

$L_{ij} \phi_j = b_i$ $\quad$ (Fredholm - Integral second kind, Existence, stability)

Dense!

$\Rightarrow$ Don't form L! Just need how it operates on ϕ_i

$\Rightarrow$ Use FMM to compute $\int G(x,y)\, q$, $\int \frac{\partial G}{\partial \nu} \phi$ $\Rightarrow O(N)$! not $O(N^2)$!

$\Rightarrow$ Nonlinear? Still use GMRES / JFNK w/ FMM