A FAST introduction to The Fast Multipole Method

A FAST ALGORITHM FOR PARTICLE SIMULATIONS

Authors: GREENGARD L, ROKHLIN V, Journal: JCP, and Published: DEC 1987

presented by Claudio Torres

April 4, 2016

An intro to N-Body problem

Let's recall the Newton's law of universal gravitation for 2 point masses

$$\mathbf{F}_{1,2} = G\frac{m_1 m_2 \left(\mathbf{x}_2 - \mathbf{x}_1\right)}{\left\|\mathbf{x}_2 - \mathbf{x}_1\right\|^3}. \tag{1}$$

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or

$$m_j \ddot{\mathbf{q}}_j = \sum_{k \neq j} \mathbf{F}_{k,j} = \gamma \sum_{k \neq j} \frac{m_j m_k (\mathbf{q}_k - \mathbf{q}_j)}{|\mathbf{q}_k - \mathbf{q}_j|^3}, \quad j = 1 \dots N. \tag{3}$$

Now, let's go to FMM

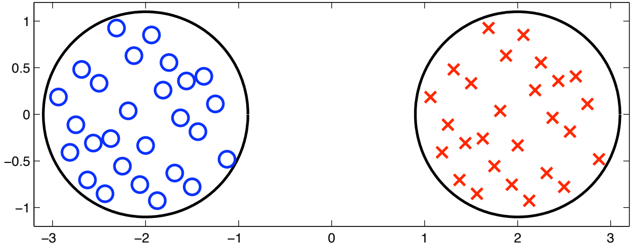

Figure: Two dimensional problem, where the interactions are pairwise

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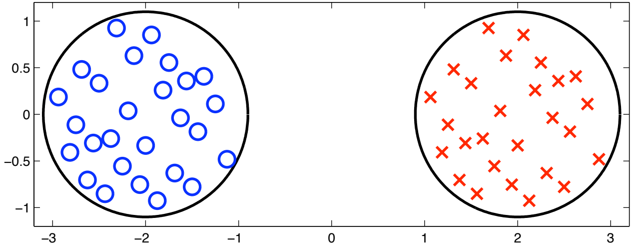

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From now on, let's define $\log(z)$ as the potential due to a charge.

Lemma

Let a point charge of intensity q be located at z_0. Then for any z such that $|z| > |z_0|$,

$$\phi_{z_0}(z) = q \log(z - z_0) = q \left(\log(z) - \sum_{k=1}^{\infty} \frac{1}{k} \left(\frac{z_0}{z} \right)^k \right) \qquad (4)$$

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Proof.

Since $\log(z - z_0) = \log(z) + \log(1 - z_0/z)$, for $\omega := |z_0/z| < 1$, and

$$\frac{1}{1-\omega} = \sum_{k=0}^{\infty}\omega^k \quad \Rightarrow_{\int \text{ and shifting}} \log(1-\omega) = (-1)\sum_{k=1}^{\infty}\frac{\omega^k}{k} \tag{5}$$

$\square$

Keep in mind the following expression:

$$\phi(z) = \sum_{i=1}^{m} q_i \log(z - z_i).$$

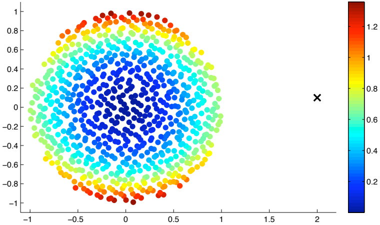

Figure: The simplest experiment: multiple sources and one target

Theorem

[Multipole Expansion] *Suppose that m charges of strengths q_i are located at points z_i for $i = 1 : m$, with $|z_i| < r$. Then for any $z \in \mathbb{C}$ with $|z| > r$, the potential $\phi(z)$ is given by*

$$\phi(z) = Q \log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k} \tag{6}$$

where

$$Q = \sum_{i=1}^{m} q_i \qquad \text{and} \qquad a_i = \sum_{k=1}^{m} \frac{-q_i z_i^k}{k} \tag{7}$$

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Furthermore, for any $p \geq 1$*,*

$$\left| \phi(z) - Q \log(z) - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \left(\frac{A}{c-1} \right) \left(\frac{1}{c} \right)^p \tag{8}$$

Furthermore, for any $p \geq 1$,

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where

$$c = \left|\frac{z}{r}\right| \qquad \text{and} \qquad A = \sum_{i=1}^{m} |q_i| \tag{9}$$

Understanding the multipole expansion

L. 1

$$
\begin{aligned}
q\log(z-z_0) &= q\left(\log(z) - \sum_{k=1}^{\infty}\frac{1}{k}\left(\frac{z_0}{z}\right)^k\right)\\
&= q\log(z) + \sum_{k=1}^{\infty}\frac{-q\,z_0^k}{k}\frac{1}{z^k}
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So, it is easy to see,

$Q = \sum_{i=1}^{m} q_i$ and $a_k = \sum_{k=1}^{m}\frac{-q_i z_i^k}{k}$

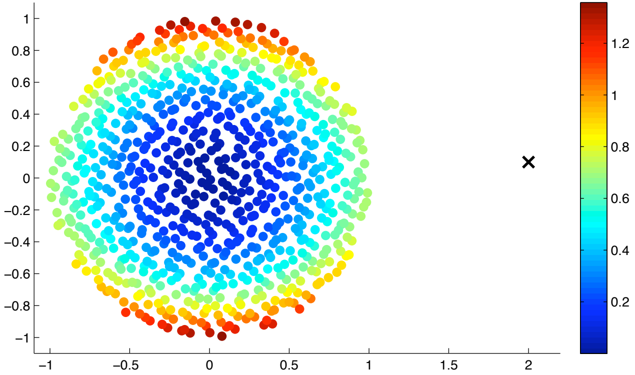

Figure: Set up of experiment with 787 sources and 1 target

The experiment try to give numerical evidence that the p-sum is a good idea to approximate potential fields.

$$\phi(z) = Q\log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k} \approx Q\log(z) + \sum_{k=1}^{p} \frac{a_k}{z^k} =: \phi(z,p) \quad (10)$$

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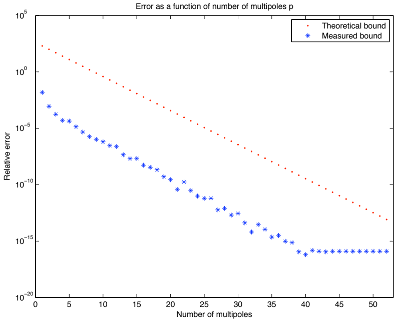


Figure: Numerical simulation

recall: p-error bound

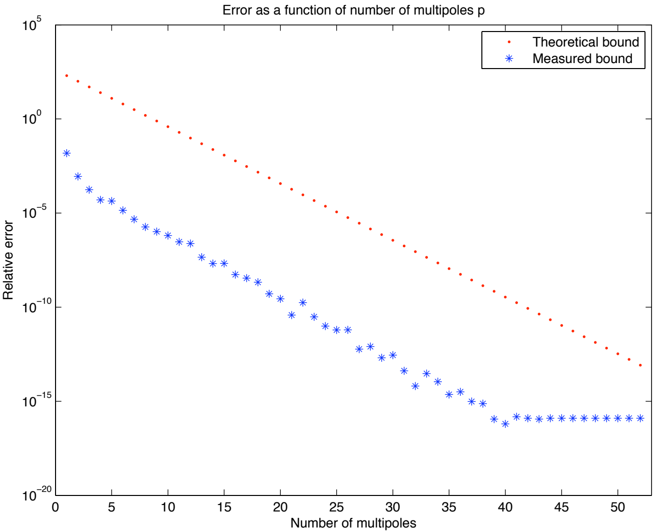
$$|\phi(z) - \phi(z,p)| \leq \left(\frac{A}{c-1}\right)\left(\frac{1}{c}\right)^p$$

with

$$c = \left|\frac{z}{r}\right|$$

and

$$A = \sum_{i=1}^{m} |q_i|$$



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Why do we call it *Fast* multipole method?

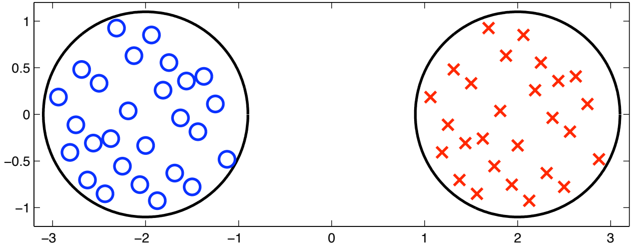

Figure: m sources at x_i(blue) and n targets at y_i(red)

Direct evaluation of potential field, due to m charges located at x_i, evaluated at y_i is $\mathcal{O}(nm)$.

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Therefore, the work has been reduced from $\mathcal{O}(nm)$ to $\mathcal{O}(pm + pn)$!, and since p is constant we only have $\mathcal{O}(m + n)$.

Shifting the multipole expansion

Lemma

Suppose that

$$\phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \tag{11}$$

is a multipole expansion of the potential due to a set of m charges of strengths q_i, with $i = 1 : m$, all of which are located inside the circle D of radius R with center at z_0. Then for z outside the circle D_1 of radius $(R + |z_0|)$ and center at the origin we have the following multipole expansion,

$$\phi(z) = a_0 \log(z) + \sum_{l=1}^{\infty} \frac{b_l}{z^l} \tag{12}$$

where

$$b_l = \left(\sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{a_0 z_0^l}{l} \tag{13}$$

Furthermore, for any $p \geq 1$

$$\left| \phi(z) - a_0 \log(z) - \sum_{l=1}^{\infty} \frac{b_l}{z^l} \right| \leq \left(A \middle/ \left(1 - \left| \frac{|z_0| + R}{z} \right| \right) \right) \left| \frac{|z_0| + R}{z} \right|^{p+1} \tag{14}$$

where

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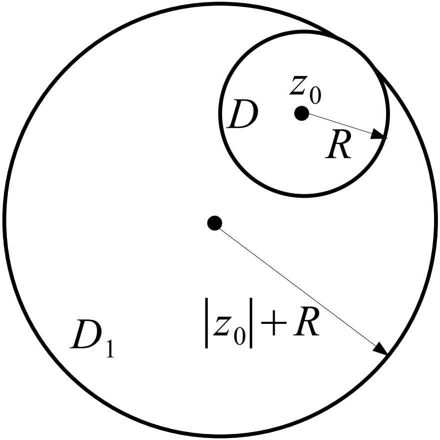
Remark: Computing b_l from a_k is *exact*!, $\Rightarrow$ we are able to shift a truncated multipole expansions without losing accuracy.


z_0
D
R
D_1
$|z_0| + R$

From multipole to local Taylor series

Lemma

Suppose that m charges of strength q_i are located inside the circle D_1 with radius R and center at z_0, and that $|z_0| > (c+1)R$ with $c > 1$. Then the corresponding multipole expansion (11) converges inside the circle D_2 of radius R centered about the origin. Inside D_2, the potential due to the charges is described by a power series:

$$\phi(z) = \sum_{l=0}^{\infty} b_l \, z^l \tag{15}$$

where

$$b_0 = \sum_{k=1}^{\infty} \frac{a_k}{z_0^k}(-1)^k + a_0 \log(-z_0) \tag{16}$$

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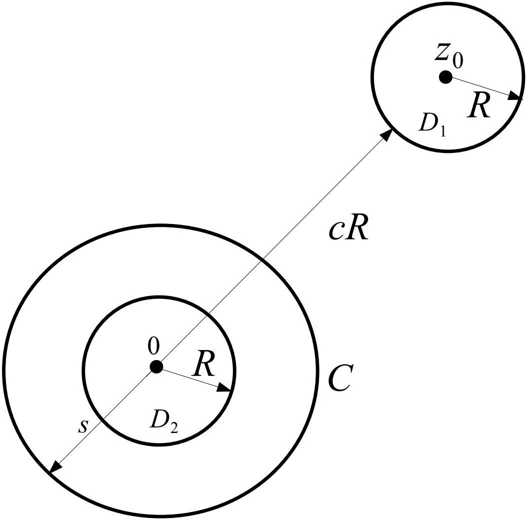
$$b_l = \left(\frac{1}{z_0^l} \sum_{k=1}^{\infty} \frac{a_k}{z_0^k} \binom{l+k-1}{k-1} (-1)^k \right) - \frac{a_0}{l \, z_0^l}, \quad \textit{for} \quad l \geq 1. \tag{16}$$

Furthermore, for any $p \geq \max(2, 2c/(c-1))$, an error bound for the truncated series is given by

$$\left| \phi(z) - \sum_{l=0}^{p} b_l \, z^l \right| < \frac{A(4e(p+c)(c+1)+c^2)}{c(c-1)} \left(\frac{1}{c}\right)^{p+1} \qquad (17)$$



z_0
R
D_1
cR
0
R
C
s
D_2

Lemma

For any complex z_0, z, *and* $\{a_k\}$, *for* $k = 0 : n$

$$\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{l=0}^{n} \left(\sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right) z^l \qquad (18)$$

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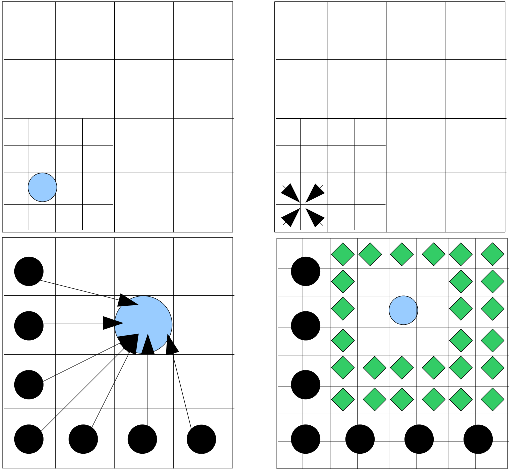
8. Add far field and near field interactions.



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2. It has been $\sim$ 2275 times cited!! (04/04/2016) *.

* Source: Web of Science.

The End