**AMSC/CMSC 661 Scientific Computing II**
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**The Fast Multipole Method**
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## The Fast Multipole Method

**References:**

Idea due to Greengard and Rokhlin.

Xiaobai Sun and Nikos P. Pitsianis, A matrix version of the fast multipole method, SIAM Review 43 (2001) 289-300.

Nail A Gumerov and Ramani Duraiswami, Fast Multipole Methods for the Helmholtz Equation in Three Dimensions (The Elsevier Electromagnetism Series)

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## What is the FMM?

In many applications, it is important to compute, for example,

- the gravitational potential arising from a distribution of masses
- electrostatic potential arising from a distribution of charges

Picture. We'll talk about charges, for definiteness.

Suppose that the charge on **source** particle $j$, which is located at position $s_j$, is $q_j$, $j = 1, \ldots, n$. Then to compute the potential $p_k$ at **target** particle $k$, located at position $t_k$, we compute

$$p_k = \sum_{j=1}^{n} \frac{q_j}{\|t_k - s_j\|^\beta}.$$

$k = 1, \ldots, m$.

For notational convenience, we take $\beta = 1$, but it really doesn't matter.

Notice that computing **all** of the potentials is just a **matrix-vector product**

$$\mathbf{p} = \mathbf{A}\mathbf{q}$$

where

$$a_{kj} = \frac{1}{\|t_k - s_j\|}.$$

The **Fast Multipole Method (FMM)** provides a fast way to **approximately** evaluate $\mathbf{A}\mathbf{q}$.

## What is the underlying idea?

$$\mathbf{p} = \mathbf{A}\mathbf{q}$$

where

$$a_{kj} = \frac{1}{\|t_k - s_j\|}.$$

- Suppose that many of the source particles were located at the same place. Then several **columns** of the matrix $\mathbf{A}$ would be identical, and we could compress the matrix to one with fewer columns by adding the corresponding elements of $\mathbf{q}$.
- Similarly, if several of the target particles were at one location, then we could delete the redundant **rows** of the matrix $\mathbf{A}$.

In either case, we end up with an equivalent problem with a smaller matrix and therefore a faster matrix-vector product.

## An approximation

The FMM is built on the idea of **approximating** the matrix-vector product by **moving** source particles that are close to each other, and far from the target, to their centroid, and doing the same with the targets.

This means that the matrix $\mathbf{A}$ is replaced by a matrix $\mathbf{A}_r$ of rank $r < m, n$, and the cost of matrix-vector product is reduced from $O(mn)$ to $O(mr + nr)$.

If the approximation is not accurate enough, a **correction** term can be computed.

All of this can be done **recursively**.

## The approximation for single clusters of sources and targets

**Theorem:** Suppose we have a set of sources, centered at $s_c$, and a set of targets, centered at $t_c$, with $\alpha < 1$ chosen so that

$$\max_j \|s_j - s_c\| + \max_k \|t_k - t_c\| \le \alpha \|t_c - t_s\|.$$

Then given any integer $p \ge 0$

$$\mathbf{A} = \mathbf{A}_r + \mathbf{A} \odot \mathbf{E}$$

where

- $\mathbf{A}_r$ has rank at most $r = (p+1)(2p+1)$.
- $\odot$ denotes the **Hadamard matrix product**

$$(\mathbf{A} \odot \mathbf{B})_{kj} = a_{kj} b_{kj}.$$

- The elements of $\mathbf{E}$ are bounded by

$$|e_{kj}| \le \frac{1+\alpha}{1-\alpha} \alpha^{p-1}.$$

**Note:** We can make this arbitrarily accurate by choosing $r$ large enough. ($r = \min(m, n)$ gives the exact result)

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## What if the sources and targets are interspersed?

Then partition them!

In 1-d, for example, divide the sources into those centered around $s_o < 0$ and those not, and divide the targets in a similar way. Then

$$\mathbf{A} = \mathbf{A}_f + \mathbf{A}_n$$

where

$$\mathbf{A}_f = \begin{bmatrix} 0 & \mathbf{A}_{o,n} \\ \mathbf{A}_{n,o} & 0 \end{bmatrix}$$

represents the **far-field interactions** and

$$\mathbf{A}_n = \begin{bmatrix} \mathbf{A}_{o,o} & 0 \\ 0 & \mathbf{A}_{n,n} \end{bmatrix}$$

represents the **near-field interactions**.

Then multiplication by $\mathbf{A}_f$ can be done by FMM.

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## The recursion

We are left with the problem of forming $\mathbf{A}_{o,o}\mathbf{q}_o$ and $\mathbf{A}_{n,n}\mathbf{q}_n$. These are two smaller problems of the same form, so we just recurse!

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## One final trick

If the original sources and targets are located at the **mesh points of a grid**, then the matrix $\mathbf{A}$ has **Toeplitz** or **block-Toeplitz** structure, and the multiplication can be done very quickly using **FFTs**.

## The work

The FMM has number of multiplications and additions proportional to $O(n \log_2 n)$ (when $n \geq m$). This is a great savings over the $O(mn)$ count of the original algorithm.

## A connection with PDEs

**Green's functions** can be interpreted as charge distributions.