

An introduction to Fast Multipole Methods

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Seminar Scientific Computing

Overview

1. Multipole methods

- Definition
- Principles
- Example: Charged particles
- Multipole expansion
- Well-separated
- Several multipole implementations

2. Fast Multipole Method

3. Another example: BEM

4. Areas of application

1. Multipole methods

Definition:

Multipole methods are methods for N-body problems, whereby “far-away” points are clustered, in order to speed up the computation.

N-body problems:

- point charges
- point vortices
- gravitational particle interaction

Multipole methods

Principles:

Multipole Methods can be used in applications where interactions must be computed.

The main idea is that the effect of all points working on all points, yields a method with $O(N^2)$ computations.

But, if points are well separated, we can deal with the “far-away” points as one point. This yields a method of $O(N)$ or $O(N \log N)$.

2. Example: charged particles

Suppose a point charge of strength q in \mathbf{x}_0 .
Then the potential in point \mathbf{x} is given by:

$$\phi_{\mathbf{x}_0}(\mathbf{x}) = -q \log(\|\mathbf{x} - \mathbf{x}_0\|)$$

Potential is a key property here, because force can be derived from it.

Further, take $x + iy = z \in \mathbb{C}$.

Then:

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

Multipole expansion

Suppose m charges of strength q_i are located in z_i with $|z_i| < r$. Then for any $z \in \mathbb{C}$ with $|z| > r$, the potential is given by

$$\phi(z) = \sum_{i=1}^m \phi_{z_i}(z) = Q \log(z) + \sum_{k=1}^{\infty} \frac{a_k}{z^k}$$

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

But, if we take a sum to p in stead of ∞ , the error will be:

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

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

Accuracy ε is a function of p :

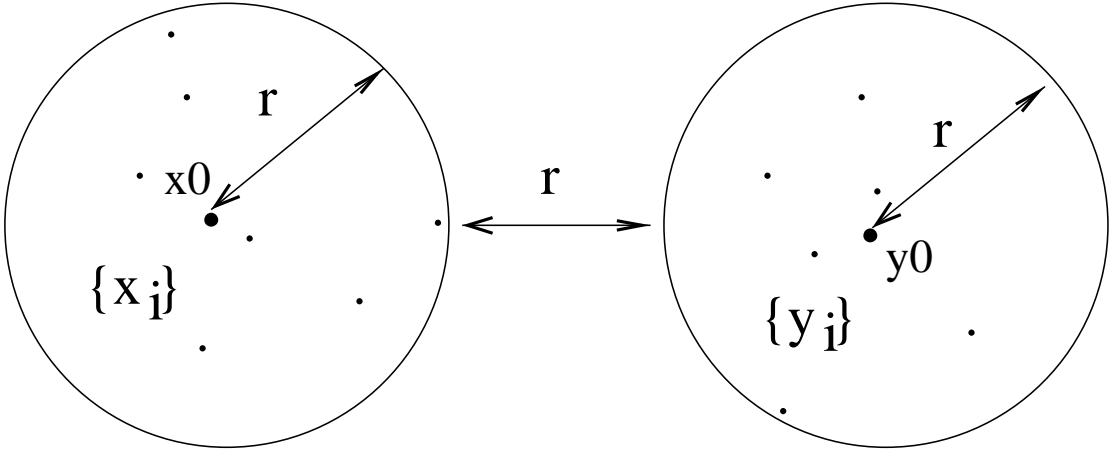
$$p = {}^c \log(\varepsilon)$$

Well-separated

The set of points $\{x_i\}$ is *well-separated* from the set $\{y_i\}$ if:

there exist points x_0 and y_0 and $r > 0$ such that:

$$\begin{aligned} |x_i - x_0| &< r && \text{for all } i = 1, \dots, m \\ |y_j - y_0| &< r && \text{for all } j = 1, \dots, n \\ |x_0 - y_0| &> 3r && \end{aligned}$$



The potential at the points y_i due to the charges at points $\{x_i\}$:

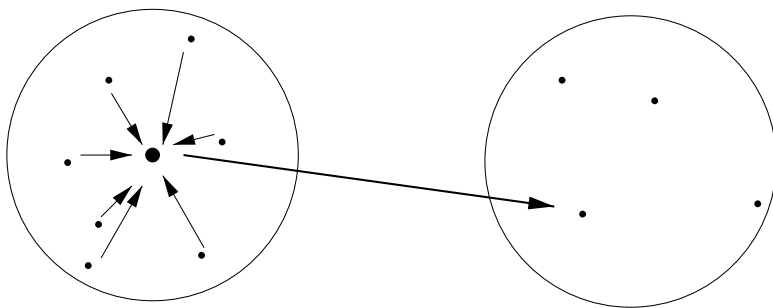
$$\sum_{i=1}^m \phi_{x_i}(y_j) \quad \text{for all } j = 1, \dots, m$$

(order nm work) can now be approximated by:

1. Calculating a p -term multipole-expansion about x_0 (which is order np work)
2. Calculating the resulting multipole expansion in points y_j :

$$\sum_{i=1}^m \phi_{x_i}(y_j) = Q \log(y_i - x_0) + \sum_{k=1}^p \frac{a_k}{|y_j - x_0|^k}$$

(which is order mp work)



Several multipole implementations

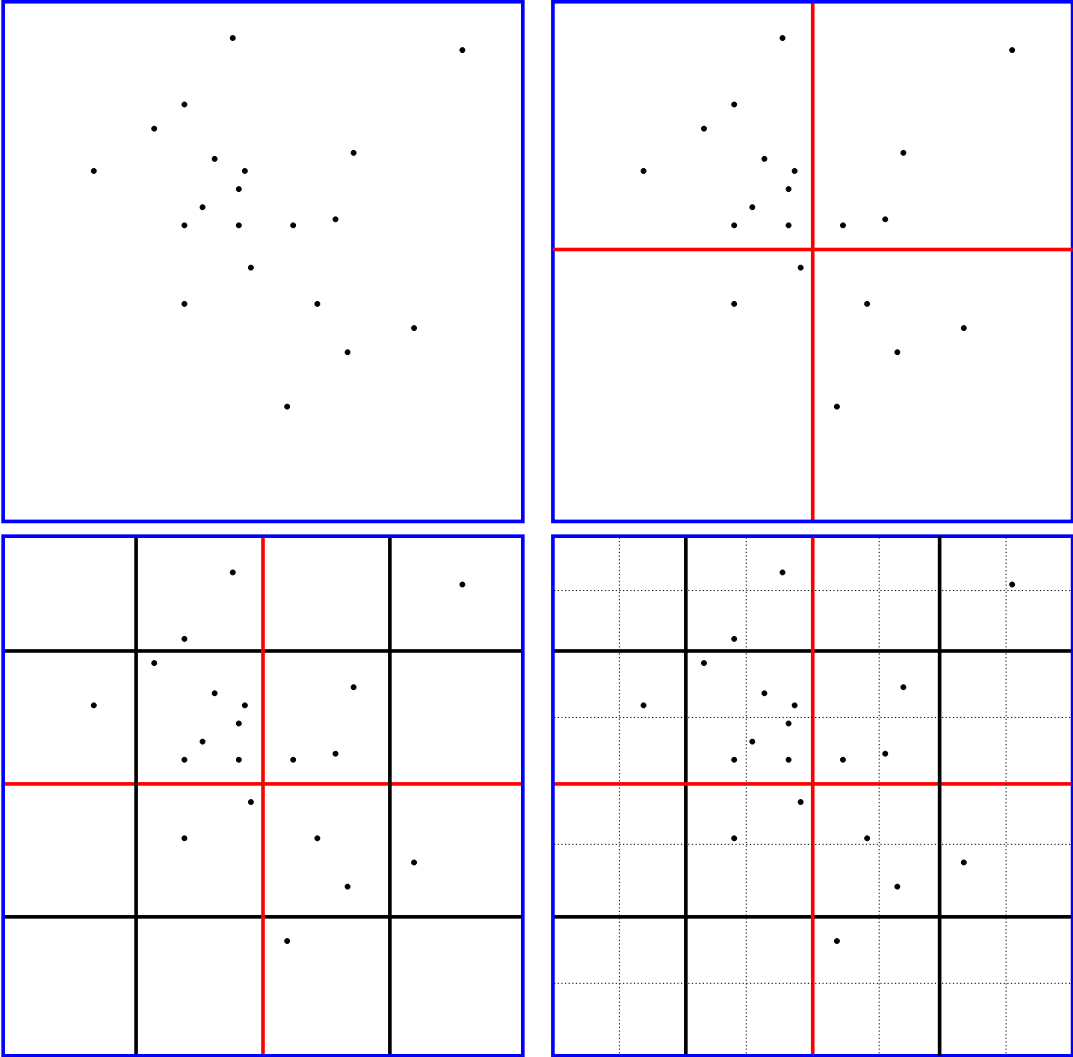
- **Fast Multipole method** [Greengard and Rokhlin]
 $O(n)$
- Tree Method [Appel, Barns and Hut]
 $O(n \log n)$
- Panel clustering method [Hackbush, Nowak]
 $O(n(\log n)^{d+2})$
- Wavelet-based methods [Beylkin, Coifman, Rokhlin] $O(n \log n)$

2. Fast Multipole Method

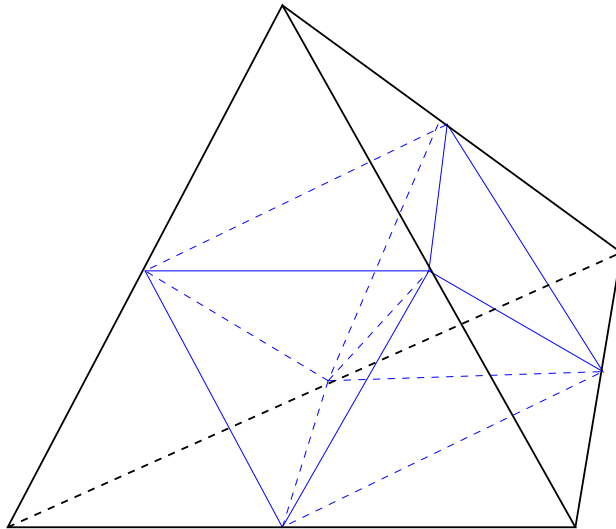
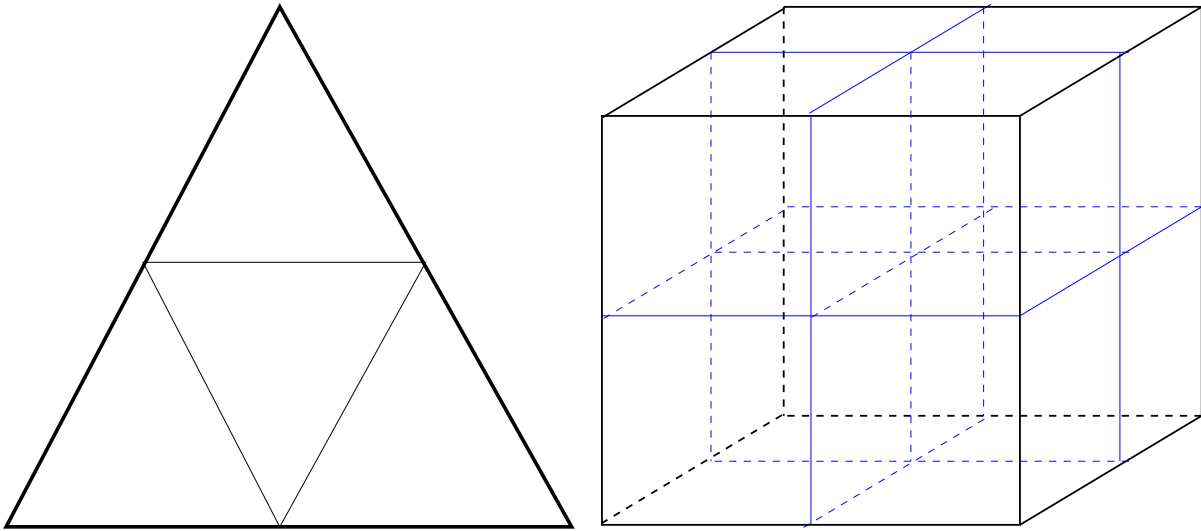
- An efficient way to implement this approximation
- An $O(n)$ method
- Region is divided such that $c = \left| \frac{z}{r} \right| = 2$
- 2D and 3D
- Global introduction (Ivo will re-address this next time)

Fast Multipole Method (cont'd)

Divide the region in 4 subregion and repeat this in several levels

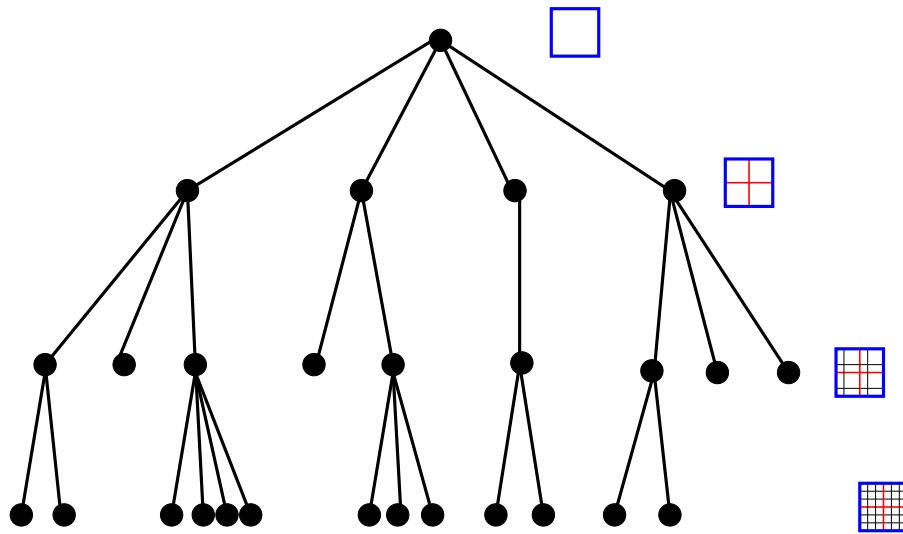


Other shapes



Fast Multipole Method (cont'd)

What we have done here, can be put in a tree:

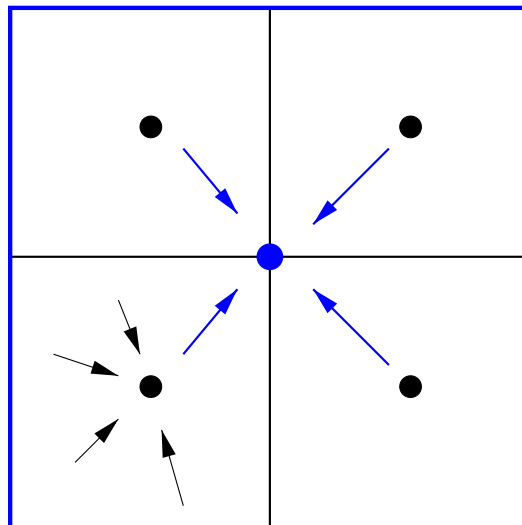


FMM consists of two parts:

1. Upward Pass
2. Downward Pass

Upward Pass (FMM)

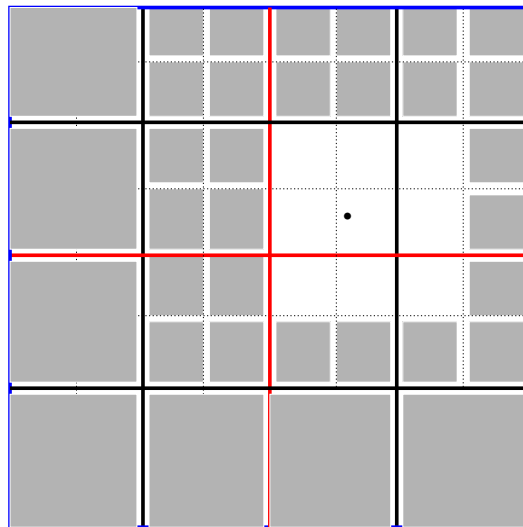
1. Calculate the multipole expansions about the centers of the cells in finest grid
2. Combining 4 finer grid centers, calculate the multipole expansion about the centers of the cells in higher grid.



Downward Pass (FMM)

Consider one particle.

1. Until finest level: Refine and calculate interaction of well-separated cells
2. Calculate the local expansion of the cells and its neighbours on finest level

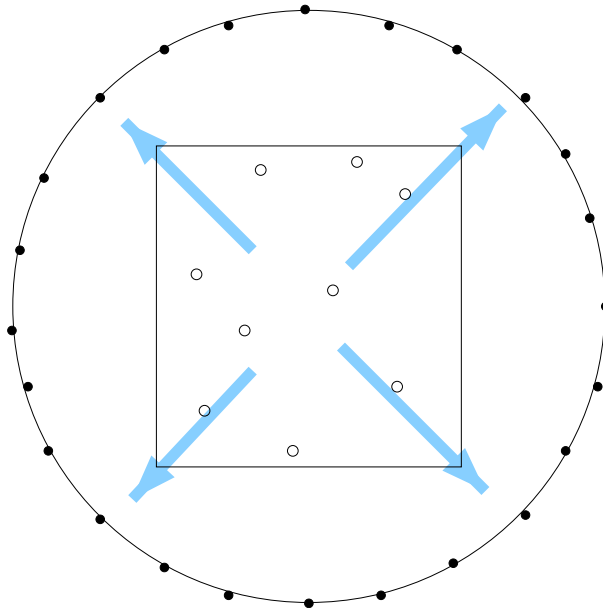


Add (1) and (2)

Be careful!

- ... in choosing the accuracy
- Is FMM really an $O(n)$ method?
At least, all steps in the algorithm are $O(n)$
- ... in choosing the level of grid refining
Depends on the number and density of the particles
- It is not necessary to use a multipole as approximation, a ring for instance can also be used.

Instead of calculating the multipole expansion about some center, it is sometimes useful to use a ring [Anderson]:



More general than point charges/vortices

Can be combined in the same way as centers
Robin Schoemaker will talk about this in his talk.

3. An other example: BEM

In many areas a BIE can arise:

$$f(x) = \int K(x, y)\varphi(y)dS$$

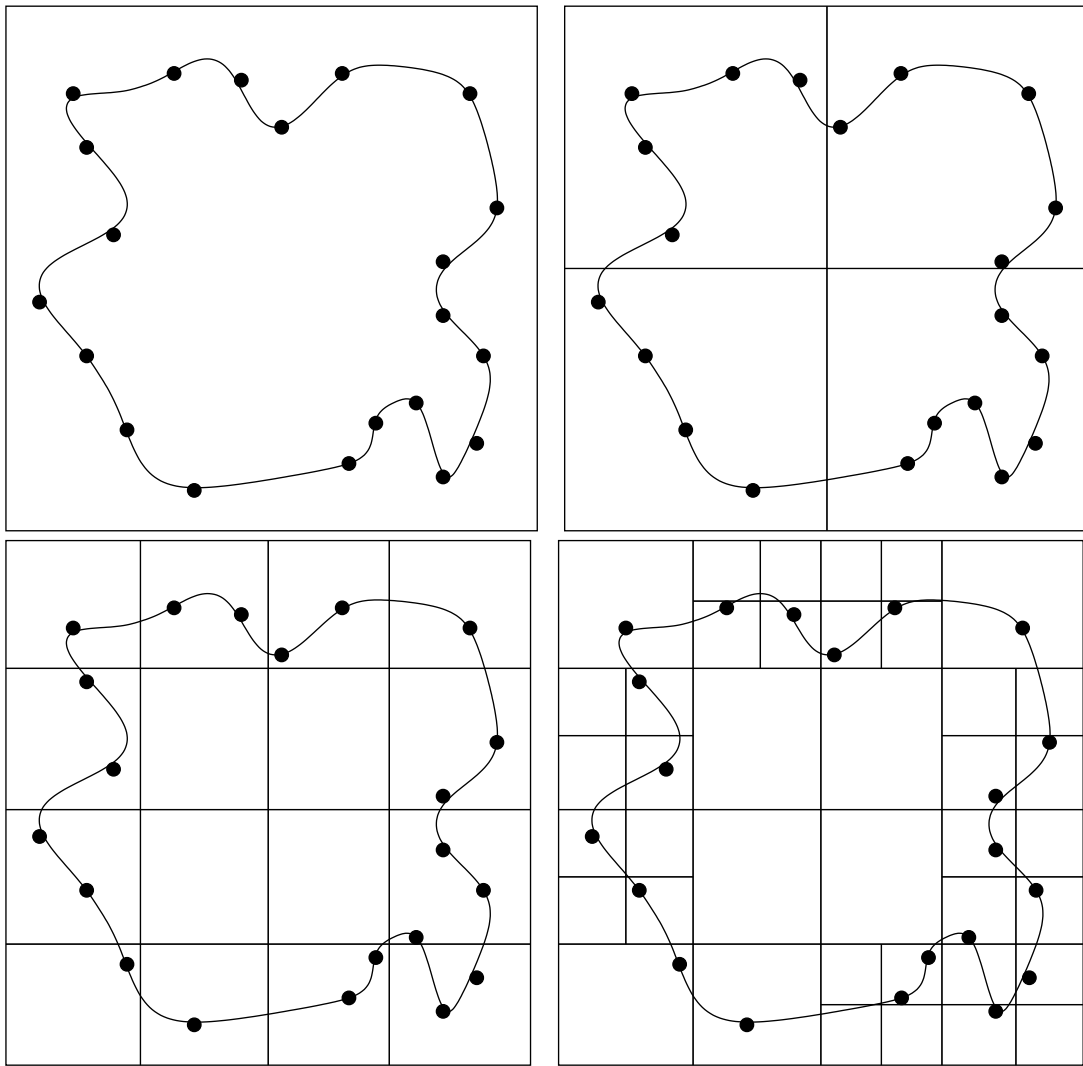
Discretize the boundaries, the unknown φ and the kernel K using a collocation method:

$$\mathbf{K}\mathbf{x} = \mathbf{f}$$

Green's function can occur in the kernel \mathbf{K} :

$$G(x, y) = \frac{e^{-jk|x-y|}}{|x-y|}$$

Green's function can be expanded and shifted.



In cases where the interaction is proportional to $\frac{1}{r}$, FMM can speed up calculations and make large and complex geometries computable.

4. Areas of application

Interaction computations in:

- Electrostatics
- Astrophysics
- Molecular dynamics
- Comp. Fluid dynamics
- Elastodynamics
- Comp. Electromagnetics
 - “Fast and efficient algorithms in computational electromagnetics” Weng Cho Chew e.a., 2001
- ... many others

Next seminar on FMM:

Ivo Severens

The FMM and an application