An implementation of the Fast Multipole Method without multipoles

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Overview

- Fast Multipole Algorithm
- Anderson’s method
  - Poisson’s formula instead of multipole expansions
- Application
\( N \)-body interactions (1)

- Particle simulations in physical systems require the evaluation of a potential function \( \phi(\mathbf{r}) \), (yielding a force field);
- These pairwise interactions are Coulombic/gravitational in nature:

\[
\phi(\mathbf{r}_j) = \sum_{i=1}^{N} q_i \log |\mathbf{r}_j - \mathbf{r}_i|, \quad j = 1, \ldots, N
\]

for a system of \( N \) charged particles in 2 dimensions with strengths \( q_i \).
If $N$ is the total number of particles involved, the temporal complexity of such a system is $O(N^2)$.
Multipole expansion

For \( m \) charges of strengths \( \{q_i, i = 1, \ldots, m\} \) located at points \( \{z_i, i = 1, \ldots, m\} \), with \( |z_i| < r \), the potential \( \phi(z) \) is approximated by the multipole expansion

\[
\phi(z) \equiv \log(z) \sum_{i=1}^{m} q_i + \sum_{k=1}^{p} \frac{a_k}{z^k} \quad \text{with} \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k},
\]

for any \( z \in \mathbb{C} \) with \( |z| > r \).
For $A = \sum_{i=1}^{m} |q_i|$ and any $p \geq 1$, 

$$\left| \phi(z) - \log(z) \sum_{i=1}^{m} q_i - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \leq \left( \frac{A}{|z/r| - 1} \right) \left( \frac{1}{|z/r|} \right)^p$$

$$\leq A \left( \frac{1}{2} \right)^p, \text{ for } |z/r| \geq 2.$$
Two sets of charges are well-separated:

\[ |x_i - x_0| < r \quad \text{for } i = 1, \ldots, m, \]
\[ |y_j - y_0| < r \quad \text{for } j = 1, \ldots, n, \]
\[ |x_0 - y_0| > 3r. \]
Example of speed-up (2)

The potential at the points \( \{y_i\} \) due to charges at \( \{x_j\} \) is computed directly via
\[
\phi_{x_i}(y_j) \quad \text{for all } j = 1, \ldots, n \quad \text{and requires } O(nm) \quad \text{computations (evaluating m fields at n points).}
\]
Example of speed-up (3)

- A $p$-term multipole expansion due to charges $q_1, \ldots, q_m$ about $x_0$ requires $O(mp)$ operations;
- Evaluating this expansion at all $\{y_i\}$: $O(np)$ operations; total: $O(mp + np)$

The $O(p)$ operations can be neglected for large $m$ and $n$, resulting in

$$O(m) + O(n) \ll O(mn).$$
Translation operators

- Shifting the centre of a multipole expansion: \texttt{M2M};
- Convert a shifted expansion into a local (Taylor) expansion: \texttt{M2L};
- Shifting the centre of a local (Taylor) expansion: \texttt{L2L}. 
\[ \phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{p} \frac{a_k}{(z - z_0)^k} \]

\[ \phi(z) = a_0 \log(z) + \sum_{l=1}^{p} \frac{b_l}{z^l} \text{ with} \]

\[ b_l = \left( \sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{a_0 z_0^l}{l} \]
\[ |z_0| > (c + 1)R \quad \text{with} \quad c > 1 \]

\[
\phi(z) = \sum_{l=0}^{p} b_l \cdot z^l
\]

with

\[
b_0 \doteq \sum_{k=1}^{p} \frac{a_k}{z_0^k} (-1)^k + a_0 \log(-z_0)
\]

\[
b_l \doteq \left( \frac{1}{z_0^l} \sum_{k=1}^{p} \frac{a_k}{z_0^k} \left( \frac{l + k - 1}{k - 1} \right) (-1)^k \right) - \frac{a_0}{l \cdot z_0^l} \quad \text{for} \quad l \geq 1
\]
Shifting a Taylor expansion via an exact translation operation with a finite number of terms:

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

$$
\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{l=0}^{n} \left( \sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right) z^l.
$$
Hierarchy: FMA (1)

Well separated cells

- Parent cell A
- Children of A
- Parent cell B
- Children of B

Connections:
- M2L
- M2M
- L2L
Levels of refinement
Anderson’s method

- FMM: $\phi(z)$ due to large numbers of particles;
- Not forced to use a multipole expansion as the ‘computational element’.

Instead use Poisson’s formula
Solving Laplace’s equation for the potential outside a disk with radius \( a \) containing ‘sources’:

\[
\phi(r, \theta) = \kappa \log(r) + \frac{1}{2\pi} \int_{0}^{2\pi} \left( \phi(a, s) - \kappa \log(a) \right) \left[ \frac{1 - \left(\frac{a}{r}\right)^2}{1 - 2\left(\frac{a}{r}\right)^2 \cos(\theta - s) + \left(\frac{a}{r}\right)^2} \right] \, ds
\]

for \( r > a \).
...and for the potential inside a hole with radius $a$ from ‘sources’ outside:

$$\phi(r, \theta) = \frac{1}{2\pi} \int_0^{2\pi} \phi(a, s) \left[ \frac{1 - \left(\frac{r}{a}\right)^2}{1 - 2\left(\frac{r}{a}\right)^2 \cos(\theta - s) + \left(\frac{r}{a}\right)^2} \right] ds$$

for $r < a$. 
Outer ring approximation (1)

Numerical representation:

With $M$ an integer and $K = 2M + 1$, we set

$$h = \frac{2\pi}{K} \text{ and } s_i = (a \cos(ih), a \sin(ih)), \quad i = 1, \ldots, K$$

$$\phi(r, \theta) = \kappa \log(r) +$$

$$\frac{1}{2\pi} \sum_{i=1}^{K} \left( \phi(a, s_i) - \kappa \log(a) \right) \left[ \frac{1 - \left(\frac{a}{r}\right)^2}{1 - 2\left(\frac{a}{r}\right)^2 \cos(\theta - s_i) + \left(\frac{a}{r}\right)^2} \right] h$$
Outer ring approximation (2)

\[ \phi(r, \theta) \]
Parent outer rings

Construction via Poisson’s formula:
Inner ring approximation

Similar as the outer ring construction:

With $M$ an integer and $K = 2M + 1$, we set

$h = \frac{2\pi}{K}$ and $s_i = (a \cos(ih), a \sin(ih))$, $i = 1, \ldots, K$:

$$\phi(r, \theta) \doteq \frac{1}{2\pi} \sum_{i=1}^{K} \phi(a, s_i) \left[ \frac{1 - \left(\frac{a}{r}\right)^2}{1 - 2\left(\frac{a}{r}\right)^2 \cos(\theta - s_i) + \left(\frac{a}{r}\right)^2} \right] h$$

for $r < a$. 
Children inner rings
Hierarchical tree

Levels of refinement
Hierarchy in action
Temporal complexity (1)

Seven steps in the hierarchy:
1. Finest level direct interactions $\propto N^2$;
2. Finest level outer ring construction $\propto KN$;
3. Finest level contribution by outer rings in well-separated area $\propto KN$;
4. Outer ring approximations $\propto K^2$;
5. Inner ring approx. by outer rings $\propto K^2$;
6. Inner ring approx. by inner ring parent $\propto K^2$;
7. Finest level contribution by inner ring parent $\propto KN$. 
Temporal complexity (2)

- Total operation count depends on $I_f$, $N$, and $K$; with $K \ll N$ and $I_f = f(N)$.
- For large $I_f$ this leads to:

\[
\text{Complexity} \sim \alpha 4^{-I_f} N^2 + \beta K N + \gamma 4^{I_f} K^2
\]

with $\alpha, \beta, \gamma$, and $K$ of order $O(10)$ for a uniform distribution of particles, resulting in
Temporal complexity (3)

an operation count linear in \( N \)

Uniform distribution

Non-uniform distribution
Numerical method for simulating:

- 2D, inviscid, incompressible vortex flows;
- Patches of uniform vorticity;
- Velocity field determined by the evolution of the contour bounding the patch:

\[
\mathbf{u}(\mathbf{r}, t) = \oint_{C(t)} \ln | \mathbf{r} - \mathbf{r}' | \, d\mathbf{r}'.
\]
Contour dynamics (2)
An $O(N^2)$ method
Contour dynamics (4)

- **Simple case**: $N = \mathcal{O}(10^2)$:

- **Hard case**: $N = \mathcal{O}(10^4)$:
Apply Anderson’s method

Instead of point sources, use source distributions like vorticity:
Accuracy of Poisson kernel (1)

Kernel is very inaccurate for \( r \to a \):

\[
\phi(r, \theta) = \frac{1}{2\pi} \sum_{i=1}^{K} \phi(a, s_i) \left[ \frac{1 - (\frac{a}{r})^2}{1 - 2(\frac{a}{r})^2 \cos(\theta - s_i) + (\frac{a}{r})^2} \right] h
\]

Accuracy of Poisson kernel (2)

Advantages of AM/HEM

• Not only point sources!
• Operations for constructing and combining elements are easy to formulate: only function evaluation;
• These operations are almost identical in 2 and 3 dimensions (not discussed);
• HEM more accurate than AM;
• \( O(N) \).