A FAST MULTIPOLE METHOD TO EVALUATE THE SELF-INTERACTION OF POINTS

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1. Introduction

In this paper, I discussed an algorithm of complexity $O(N^{4/3})$ for the evaluation of the potential field of large-scale ensembles of particles with Laplacian kernel.

Suppose that a point with charge q is located at $z \in \mathbb{R}^2$, then the potential due to this charge is described by $\phi(z) = q * \ln(\frac{1}{|z-y|})$. If we identify $\mathbb{R}^2$ with $\mathbb{C}$ in the usual way, then $\phi(z) = Re(q * \ln(\frac{1}{|z-y|}))$. So the direct evaluation requires order $O(N^2)$ operations.

2. Analytic Tools

Following are two theorems used to obtain the local expansion of potential of well separated particles:

(1) Theorem 1{Multipole expansion}

Suppose that m charges of strengths $q_i, i = 1, ..., m$ are located at points $z_i, i = 1, ..., m$, all of which are located inside the circle D of radius R with center at z_0. Then for any $z \in \mathbb{C}$ with $|z - z_0| > R$, the potential $\phi(z)$ is given by

$$\phi(z) = c_0 * \ln(z - z_0) + \sum_{n=1}^{\infty} \frac{c_n}{(z-z_0)^n}$$

with $c_0 = \sum q_i$ and $c_m = \sum \frac{1}{m} * q_i * (z - z_0)^m$.

(2) Theorem 2 {Multipole to local}:

Suppose that

$$\phi(z) = c_0 * \ln(z - z_0) + \sum_{n=1}^{\infty} \frac{c_n}{(z-z_0)^n}$$

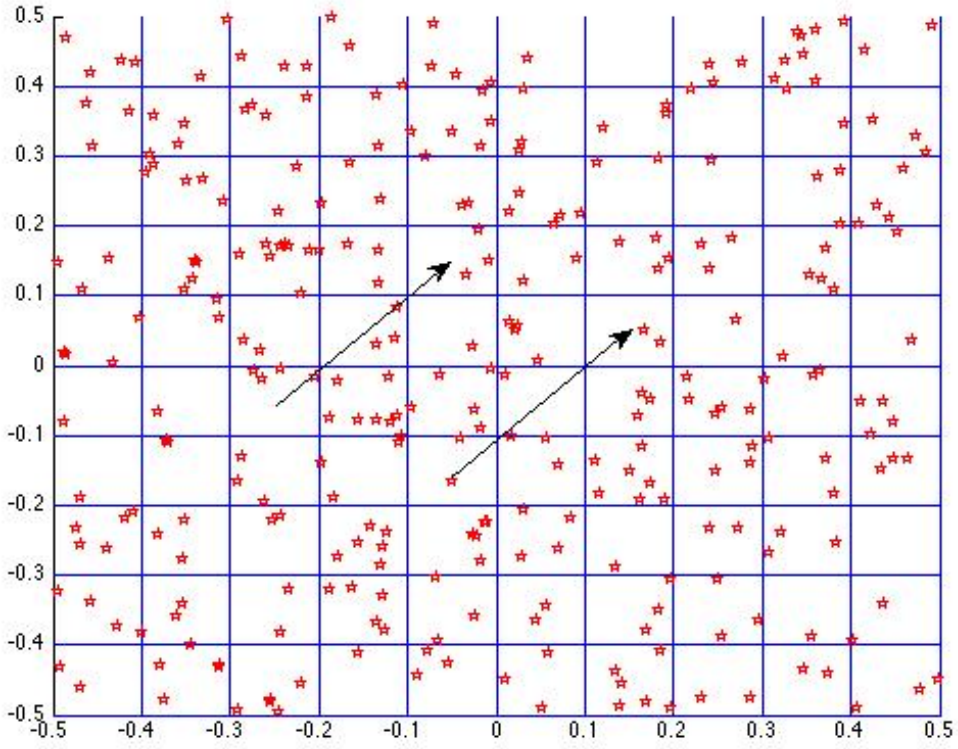
is a multipole expansion of the potential due to a set of m charges of strengths $q_1, q_2, ..., q_m$, all of which are located inside the circle D. If $|z_0| \geq 2R$ then for z with $|z| < R$,

$$\phi(z) = \sum_{m=0}^{\infty} a_m * z^m$$

with $a_0 = \ln \frac{1}{z_0} * c_0 + \sum_{n=1}^{\infty} (-1)^n * z_0^{-n} * c_n$, and $a_m = \frac{1}{m} * z_0^{-m} * c_0 + \sum_{n=1}^{\infty} (-1)^n * \binom{n+m-1}{m} * \frac{1}{m} * z_0^{-n-m} * c_n$.

3. General Strategy

The general strategy consists of clustering particles at a fixed spatial length and computing interactions between well-separated clusters using localized multipole expansions. The interactions between nearby clusters are computed directly.



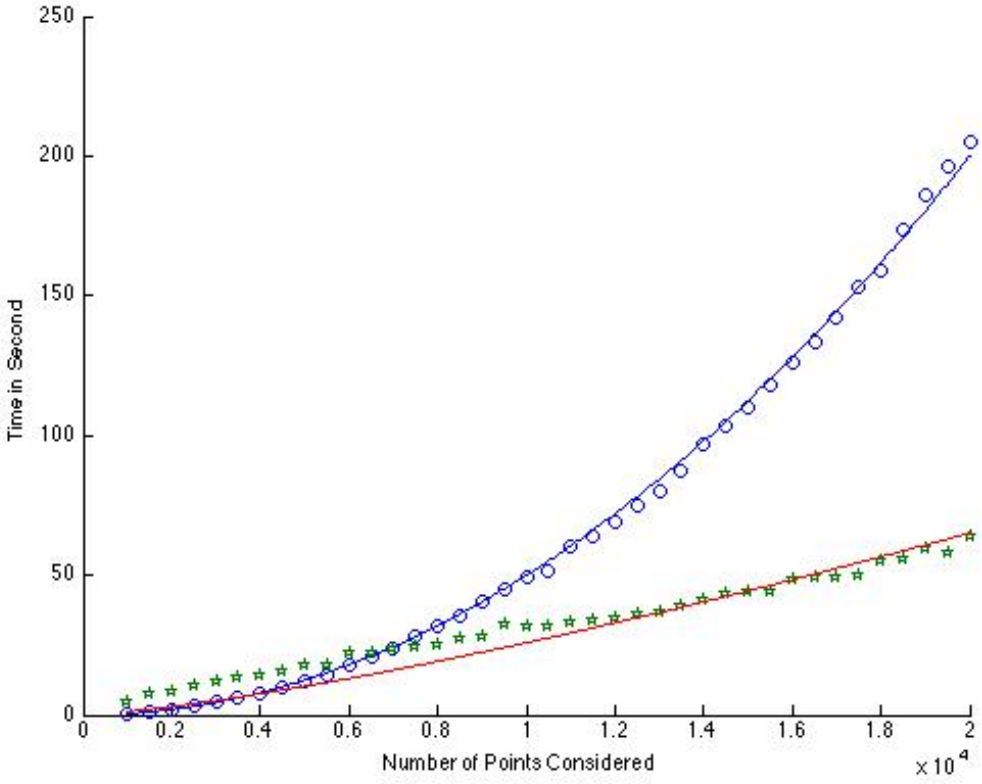
In the above picture, there are 300 points and 10^2 computation boxes. Those arrows are there to illustrate that the displacement vectors between boxes where the heads of arrows are and boxes with the tails of the arrows are the same.

4. Description of the algorithm

(1) let $m = ceil(N^{1/3})$ and divide the computation area into m^2 boxes. Choose $p = 15$, the number of terms in all sums.
(2) For each box (i, j), compute $C_{i,j}$.

(3) Instead of compute $A_{i,j}$ by summing over all boxes, build the transaction matrix $T : C- > A$, which can speed up the codes a lot.
(4) evaluate local expansions at all boxes.
(5) Finally, compute potential due to nearest neighbors directly. Add direct and well-separated terms together.

5. Numerical results



The red line is $y(x) = 1.2 * 10^{-4} * x^{4/3}$;The blue line is $y(x) = 5 * 10^{-7} * x^2$; $N = 10^6$, $T = 4932s$.
The errors for $N \in [10^3, 2 * 10^4]$ are of order $O(10^{-7})$, due to the fixed choice of $P = 15$.

6. The Bibliography

(1) L. GREENGARD and V. ROKHLIN, Journel of Computational Physics 73, 325-348 (1987).

(2) J. CARRIER, L. GREENGARD and V. ROKHLIN, SIAM J.SCI. STAT. COMPUT. Vol 9, No. 4, (July 1988)