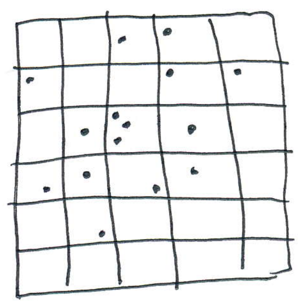
Fast multipole method

Based on classic paper: L. Greengard and V. Rokhlin, A fast algorithm for particle simulations, J. Comput. Phys., 73, 325–348 (1987). The last paper on Trefethen's list of 13 classic papers in applied mathematics.

Motivation: wanted to simulate systems of many particles that have Coulombic or gravitational interactions. Simple approach: N particles gives $O(N^2)$ work. Impractical for large systems.



One previously known approach: "particle-in-cell" method:

- interpolate source density to a mesh
- solve Poisson equation on mesh
- compute potential/force at particle positions via interpolation

If there are M grid points, then G+R say work is $O(N+M \lg M)$, based on solving Poisson via the FFT. Could do better with multigrid, $O(N+M)$ but still involves messy interpolation, and limited resolution if particles are clustered together.

For gravitation, consider particles of mass m_i at positions $\underline{x}_i$. The N-body problem requires evaluating

Let $r_{ij} = \|\underline{x}_i - \underline{x}_j\|_2$

$$\Phi(\underline{x}_j) = \sum_{\substack{i=1 \\ i\neq j}}^{N} \frac{m_i}{r_{ij}} \qquad\qquad \underline{E}(\underline{x}_j) = \sum_{\substack{i=1 \\ i\neq j}}^{N} m_i \frac{\underline{x}_j - \underline{x}_i}{r_{ij}^3}$$

Potential $\qquad\qquad$ Gravitational field.

Could also evaluate at a set of arbitrary points $\underline{y}_j$.

$$\Phi(\underline{y}_j) = \sum_{i=1}^{N} \frac{m_i}{\|\underline{x}_i - \underline{y}_j\|_2}$$

Many possible variations.

- Acoustic scattering $\Phi(\underline{x}_j) = \sum_{\substack{i=1 \\ i\neq j}}^{N} w_i \frac{e^{ikr_{ij}}}{r_{ij}}$

- Continuous mass distribution $\underline{E}(\underline{y}) = -\int m(\underline{x}) \frac{\underline{y}-\underline{x}}{|\underline{y}-\underline{x}|^3} d\underline{x}$

- Heat diffusion from point sources

$$u(\underline{x}_j) = \frac{1}{\sqrt{(4\pi T)^3}} \sum_{i=1}^{N} w_i e^{\frac{-r_{ij}^2}{4T}} \qquad u_t = \Delta u$$

$$\boxed{\text{All of these involve sums over kernels:} \quad \underline{u}(\underline{x}) = \int K(\underline{x},\underline{y}) w(\underline{y}) d\underline{y}, \quad \underline{u}(\underline{x}) = \sum_{i=1}^{N} w_i K(\underline{x},\underline{y}_i).}$$

Can see why it would be expensive. Suppose that the kernel can be expressed as a finite series

$$K(\underline{x},\underline{y}) = \sum_{k=1}^{p} \phi_k(\underline{x}) \psi_k(\underline{y}).$$

Then if one computes moments

$$A_k = \sum_{i=1}^{N} w_i \psi_k(\underline{y}_i)$$

the potential becomes easy to evaluate with

$$\underline{u}(\underline{x}) = \sum_{k=1}^{p} A_k \phi_k(\underline{x})$$

This is the key idea behind the fast multipole method and related techniques.

FMM in two dimensions

Consider point charge at $\underline{x}_0 = (x_0, y_0)$. The potentials is

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

And the electric field is

$$\underline{E}_{x_0}(\underline{x}) = \frac{\underline{x} - \underline{x}_0}{\|\underline{x} - \underline{x}_0\|}$$

Potential is harmonic away from $\underline{x}_0$ and satisfies

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.$$

For every harmonic function u there exists an analytic function w such that $u = \mathrm{Re}(w)$. Have

$$\phi_{\underline{x}_0}(\underline{x}) = \mathrm{Re}(-\log(z - z_0))$$

Can also write electric field as $\underline{E}(\underline{x}) = \nabla u = (u_x, u_y) = (\mathrm{Re}(w'), -\mathrm{Im}(w'))$

Consider point charge of strength q, located at z_0.

$$\phi_{z_0}(z) = q \log(z - z_0) = q\left[\log z + \log 1 - \frac{z_0}{z}\right]$$

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

Suppose m charges of strengths $\{q_i, i = 1, \ldots, m\}$ are located at points $\{z_i, i = 1, \ldots, m\}$ with $|z_i| < r$, Then for any z with $|z| > r$,

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

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

For $p \geq 1$,

$$\left|\phi(z) - Q \log z - \sum_{k=1}^{p} \frac{a_k}{z^k}\right| \leq \frac{1}{p+1} \alpha \left|\frac{r}{z}\right|^{p+1}$$

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

$$c = \left|\frac{z}{r}\right| \qquad A = \sum_{i=1}^{m} |q_i| \qquad \alpha = \frac{A}{1 - \left|\frac{r}{z}\right|}.$$

To prove, note that

$$\left| \phi(z) - Q \log z - \sum_{k=1}^{p} \frac{a_k}{z^k} \right| \le \left| \sum_{k=p+1}^{\infty} \frac{a_k}{z^k} \right|.$$

$$\le A \sum_{k=p+1}^{\infty} \frac{r^k}{k|z|^k}$$

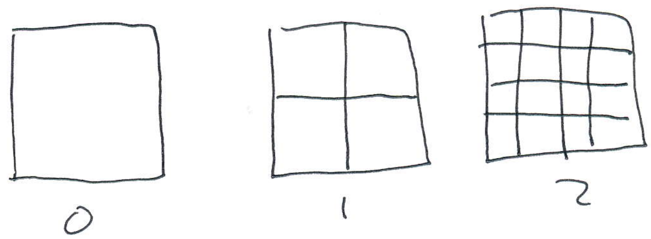
$$\le \frac{A}{p+1} \sum_{k=p+1}^{\infty} \left|\frac{r}{z}\right|^k$$

$p = \log_2 \frac{1}{\varepsilon}$.

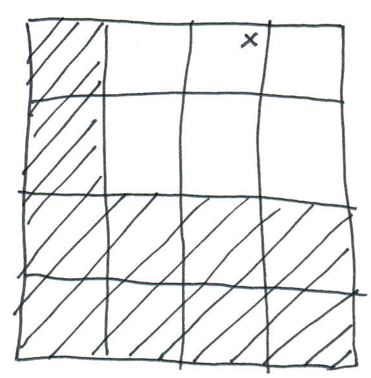
$$= \frac{\alpha}{p+1} \left|\frac{r}{z}\right|^{p+1} = \left(\frac{A}{p+1}\right)\left(\frac{1}{c-1}\right)\left(\frac{1}{c}\right)^p$$

N log N algorithm

Grid hierarchy.



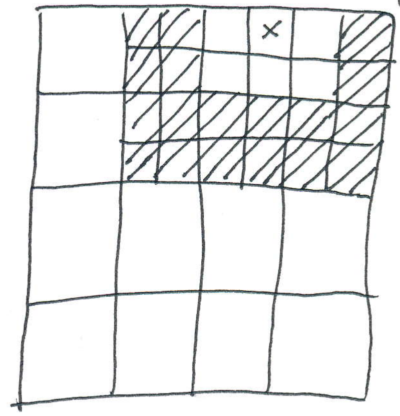
- Two boxes are near neighbors if they ar at the same level and share a boundary point. A box is an NN of itself.
- Two boxes are well separated if they are at the same refinement level and are not near neighbors
- Each box has an interaction list, consisting of the children of the near neighbors of is parent that are well-separated from i.



Look at level 2: some boxes will be well separated. They can be dealt with using multipole expansions.

Now look at level 3. Cand deal with other boxes using multipole expansions.

Use $\log N$ levels of refinement.



Work done to make multipole expansions is Np.

Up to $27Np$ operations to evaluate expansions in up to 27 boxes at each level.

$\sim 28 Np \log N$ $\qquad O(N \log N)$.

How to do better, and obtain $O(N)$?

Translation of a multipole expansion

Suppose that

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

is a multipole expansion of the potential due to a set of m charges of strengths $q_1, q_2, \dots, q_m$ within the circle D of radius R, centered at z_0. Then for z outside D_1, a circle of radius $(R+|z_0|)$ and center at the origin,

$$\phi(z) = a_0 \log z + \sum_{k=1}^{\infty} b_l z^{-l}$$

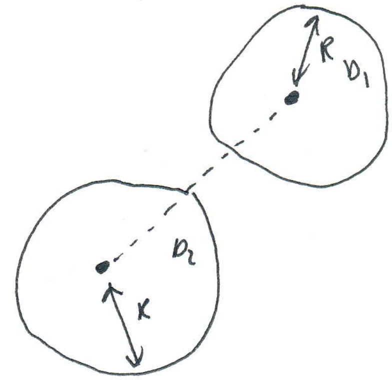
$$b_l = \frac{-a_0 z_0^l}{l} + \sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1}.$$

For any $p \geq 1$

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

Error bound follows from the uniqueness of the multipole expansion. One obtained indirectly must match one obtained directly.

Conversion of a multipole expansion into a local expansion



Assume $|z_0| > (c+1)R$, $c > 1$.

Original multipole expansion converges in D_2

Inside D_2, potential due to the charges is given by a power series

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

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

$$b_l = \frac{-a_0}{l z_0^l} + \frac{1}{z_0^l} \sum_{k=1}^{\infty} \frac{a_k}{z_0^k} \binom{l+k-1}{k-1} (-1)^k$$

Error bound

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

Use expressions

$$\log(z-z_0) = \log\left(-z_0\left(1-\frac{z}{z_0}\right)\right)$$

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

$$(z-z_0)^{-k} = \left(\frac{-1}{z_0}\right)^k \sum_{l=0}^{\infty} \binom{l+k-1}{k-1} \left(\frac{z}{z_0}\right)^l$$

- Can combine multipole expansions at four children into one
- Can ~~combine~~ transmit a local expansion of the field to four children.