Lecture 5

Last time: The FMM:

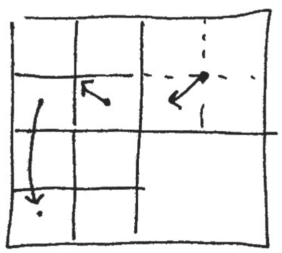
M2M, L2L, M2L operators

Op count: (per box) (n boxes)

M2M: $O(p^4)$

M2L: $O(189p^4)$

L2L: $O(8p^4)$



Option 1 for decreasing op count:

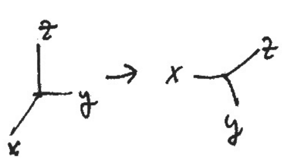
Point & Shoot

(1) Rotate O_ℓ^m, I_ℓ^m expansion to point $\theta = 0$ at the new origin $(O(p^3))$

(2) Translate: $O(p^3)$

(3) Rotate back: $O(p^3)$

How to rotate a spherical harmonic expansion?



$\Leftrightarrow \quad r, \theta, \varphi \rightarrow r, \theta', \varphi'$ $\qquad$ r is unchanged!

We need to find the map from

$$M_{lm} \to M'_{lm}$$

$$\sum_{l=0}^{p} \sum_{m=-l}^{l} M_{lm} O_l^m = \sum_{l,m} M_{lm} C_{lm} \frac{1}{r^{l+1}} \cancel{Y_l^m(\theta,\varphi)} P_l^m(\cos\theta)\, e^{im\varphi}$$

$$= \sum_{l,n} M'_{lm} C_{lm} \frac{1}{r^{l+1}} P_l^m(\cos\theta')\, e^{im\varphi'}$$

These expansions must be exact.

Ex: Rotate about z-axis.

$$\Rightarrow \varphi' = \varphi + \beta$$

$$e^{im\varphi} = e^{im\varphi'} - e^{im\beta}$$

$$\Rightarrow e^{im\varphi'} = e^{im\beta} e^{im\varphi}$$

$$\Rightarrow M'_{lm} = M_{lm} e^{im\varphi} \qquad (O(p^2))$$

$(R_z(\beta))$

Ex: Rotate about y-axis. (see quantum mechanics lit.)

$$\Rightarrow M'_{lm} = \sum_{m'=-l}^{l} R(l,m,m',\alpha) M_l^{m'} \qquad (\text{preserves } \theta)$$

$O(p^3)$ application

$(R_y(\alpha))$

Translation are simpler as well:

<u>M2M</u> If $\phi(\vec{x}-\vec{x}') = \phi(\rho,\alpha,\beta)$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} M'_{lm}\, O_l^m(\rho,\alpha,\beta)$$

then for $\|\vec{x}\| > D$ (enclosing disk) we have..

$$\phi(\vec{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} M_{lm}\, O_l^m(r,\theta,\varphi)$$

with $$M_{lm} = \sum_{l'=0}^{l} \sum_{m'=-l'}^{l'} T_{lm,l'm'}\, M'_{l-l',m-m'}\, r'^{\,l'}\, Y_{l'}^{-m'}(\theta',\varphi')$$

<u>If</u> $\vec{x}'$ is located along the z-axis, then $\theta' = 0$. (or π).

$$\Rightarrow \quad M_{lm} = \sum_{l'=0}^{l} \sum_{m'} T_{lm,l'm'}\, M'_{l-l',m-m'}\, r'^{\,l'}\, Y_{l'}^{-m'}(0,\varphi')$$

If $\sum_{lm} M'_{lm}\, C_{lm}\, O_l^m(r',\theta',\varphi') = \sum M'_{lm}\, C_{lm}\, O_l^m(r',\theta',\varphi)$

<u>exactly</u>, then in particular it should hold for any φ, including $\varphi = 0$ (also, at $\theta = 0$, φ doesn't mean anything)

$\Rightarrow$ all m modes are mapped similarly (set $m' = 0$)

$\Rightarrow$ ~~We only need to map the coefficients.~~

$$\Rightarrow \quad M_{lm} = \sum_{l'=0}^{l} M'_{l-l',m}\, r'^{\,l'}\, Y_{l'}^{0}(0,0)$$

$O(p^2 \times p) = O(p^3)$

So, the overall translation is performed as

$$\tilde{T}_{M2M} = R_z(-\beta)\, R_y(-\alpha)\, \tilde{T}^{z}_{M2M}(r')\, R_y(\alpha)\, R_z(\beta)$$

Do <u>not</u> form this matrix, rather apply each piece separately: each term is <u>sparse</u>, but we know that $\tilde{T}_{M2M}$ is <u>not</u> → no reason for a product of sparse matrices to be sparse.

Similar formulas for each of $\tilde{T}_{M2L}$, $\tilde{T}_{L2L}$.

Can we do better?

<u>Idea one</u>: all multipole translations are <u>convolutional</u> in nature. ⇒ Use FFT to accelerate.

Aside: Discrete convolution theorem:

$$q_k = \sum_j f_{k-j}\, g_j$$

$$= F^{-1}\big(F(f) \cdot F(g) \big)$$

up to zero-padding, this is an <u>exact</u> <u>discrete</u> statement.

Observation In 3D, this is a double convolution in l and m, $\Rightarrow$ 2D FFT.

~~For small p~~ This reduces the computation from $O(p^4) \to O(p^2 \log p)$, decent improvement for large p.

<u>Idea Two</u> <u>Translate</u> in Fourier space.

do <u>one</u> FFT of multipole coefficients on the first level, then perform upward pass in Fourier space: coefficients are in the correct basis already, merely <u>add them</u>.

~~Th~~ Both of these require careful analysis and scaling of the multipole translation coefficients (i.e. for small boxes, r^l is <u>very</u> small, so scale with the box size)

(see tech report 602)

Idea Three Plane Wave Expansions.

A "plane wave" is merely a phrase used to describe a particular representation of a potential in the exponential basis:

$$\frac{1}{\|\vec{x}-\vec{x}'\|} = \frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}$$

$$= \int_0^\infty e^{-\lambda|z-z'|} J_0\Big(\lambda \underbrace{\sqrt{(x-x')^2+(y-y')^2}}_{\text{in polar coordinates}}\Big)\, d\lambda$$

~~and in~~

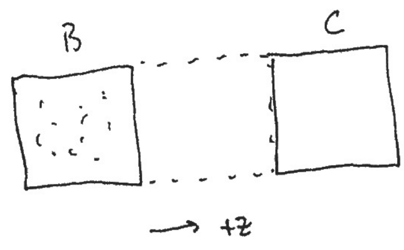
$$= \frac{1}{2\pi}\int_0^\infty e^{-\lambda|z-z'|} \int_0^{2\pi} e^{i\lambda\left((x-x')\cos\alpha + (y-y')\sin\alpha\right)}\, d\alpha\, d\lambda$$

well-known integral representation of J_0.

~~For a unit box~~ Given a quadrature rule $(w_{jk}, \alpha_j, \lambda_k)$,

we have
$$\frac{1}{\|\vec{x}-\vec{x}'\|} = \frac{1}{2\pi}\sum_{j,k} w_{jk}\, e^{-\lambda_k|z-z'|}\, e^{i\lambda_k(x-x')\cos\alpha_j}\, e^{i\lambda_k(y-y')\sin\alpha_j}$$

So Points → exponential → shift → exponential looks like:



$$\phi(\overset{\vec{x}}{\cancel{P}}) = \sum_{l=1}^{N} \frac{q_l}{\|\vec{x}-\vec{x}'_l\|}$$

$$= \sum_{l=1}^{N} q_l \frac{1}{2\pi} \int_0^{\infty} e^{-\lambda(z-z'_l)} \int_0^{2\pi} e^{i\lambda\left((x-x'_l)\cos\alpha + (y-y'_l)\sin\alpha\right)} \, d\alpha \, d\lambda$$

$\rightarrow$ discretize

$$= \frac{1}{2\pi}\sum_{l=1}^{N} q_l \sum_{j,k} w_{jk} e^{-\lambda_k(z-z'_l)} e^{i\lambda_k(x-x'_l)\cos\alpha_j} e^{i\lambda_k(y-y'_l)\sin\alpha_j}$$

$$= \sum_{j,k} V^B_{jk} e^{-\lambda_k z} e^{i\lambda_k x\cos\alpha_j} e^{i\lambda_k y\sin\alpha_j}$$

roughly $O(p^2)$ basis functions $\| \; S_{Exp}$

with $$V^B_{jk} = \frac{1}{2\pi}\sum_{l=1}^{N} q_l e^{\lambda_k z'_l} e^{-i\lambda_k x'_l\cos\alpha_j} e^{-i\lambda_k y'_l\sin\alpha_j}$$

to shift, mean to center the expansion about the center of the new box, ~~with~~ C with center x_0, y_0, z_0:

$$\phi(\vec{x}) = \sum_{j,k} V^B_{jk} e^{-\lambda_k(z_0-z_0)} e^{i\lambda_k(x_0-x_0)\cos\alpha_j} e^{i\lambda_k(y_0-y_0)\sin\alpha_j}$$
$$\times e^{-\lambda_k z'} e^{i\lambda_k x\cos\alpha_j} e^{i\lambda_k y\sin\alpha_j}$$

$$= \sum_{j,k} \tilde{V}^C_{jk} e^{-\lambda_k(z-z_0)} e^{i\lambda_k(x-x_0)\cos\alpha_j} e^{i\lambda_k(y-y_0)\sin\alpha_j}$$

$$\tilde{V}^C_{jk} \doteq V^B_{jk} \times E_{jk}(\vec{x}_0)$$

(diagonal! $S_{Exp} = O(p^2)$)