Lecture 6

Last time:

accelerated translation operators.

- point and shoot
  - rotate
  - translate
  - rotate back

- ~~expone~~ diagonal plane wave representation.

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

$$= \sum_{j,k} w_{j,k} \, e^{-\lambda \cdots} \, e^{i \cdots}$$

"Translation" means re-centering about a box. $\Rightarrow$ only need to scale $w_{j,k}$ by exponentials.

Points to Exponentials is not the common operation.

MP to Exponentials is.

Recall:
$$\frac{Y_l^{\pm m}(\theta,\varphi)}{r^{l+1}} = A_{lm}\left(\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y}\right)^m \left(\frac{\partial}{\partial z}\right)^{l-m} \frac{1}{\|\vec{x}\|}$$

Usually we will ~~not~~ map from points to exponentials, but from multipole expansions to exponentials:

Recall: since

$$\frac{Y_l^{\pm m}(\theta,\varphi)}{r^{l+1}} = A_{lm}\left(\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y}\right)^m \left(\frac{\partial}{\partial z}\right)^{l-m} \frac{1}{\|\vec{x}\|}$$

for $m \geq 0$

(2)

we have that in terms of plane waves: (for $z > 0$

$$\frac{Y_l^{\pm m}(\theta,\varphi)}{r^{l+1}} = A_{lm}(\ )^m(\ )^{l-m}\frac{1}{2\pi}\int_0^\infty e^{-\lambda z}\int_0^{2\pi} e^{i\lambda(x\cos\alpha + y\sin\alpha)}\,d\alpha\,d\lambda$$

$$= A_{lm}\frac{1}{2\pi}\int_0^\infty (-1)^{l-m}\lambda^{l-m} e^{-\lambda z}\int_0^{2\pi}(i\lambda)^m(\cos\alpha \pm i\sin\alpha)^m e^{i\lambda(\ )}\,d\alpha\,d\lambda$$

$$= A_{lm}\frac{1}{2\pi}(-1)^{l-m}(i)^m\int_0^\infty \lambda^l e^{-\lambda z}\int_0^{2\pi} e^{\pm im\alpha} e^{i\lambda(x\cos\alpha + y\sin\alpha)}\,d\alpha\,d\lambda$$

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

$$\phi(\vec{x}) = \sum_{j,k} V_{jk}\, e^{-\lambda_k z}\, e^{i\lambda_k(x\cos\alpha_j + y\sin\alpha_j)}$$

with $V_{jk} = W_{jk}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(i)^m(-1)^{l-m}}{2\pi}\lambda_k^l e^{\pm im\alpha_j} M_{lm}$

$O(p^2)$ Why!

$O(p^2)$

$\Rightarrow O(p^4)$ computation naively...

For a p^{th} order expansion, interchanging the sums since

$$\sum_{l=0}^{p}\sum_{m=-l}^{l} = \sum_{m=-p}^{p}\sum_{l=|m|}^{p}$$

we have:

~~Exp2M~~

M2Exp

$$V_{jk} = \frac{W_{jk}}{2\pi}\sum_{m=-p}^{p} (-i)^m e^{\pm i m \alpha_j} \underbrace{\sum_{l=|m|}^{p} (-1)^l \lambda_k^l M_{lm}}$$

For each $k \sim O(p)$ m, $2p+1$ of them, do a sum with $\leq p$ terms.
$\Rightarrow O(p^3)$

do a sum with $2p+1$ terms for each α_j $\Rightarrow O(p^2)$

~~for each jk, $O(p^2)$~~

via FFT? still dominated by $O(p^3)$ term.

and likewise, the Exp2L operator is given by a similar expression.

So we can factorize T_{M2L} as

$$T_{M2L} = C_{X2L} D_{BC} C_{M2X}.$$

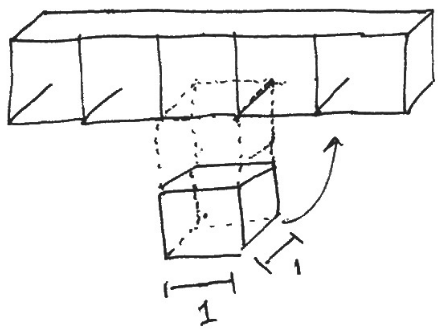
The cost of one is $O(p^3)$, can we ammortize this? Accumulate the PW expansions, then apply C_{X2L}

Quadrature ~~and~~ for discretization

We need to accurately evaluate the integral

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

For translating <u>up</u> in $+z$ direction:



We <u>know</u> for a unit box: that

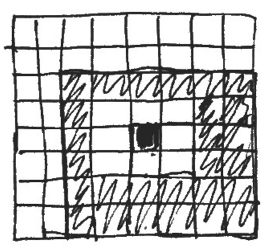
for some source $\vec{x}'$ and target $\vec{x}$

$z - z' \in (1,4)$

$|x - x'| \in (0,4)$

$\Rightarrow x - x' \in (-4,4)$

$y - y' \in (-4,4)$



We want the most efficient and accurate quadrature rule for all the range of these parameters:

α integral: trapezoidal rule

λ integral: For each α_j in design a Generalized Gaussian rule.

Quadrature Rules for Diagonal Forms:

For $z \in (1,4)$

$x \in (-4,4)$

$y \in (-4,4)$ integrate

$$\int_0^\infty e^{-\lambda z} \underbrace{\int_0^{2\pi} e^{i\lambda(x\cos\alpha + y\sin\alpha)}}_{\text{periodic, trapezoidal, } |\cdot| \le 1} d\alpha \, d\lambda$$

For $z = 1$, $\lambda = 30 \Rightarrow |\cdot| = 10^{-13}$ ← (Worst case) slowest decay.

$z = 4$, $\lambda = 8 \Rightarrow |\cdot| = 10^{-14}$

<u>Goal</u>: For λ_j nodes, find n_j = number of nodes need to integrate $e^{i\lambda_j 4(\cos\alpha + \sin\alpha)}$.

Ex: Discretize on $\lambda \in (0,30)$
$\alpha \in (0, 2\pi)$

~~Ex: $\lambda = .5$, $n = 10 \Rightarrow 10^{-15}$ error~~

~~$\lambda = 1$, $n = 10 \Rightarrow 10^{-15}$ error~~

~~$\lambda = 10$,~~

$\boxed{\text{Update}}$

In summary:

Use multipole expansion for L2L, M2M,

Exponential expansion for M2L

<u>Moving on</u> The Helmholtz equation.

$$(\Delta + k^2)\, u = 0$$

The important take-home message: For "k × size of domain" small, the physics of the problem is very close to the Laplace case. For "k × size" large, it is very different.

<u>Separation of variables solution:</u>

$$u = R(r)\,\Theta(\theta)\,\Phi(\varphi)$$

$$\Rightarrow \quad u =$$

$$= \sum_{l,m} \left(a_{lm}\, j_l(kr) + b_{lm}\, h_l(kr) \right) Y_l^m(\theta,\varphi)$$

spherical Bessel functions.

These function satisfy the radial ODE:

$$\left(r^2 \frac{d^2}{dr^2} + 2r\frac{d}{dr} + \left(r^2 - n(n+1)\right)\right) \varphi_n(r) = 0$$

$$j_n(r) = \sqrt{\frac{\pi}{2r}}\, J_{n+\frac{1}{2}}(r)$$

$$h_0(r) = \frac{e^{ir}}{ir} = \text{Greens Function for the Helmholtz equation}$$

$$(\Delta + k^2)\frac{h_0(kr)(ik)}{4\pi} = \delta(r) \qquad g_k(r) = \frac{e^{ikr}}{4\pi r}$$

Multipole Expansions $\Rightarrow$ Partial Wave Expansions:

$$\sum_{l,m} \frac{M_{lm}}{r^{l+1}} Y_l^m(\theta,\varphi) \Rightarrow \sum_{l,m} \alpha_{lm} h_l(kr)\, Y_l^m(\theta,\varphi)$$

Local Expansions $\Rightarrow$ $\sum_{l,m} \beta_{lm}\, j_l(kr)\, Y_l^m(\theta,\varphi)$

Main Addition Theorem:

$$g_k(r) = \frac{e^{ikr}}{4\pi r} = \frac{e^{ik\|\vec{x}-\vec{x}'\|}}{4\pi\|\vec{x}-\vec{x}'\|} \quad \text{for } r > r'$$

$$= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} (-1)^l j_l(kr')\, h_l(kr)\, Y_l^{-m}(\theta',\varphi')\, Y_l^m(\theta,\varphi)$$

(Up to signs! and $\pm i$'s)

Diagonal Plane-Wave Representation

Similar to Laplace $\frac{1}{r}$:

$$(*) \qquad \frac{e^{ikr}}{r} = \frac{1}{2\pi} \int_0^\infty \underbrace{\frac{e^{-\sqrt{\lambda^2-k^2}}}{\sqrt{\lambda^2-k^2}}} \int_0^{2\pi} e^{i\lambda(x\cos\alpha + y\sin\alpha)} \, \lambda \, d\alpha \, d\lambda$$

<u>Cannot</u> discretize directly along $\lambda = 0 \to \infty \ldots$

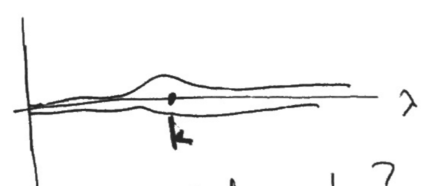
The integrand in (*) has two qualitatively different behaviors: $\lambda < k$, $\lambda > k$. (assume $\mathrm{Im}(k) \geq 0$).

If $\lambda < k$, then $\sqrt{\lambda^2 - k^2} = i\,\mathrm{Re}\ldots$ "Propagating"

$\lambda > k$, then $\mathrm{Re}\left(\sqrt{\lambda^2-k^2}\right) > 0$ "Evanescent."

~~Two~~ Options: Contour deformation / change of variables.

~~Assume~~. Singularity at <u>$\lambda = k$</u>.



which side?

The physically meaningful side, $\mathrm{Im}(k) \geq 0$, has to correspond to <u>decaying</u> waves.

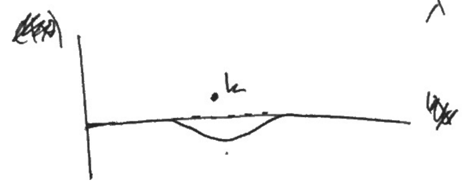
~~The original wave equation~~

If $\mathrm{Im}(k) > 0$, then

$$\frac{e^{ikr}}{r} = \frac{e^{i\mathrm{Re}(k) r} \, e^{-\mathrm{Im}(k) r}}{r} \to 0 \text{ as } r \to \infty.$$

So any contour must not cross k:

λ plane.

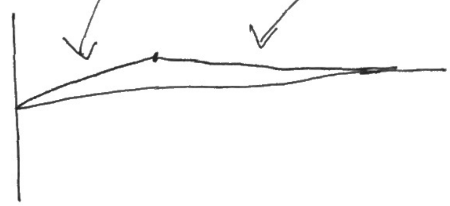


$\lambda^2 - k^2 = -k^2\cos^2\theta$

$d\lambda = k\cos\theta$

$\lambda = k\sin\theta$

$\lambda^2 = \sigma^2 + k^2$

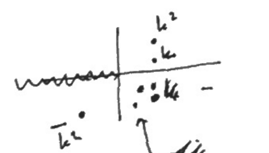


<u>Ex:</u> Deform to: $\int_0^\infty \rightarrow$

So $$\int_0^\infty = \underbrace{\int_0^{\pi/2} e^{ik\cos\theta z} \int_0^{2\pi} d\alpha \, \frac{k^{\cancel{2}} \cancel{\cos\theta} \sin\theta \, d\theta}{-i\cancel{k}\cos\theta}}$$

$\sqrt{\lambda^2 - k^2} = \sqrt{-k^2\cos^2\theta}$

$>$ Im   Re



$$ik \int_0^{\pi/2} e^{ik\cos\theta z} \int_0^{2\pi} d\alpha \, \sin\theta \, d\theta.$$

$$+ \underbrace{\int_0^\infty e^{-\sigma z} J_0\left(\sqrt{\sigma^2+k^2}\sqrt{x^2+y^2}\right) d\sigma}_{\text{Similar to Laplace quadrature.}}$$

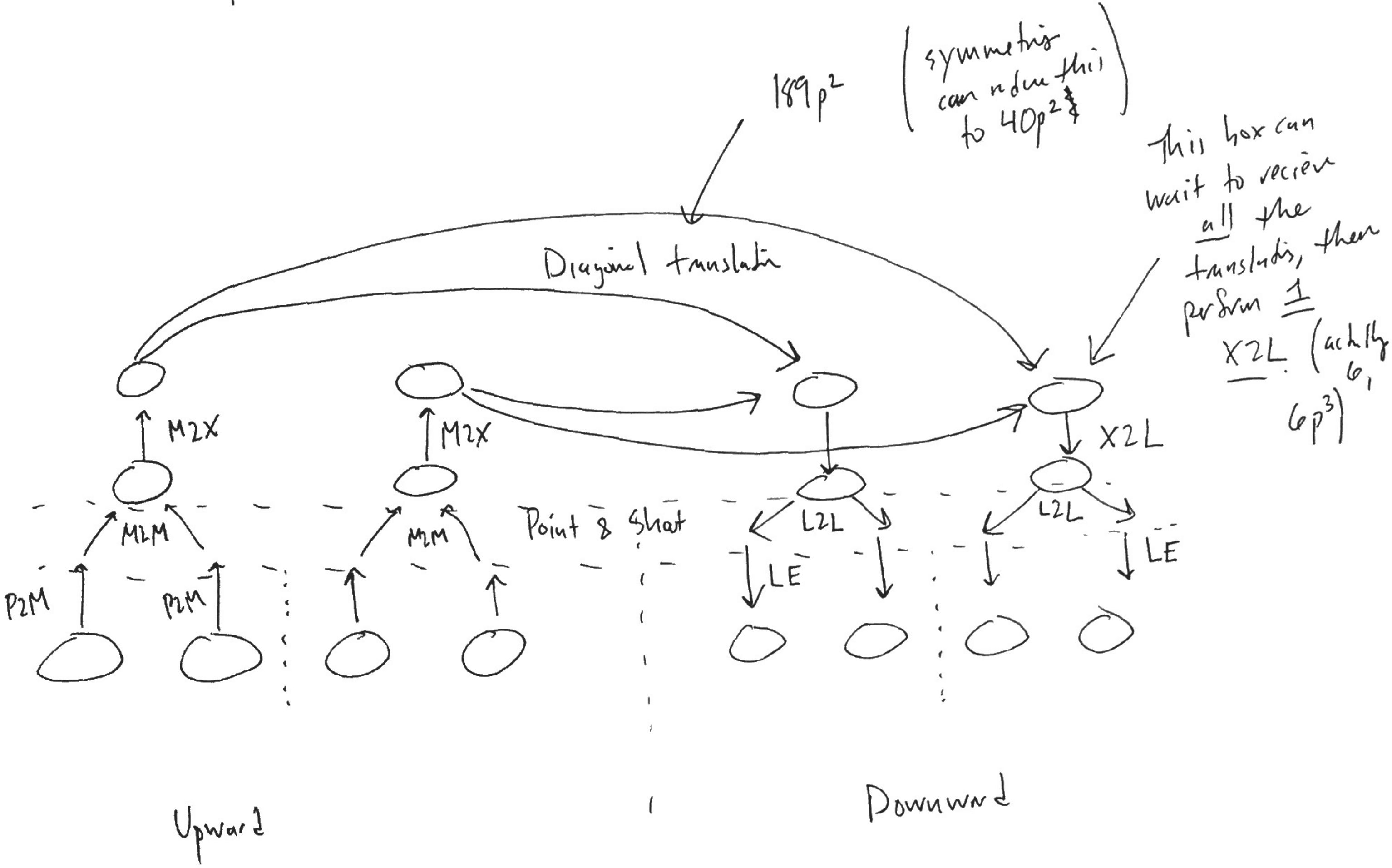
for θ: Gauss-Legendre

α: Trapezoidal

Infinitely more contour deformations exist...

& Quadrature scaling is more sensitive to box size, size of k, etc.

To recap ~~the~~ where the diagonal forms enter:



Maxwell

$$\nabla \times \vec{E} = ik\vec{H} \qquad \nabla \cdot \vec{E} = 0$$

$$\nabla \times \vec{H} = -ik\vec{E} \qquad \nabla \cdot \vec{H} = 0$$

$$\Rightarrow \quad \nabla \times \nabla \times \vec{E} - k^2 \vec{E} = 0.$$

Vector wave equatin.

$$\Rightarrow \quad H = \nabla \times S_k \vec{J}$$

$$E = ik S_k \vec{J} - \nabla S_k \rho$$

$$\int g_k(\cdot)\, \vec{J}\, ds$$

Optin 1.

This has ~~a~~ ~~ge~~ the Green's Functin:

$$G_k^E = \left(I + \frac{1}{k^2} \nabla\nabla \right) \frac{e^{ikr}}{4\pi r}$$

In either case, an integral with the Greens functin is merely sums of derivatis of e^{ikr}/r ...