

Fourier Based MLFMM for the Helmholtz Equation

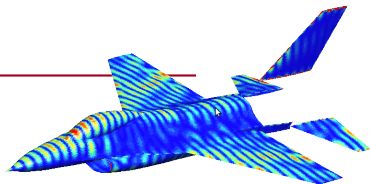
Cris Cecka Eric Darve

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Institute for Computational and Mathematical Engineering
Stanford University

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Research Group Meeting



Solving Helmholtz



The Helmholtz equation over $\Omega \subset \mathbb{R}^3$,

$$(\nabla^2 + \kappa^2)u(\mathbf{x}) = \rho(\mathbf{x})$$

has solution

$$u(\mathbf{x}) = \int_{\Omega} \frac{e^{i\kappa|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \rho(\mathbf{y}) \, d\mathbf{y}$$

Taking a set of point sources $\{\mathbf{y}_j\}_{j=1}^N$ and field points $\{\mathbf{x}_i\}_{i=1}^N$,

$$u(\mathbf{x}_i) = \sum_{\mathbf{y}_j \neq \mathbf{x}_i} \frac{e^{i\kappa|\mathbf{x}_i-\mathbf{y}_j|}}{4\pi|\mathbf{x}_i-\mathbf{y}_j|} \rho_j$$

requiring $\mathcal{O}(N^2)$ operations. MLFMM reduces this to $\mathcal{O}(N \log N)$.



Low Rank Approximation

The Helmholtz MLFMM is based on the plane wave expansion

$$\frac{e^{i\kappa|\mathbf{r}_0+\mathbf{r}|}}{|\mathbf{r}_0+\mathbf{r}|} = \lim_{\ell \rightarrow \infty} \int_{S^2} e^{i\kappa\hat{\mathbf{s}}\cdot\mathbf{r}} T_{\ell,\mathbf{r}_0}(\hat{\mathbf{s}}) dS(\hat{\mathbf{s}})$$

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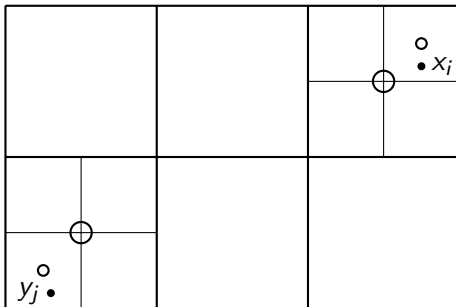


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We define fields over the 2-sphere at the nodes of a tree:

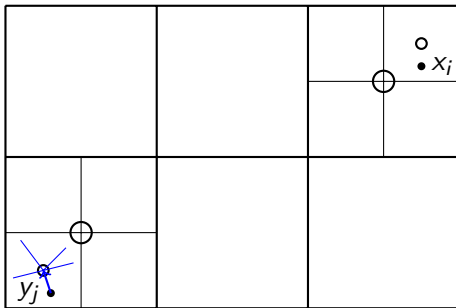


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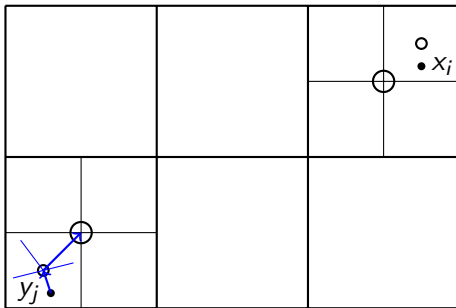


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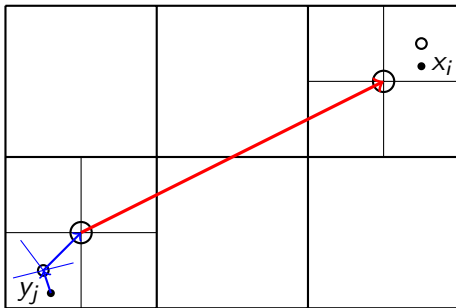


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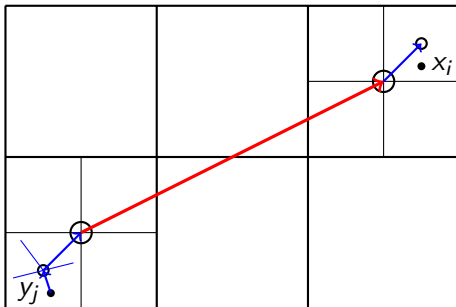


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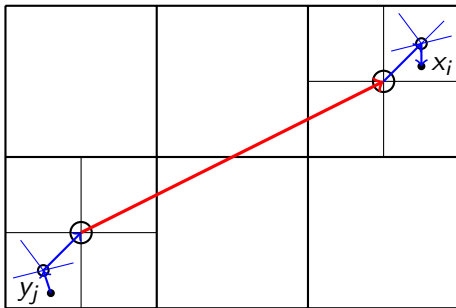


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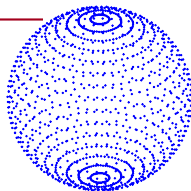
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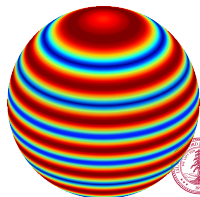
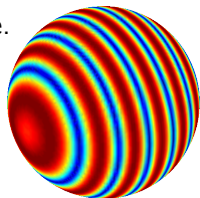
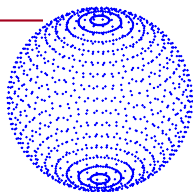
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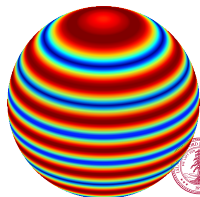
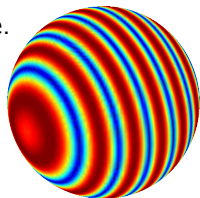
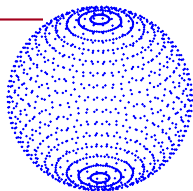
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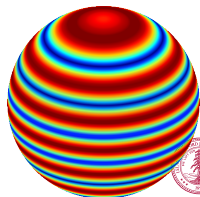
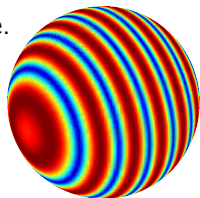
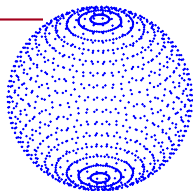
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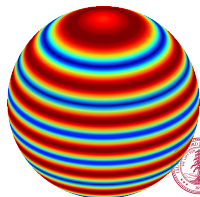
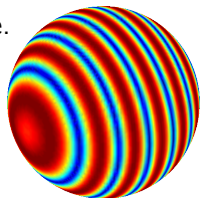
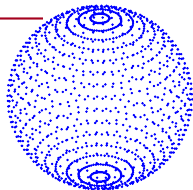
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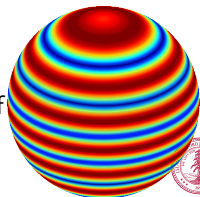
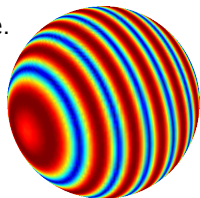
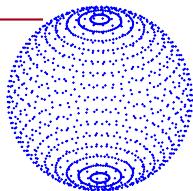
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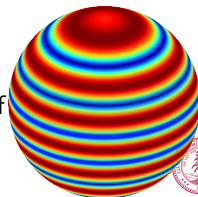
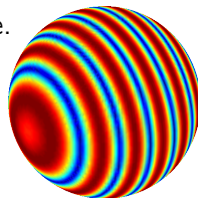
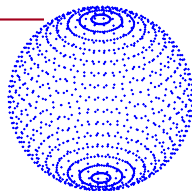
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- Moral: Want better interpolation/anterpolation.



Fourier Based Helmholtz MLFMM

Instead, use a 2D Fourier basis:

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$$T_{\ell,\mathbf{r}_0}^s(\hat{\mathbf{s}}) = \frac{1}{2} T_{\ell,\mathbf{r}_0}(\hat{\mathbf{s}}) |\sin(\theta)|$$



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- Fast, exact interpolation and anterpolation using FFTs.



Spherical Fourier

$f : [0, 2\pi) \times [0, 2\pi) \rightarrow \mathbb{C}$ with

$$f(\theta, \phi) = f(2\pi - \theta, \pi + \phi)$$

has the trigonometric polynomial representation

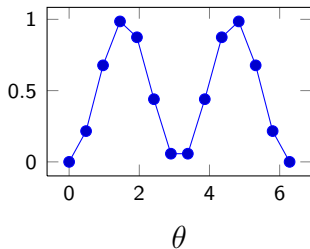
$$f(\theta, \phi) = \sum_{n=-N}^N \sum_{m=-M}^M f_{n,m} e^{i(n\theta+m\phi)} \quad \text{s.t.} \quad f_{n,m} = (-1)^m f_{-n,m}$$

Then, we can compute the inner product exactly as

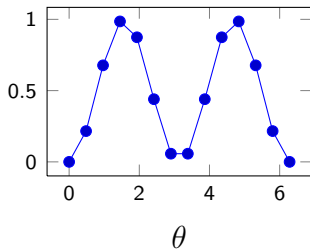
$$\begin{aligned} \langle f, g \rangle &= \int_0^{2\pi} \int_0^{2\pi} f(\theta, \phi) \overline{g(\theta, \phi)} d\theta d\phi \\ &= 4\pi^2 \sum_{n=-N}^N \sum_{m=-M}^M f_{n,m} \overline{g_{n,m}} \\ &= \frac{4\pi^2}{(2N+1)(2M+1)} \sum_{n=0}^{2N} \sum_{m=0}^{2M} f(\theta_n, \phi_m) \overline{g(\theta_n, \phi_m)} \end{aligned}$$



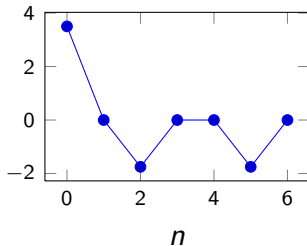
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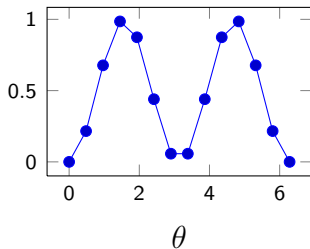
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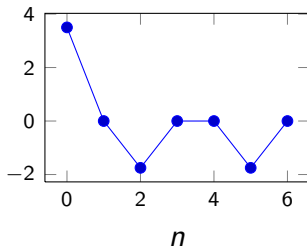
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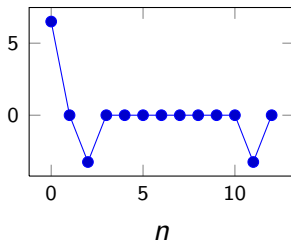
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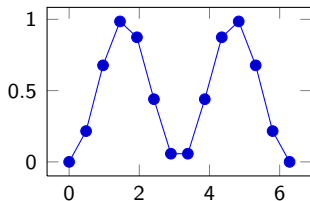
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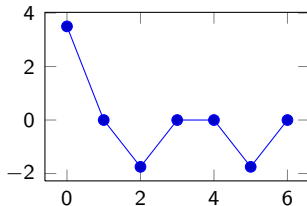
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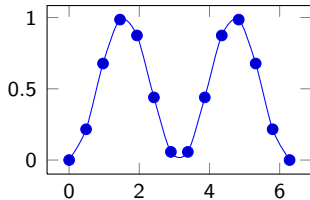
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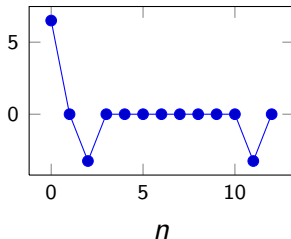
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Fourier Integration with Filtering

Consider 1D non-bandlimited functions $f, g \in L^2([0, 2\pi))$



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- Their exact integral:

$$\langle f, g \rangle = \int_0^{2\pi} \left[\sum_{n=-\infty}^{\infty} f_n e^{in\theta} \right] \left[\sum_{m=-\infty}^{\infty} \overline{g_m} e^{-im\theta} \right] d\theta = 2\pi \sum_{n=-\infty}^{\infty} f_n \overline{g_n}$$



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- Error:

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- Then, the discrete integral is

$$\langle f_N, g \rangle_K = \frac{2\pi}{K} \sum_{k=1}^K \left[\sum_{n=-N}^N f_n e^{in\theta_k} \right] \left[\sum_{m=-\infty}^{\infty} \overline{g_m} e^{-im\theta_k} \right] d\theta = 2\pi \sum_{n=-N}^N \sum_{m=-\infty}^{\infty} f_n \overline{g_{n+mK}}$$



Fourier Integration with Filtering

Instead, suppose we know (or can compute) f_n exactly.

- Construct the low-pass bandlimited version:

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- Error:

$$|\varepsilon| = |\langle f, g \rangle - \langle f_N, g \rangle_K| = 2\pi \left| \sum_{|n|>N} f_n \overline{g_n} - \sum_{|n|\leq N} \sum_{m\neq 0} f_n \overline{g_{n+mK}} \right|$$



Fourier Integration with Filtering

- Bandlimited:

$$T_{\ell, \mathbf{r}_0}(\hat{\mathbf{s}}) = \sum_{n=-\ell}^{\ell} \sum_{m=-\ell}^{\ell} t_{n,m} e^{i(n\theta + m\phi)}$$



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- Not bandlimited, and slow decay:

$$|\sin(\theta)| = \sum_{n=-\infty}^{\infty} s_n e^{in\theta}$$

- Then, $T_{\ell, \mathbf{r}_0}^{\hat{\mathbf{s}}}(\hat{\mathbf{s}}) = \frac{1}{2} T_{\ell, \mathbf{r}_0}(\hat{\mathbf{s}}) |\sin(\theta)|$ decays slowly in θ .



Low-Pass Modified Transfer Function

- Thus,

$$T_{\ell, \mathbf{r}_0}(\theta, \phi) |\sin(\theta)| = \sum_{n=-\infty}^{\infty} \sum_{m=-\ell}^{\ell} t_{n,m} e^{i(n\theta + m\phi)}$$

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$$\mathcal{F}_n[|\sin(\theta)|] = \frac{(-1)^n + 1}{\pi(1 - n^2)}$$



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- Can compute the exact coefficients by convolution:

$$\mathcal{F}_n[T(\theta)s(\theta)] = \sum_{m=-\ell}^{\ell} \mathcal{F}_m[T(\theta)] \mathcal{F}_{n-m}[s(\theta)]$$



Improved Error Analysis

With exact integration and interpolation, only two sources of error:

$$\begin{aligned} \frac{e^{i\kappa|\mathbf{r}_0+\mathbf{r}|}}{|\mathbf{r}_0+\mathbf{r}|} &\stackrel{1}{\rightarrow} \iint_0^{2\pi} e^{i\kappa\hat{\mathbf{s}}\cdot\mathbf{r}} T_{\ell,\mathbf{r}_0}^s(\hat{\mathbf{s}}) d\theta d\phi \\ &\stackrel{2}{\rightarrow} \sum_k \omega_k e^{i\kappa\hat{\mathbf{s}}_k\cdot\mathbf{r}} T_{\ell,\mathbf{r}_0}^{s,L}(\hat{\mathbf{s}}_k) \end{aligned}$$

- Error 1 - Gegenbauer series truncation.
- Error 2 - Numerical quadrature approximation.



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 - Account for error in sampling $e^{i\kappa\hat{\mathbf{s}}\cdot\mathbf{r}}$ in finite quadrature.



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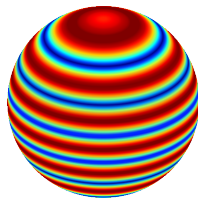
$$\begin{aligned} \frac{e^{i\kappa|\mathbf{r}_0+\mathbf{r}|}}{|\mathbf{r}_0+\mathbf{r}|} &\stackrel{1}{\rightarrow} \iint_0^{2\pi} e^{i\kappa\hat{\mathbf{s}}\cdot\mathbf{r}} T_{\ell,\mathbf{r}_0}^{\mathbf{s}}(\hat{\mathbf{s}}) d\theta d\phi \\ &\stackrel{2}{\rightarrow} \sum_k \omega_k e^{i\kappa\hat{\mathbf{s}}_k\cdot\mathbf{r}} T_{\ell,\mathbf{r}_0}^{\mathbf{s},L}(\hat{\mathbf{s}}_k) \end{aligned}$$

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 - Account for error in sampling $e^{i\kappa\hat{\mathbf{s}}\cdot\mathbf{r}}$ in finite quadrature.
 - Want to find the smallest quadrature for a given accuracy.
 - Error analysis yields constructive algorithms for quadrature.



Improved Error Analysis: N_θ

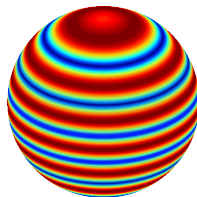
- We want to choose N_θ .



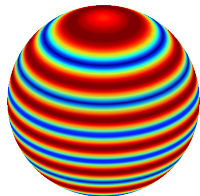
Improved Error Analysis: N_θ

- We want to choose N_θ .
- When $\mathbf{r}_0, \mathbf{r} \sim \hat{\mathbf{z}}$, then ϕ integrates out:

$$|\varepsilon_I| = 2\pi \left| \int_0^{2\pi} E(\theta) T^S(\theta) d\theta - \frac{2\pi}{N_\theta} \sum_{n=1}^{N_\theta} E(\theta_n) T^L(\theta_n) \right|$$



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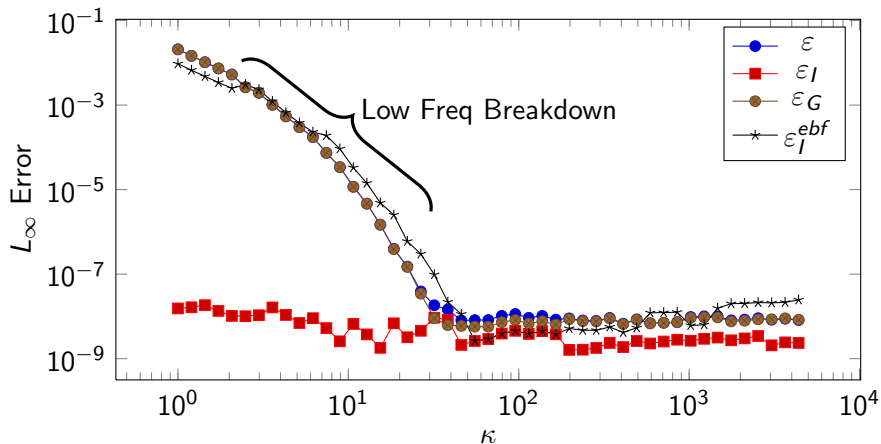
$$|\varepsilon_I| = 2\pi \left| \int_0^{2\pi} E(\theta) T^s(\theta) d\theta - \frac{2\pi}{N_\theta} \sum_{n=1}^{N_\theta} E(\theta_n) T^L(\theta_n) \right|$$

- This is exactly the 1D truncation case $|\langle f, g \rangle - \langle f_N, g \rangle_K|$.
- Using the error expression and $\mathcal{F}_n[E(\theta)] = i^n J_n(\kappa |\mathbf{r}|)$,

$$|\varepsilon_I| \leq 4\pi^2 \left[\sum_{|n| > N_\theta/2} |T_n^s| |J_n(\kappa |\mathbf{r}|)| + \sum_{|n| \leq N_\theta/2} |T_n^s| |J_{N_\theta - |n|}(\kappa |\mathbf{r}|)| \right]$$

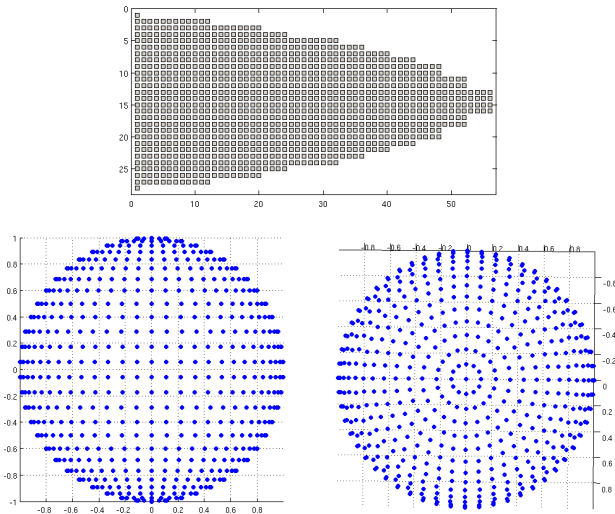


Two points: $\mathbf{r}_0 \sim \hat{\mathbf{z}}$ and boxsize 1



Quadrature Example

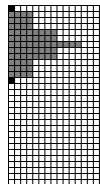
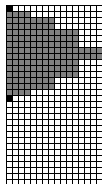
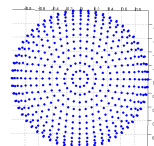
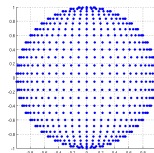
With $\kappa |\mathbf{r}| = 10$, a 1042 point quadrature is created:



Interpolation/Anterpolation Between Quadratures

Interpolate/Anterpolate from quadrature Q to Q' . Let

$$\mathcal{N}_\phi = \max(\max_{1 \leq j \leq N_\theta} N_\phi(\theta_j), \max_{1 \leq j \leq N'_\theta} N'_\phi(\theta_j))$$

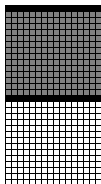
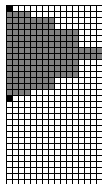
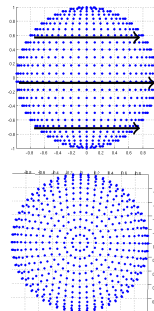


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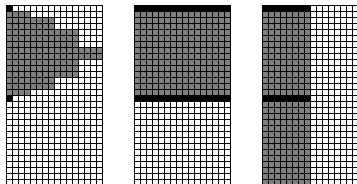
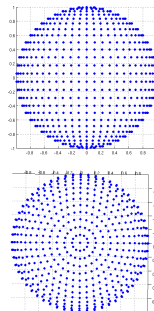


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- 2 Wrap the data to construct the θ -periodic data.

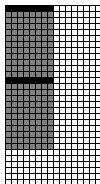
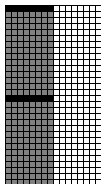
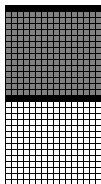
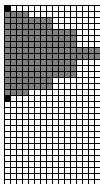
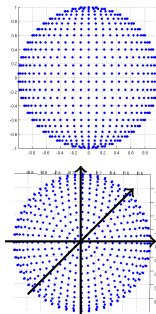


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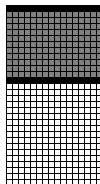
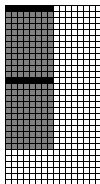
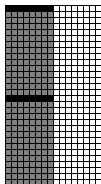
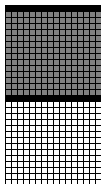
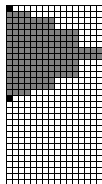
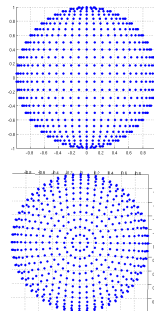


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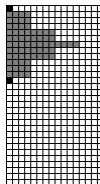
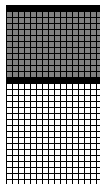
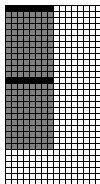
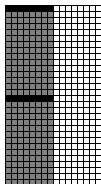
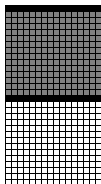
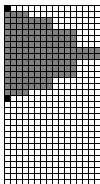
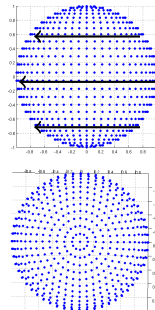


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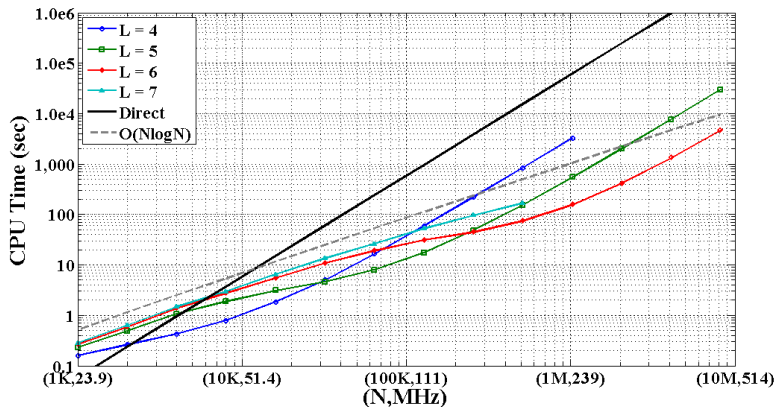
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- 5 Anterpolate from length \mathcal{N}_ϕ to $N'_\phi(\theta_j)$.



Asymptotic Running Time

With accuracy approximately 10^{-6} ,



Moral of the Story

Reasons to use the Fourier Based FMM:

- Exact interpolation/interpolation steps
- Fast with widely available, highly optimized FFT libraries
- All error can be accounted for in the precomputation stage
 - Strict error bounds to be computed before the computation.
 - Error bounds are used to determine truncation and quadrature.

