

Fast computational method for wave scattering

Min Hyung Cho

Department of Mathematical Sciences
University of Massachusetts Lowell

Joint work with
Jingfang Huang at UNC,
Alex Barnett at Dartmouth College/Simons Foundation,
Duan Chen and Wei Cai at UNC Charlotte

Introduction

Wave scattering in layered Media

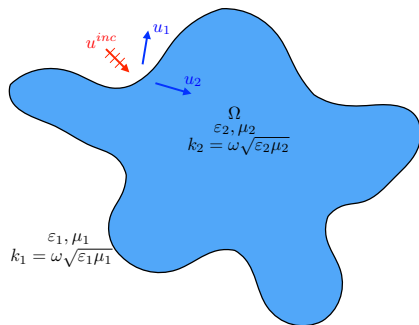
Boundary integral equation for Helmholtz equation in 2-D

Volume integral equation for Maxwell's equations in 3-D

Fast Solver - Heterogenous Fast Multipole Method

Conclusion

Boundary value problem

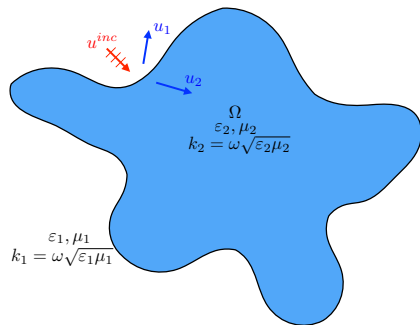


Boundary value problem

Helmholtz equations

$$\Delta u_1 + k_1^2 u_1 = 0$$

$$\Delta u_2 + k_2^2 u_2 = 0$$



Boundary value problem

Helmholtz equations

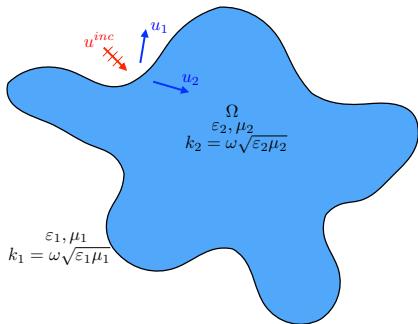
$$\Delta u_1 + k_1^2 u_1 = 0$$

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Interface conditions on $\partial\Omega$

$$u_1 + u^{inc} = u_2$$

$$\frac{\partial u_1}{\partial \mathbf{n}} + \frac{\partial u^{inc}}{\partial \mathbf{n}} = \frac{\partial u_2}{\partial \mathbf{n}}$$



Boundary value problem

Helmholtz equations

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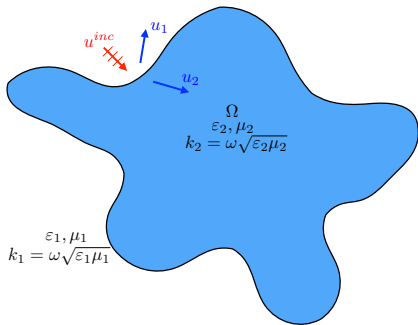
Interface conditions on $\partial\Omega$

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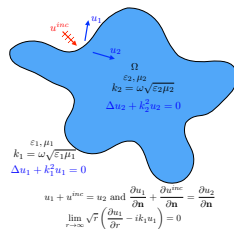
$$\frac{\partial u_1}{\partial \mathbf{n}} + \frac{\partial u^{inc}}{\partial \mathbf{n}} = \frac{\partial u_2}{\partial \mathbf{n}}$$

Sommerfeld radiation condition

$$\lim_{r \rightarrow \infty} \sqrt{r} \left(\frac{\partial u_1}{\partial r} - i k_1 u_1 \right) = 0$$

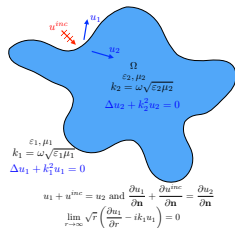


Boundary integral equation



Boundary integral equation

- ▶ Solutions in $\mathbb{R}^2 \setminus \Omega$ and Ω (Potential theory)



Boundary integral equation

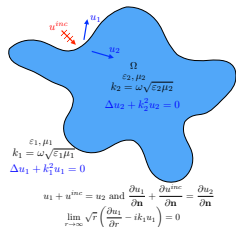
- Solutions in $\mathbb{R}^2 \setminus \Omega$ and Ω (Potential theory)

$$u_1(\mathbf{r}) = \int_{\partial\Omega} \frac{\partial G^1}{\partial \mathbf{n}'}(\mathbf{r}, \mathbf{r}') \tau(\mathbf{r}') ds_{\mathbf{r}'} + \int_{\partial\Omega} G^1(\mathbf{r}, \mathbf{r}') \sigma(\mathbf{r}') ds_{\mathbf{r}'} \quad \text{for } \mathbf{r} \in \mathbb{R}^2 \setminus \Omega$$

$$u_2(\mathbf{r}) = \int_{\partial\Omega} \frac{\partial G^2}{\partial \mathbf{n}'}(\mathbf{r}, \mathbf{r}') \tau(\mathbf{r}') ds_{\mathbf{r}'} + \int_{\partial\Omega} G^2(\mathbf{r}, \mathbf{r}') \sigma(\mathbf{r}') ds_{\mathbf{r}'} \quad \text{for } \mathbf{r} \in \Omega,$$

where

$$G^i(\mathbf{r}, \mathbf{r}') = \frac{i}{4} \underbrace{H_0^{(1)}(k_i |\mathbf{r} - \mathbf{r}'|)}_{\text{Hankel function}}$$



Boundary integral equation

- Solutions in $\mathbb{R}^2 \setminus \Omega$ and Ω

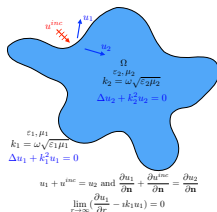
$$u_1(\mathbf{r}) = (D^1 \tau)(\mathbf{r}) + (S^1 \sigma)(\mathbf{r}) \quad \text{for } \mathbf{r} \in \mathbb{R}^2 \setminus \Omega,$$

$$u_2(\mathbf{r}) = (D^2 \tau)(\mathbf{r}) + (S^2 \sigma)(\mathbf{r}) \quad \text{for } \mathbf{r} \in \Omega,$$

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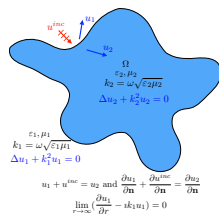
$$(D^i \tau)(\mathbf{r}) = \int_{\partial \Omega} \frac{\partial G^i}{\partial \mathbf{n}'}(\mathbf{r}, \mathbf{r}') \tau(\mathbf{r}') ds'_{\mathbf{r}'},$$

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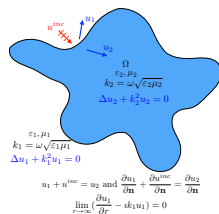
Boundary integral equation

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Boundary integral equation

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- ▶ Let $\mathbf{r} \rightarrow \mathbf{x} \in \partial\Omega$

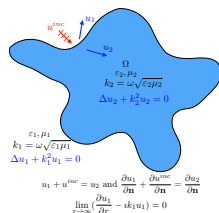


Boundary integral equation

- ▶ Matching interface conditions on $\partial\Omega$
- ▶ Let $\mathbf{r} \rightarrow \mathbf{x} \in \partial\Omega$

$$u_1(\mathbf{x}) = \frac{1}{2}\tau(\mathbf{x}) + (D^1\tau)(\mathbf{x}) + (S^1\sigma)(\mathbf{x}),$$

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Boundary integral equation

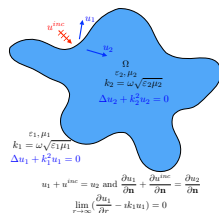
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$$\frac{\partial u_2}{\partial \mathbf{n}}(\mathbf{x}) = \frac{\partial}{\partial \mathbf{n}}(D^2\tau)(\mathbf{x}) + \frac{1}{2}\sigma(\mathbf{x}) + \frac{\partial}{\partial \mathbf{n}}(S^2\sigma)(\mathbf{x}).$$



Boundary integral equation

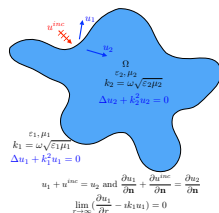
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Boundary integral equation

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Boundary integral equation

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$$\begin{aligned} \underline{u_1} + u^{inc} &= \underline{u_2} \\ \frac{\partial u_1}{\partial \mathbf{n}} + \frac{\partial u^{inc}}{\partial \mathbf{n}} &= \frac{\partial u_2}{\partial \mathbf{n}} \end{aligned}$$

Boundary integral equation

- ▶ Interface Conditions on $\partial\Omega$

$$\frac{\frac{1}{2}\tau + D^1\tau + S^1\sigma + u^{inc}}{2} = \frac{-\frac{1}{2}\tau + D^2\tau + S^2\sigma}{2}$$

$$\frac{T^1\tau - \frac{1}{2}\sigma + D^{1,*}\sigma + \frac{\partial u^{inc}}{\partial \mathbf{n}}}{2} = \frac{T^2\tau + \frac{1}{2}\sigma + D^{2,*}\sigma}{2}$$

Boundary integral equations

- ▶ Boundary integral equations (Müller '69, Rokhlin '83)

$$\begin{aligned}\tau + (D^1 - D^2)\tau + (S^1 - S^2)\sigma &= -u^{inc} \\ -\sigma + (T^1 - T^2)\tau + (D^{1,*} - D^{2,*})\sigma &= -\frac{\partial u^{inc}}{\partial \mathbf{n}}\end{aligned}$$

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or

$$\left(\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D^1 - D^2 & S^2 - S^1 \\ T^1 - T^2 & D^{2,*} - D^{1,*} \end{bmatrix} \right) \begin{bmatrix} \tau \\ -\sigma \end{bmatrix} = \begin{bmatrix} -u^{inc} \\ -\frac{\partial u^{inc}}{\partial \mathbf{n}} \end{bmatrix}$$

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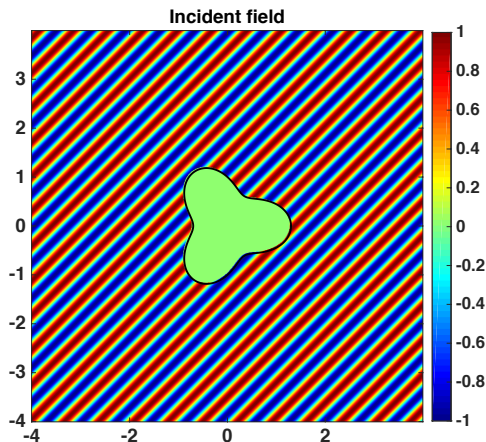
or

$$\left(\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D^1 - D^2 & S^2 - S^1 \\ T^1 - T^2 & D^{2,*} - D^{1,*} \end{bmatrix} \right) \begin{bmatrix} \tau \\ -\sigma \end{bmatrix} = \begin{bmatrix} -u^{inc} \\ -\frac{\partial u^{inc}}{\partial \mathbf{n}} \end{bmatrix}$$

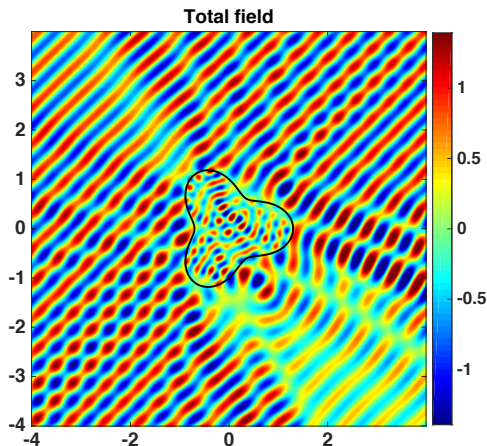
- ▶ Discretization

$$(I + A)\boldsymbol{\eta} = \mathbf{f}$$

- ▶ Smooth-star domain : $\omega = 4\pi$, $\varepsilon_1 = 1$, $\varepsilon_2 = 4$, $\mu_1 = \mu_2 = 1$, $\theta^{inc} = -\pi/4$, 400×400 matrix and 12-digit accuracy

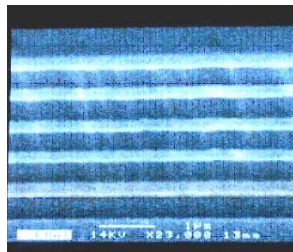
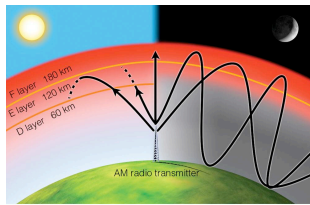
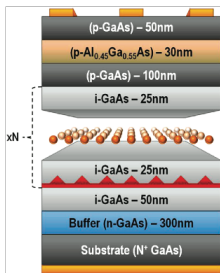


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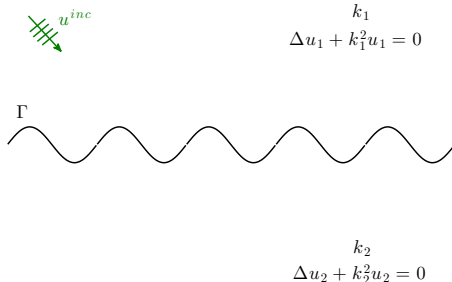


Wave scattering in layered Media

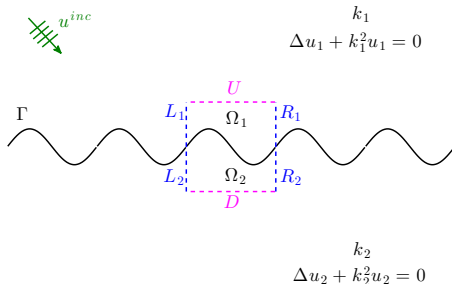
Layered media

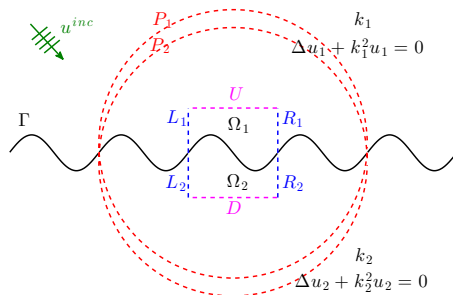


Two layers with one periodic interface (period = d)

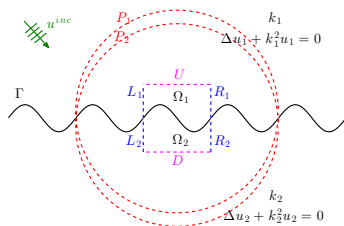


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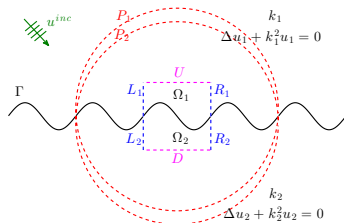


Two layers with one periodic interface (period = d)

Solution in each layer



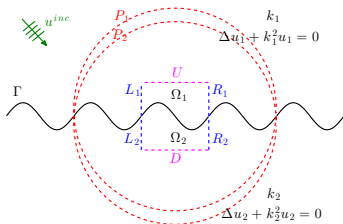
Solution in each layer



$$u_1(\mathbf{r}) = \tilde{D}_{\Omega_1}^1 \tau + \tilde{S}_{\Omega_1}^1 \sigma + \sum_{p=1}^P c_p^1 \phi_p^1$$

$$u_2(\mathbf{r}) = \tilde{D}_{\Omega_2}^2 \tau + \tilde{S}_{\Omega_2}^2 \sigma + \sum_{p=1}^P c_p^2 \phi_p^2$$

Solution in each layer



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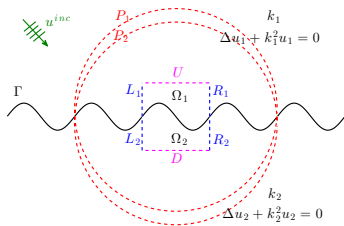
where

$$(\tilde{D}_V^i \tau)(\mathbf{r}) := \sum_{l=-1}^1 \alpha^l \int_W \frac{\partial G^i}{\partial \mathbf{n}'}(\mathbf{r}, \mathbf{r}' + l\mathbf{d}) \tau(\mathbf{r}') ds_{\mathbf{r}'}, \quad (\tilde{S}_V^i \sigma)(\mathbf{r}) := \sum_{l=-1}^1 \alpha^l \int_W G^i(\mathbf{r}, \mathbf{r}' + l\mathbf{d}) \sigma(\mathbf{r}') ds_{\mathbf{r}'},$$

$$(\tilde{T}_V^i \tau)(\mathbf{r}) := \sum_{l=-1}^1 \alpha^l \int_W \frac{\partial^2 G^i}{\partial \mathbf{n} \partial \mathbf{n}'}(\mathbf{r}, \mathbf{r}' + l\mathbf{d}) \tau(\mathbf{r}') ds_{\mathbf{r}'}, \quad (\tilde{D}_V^{i,*} \sigma)(\mathbf{r}) := \sum_{l=-1}^1 \alpha^l \int_W \frac{\partial G^i}{\partial \mathbf{n}}(\mathbf{r}, \mathbf{r}' + l\mathbf{d}) \sigma(\mathbf{r}') ds_{\mathbf{r}'},$$

$$\phi_p^i(\mathbf{r}) := \frac{\partial G^i}{\partial \mathbf{n}_p}(\mathbf{r}, \mathbf{y}_p^i) + ik_i G^i(\mathbf{r}, \mathbf{y}_p^i), \quad \mathbf{r} \in \Omega_i, \quad p = 1, 2, \quad \alpha = e^{idk_1 \cos \theta^{inc}}$$

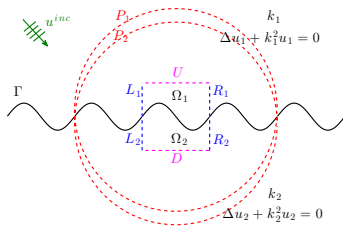
Boundary integral equations



$$u_1(\mathbf{r}) = \tilde{D}_{\Omega_1}^1 \tau + \tilde{S}_{\Omega_1}^1 \sigma + \sum_{p=1}^P c_p^1 \phi_p^1$$

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Boundary integral equations

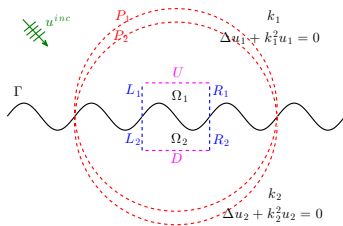


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- Interface conditions

Boundary integral equations



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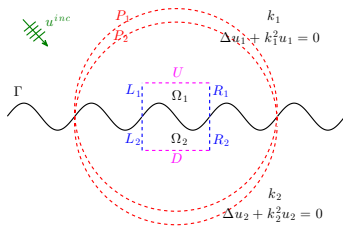
$$u_2(\mathbf{r}) = \tilde{D}_{\Omega_2}^2 \tau + \tilde{S}_{\Omega_2}^2 \sigma + \sum_{p=1}^P c_p^2 \phi_p^2$$

- Interface conditions
- Quasi-periodicity

$$u|_L - \alpha u|_R = 0$$

$$u_n|_L - \alpha u_n|_R = 0$$

Boundary integral equations



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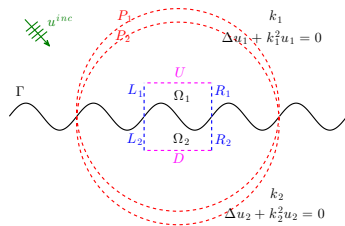
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- Interface conditions
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$$u|_L - \alpha u|_R = 0$$

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- Radiation condition
(Rayleigh-Bloch Expansion)

Boundary integral equations



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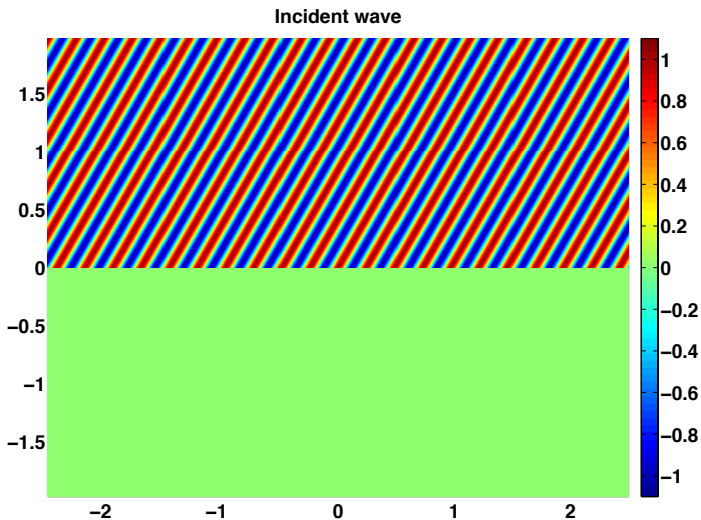
$$u_n|_L - \alpha u_n|_R = 0$$

$$\rightarrow \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{0} \\ \mathbf{C} & \mathbf{Q} & \mathbf{0} \\ \mathbf{Z} & \mathbf{V} & \mathbf{W} \end{bmatrix} \begin{bmatrix} \eta \\ \mathbf{c} \\ \mathbf{a} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

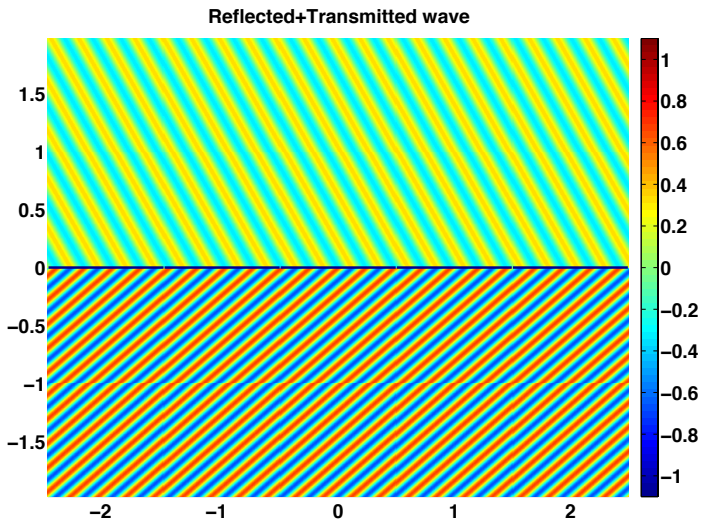
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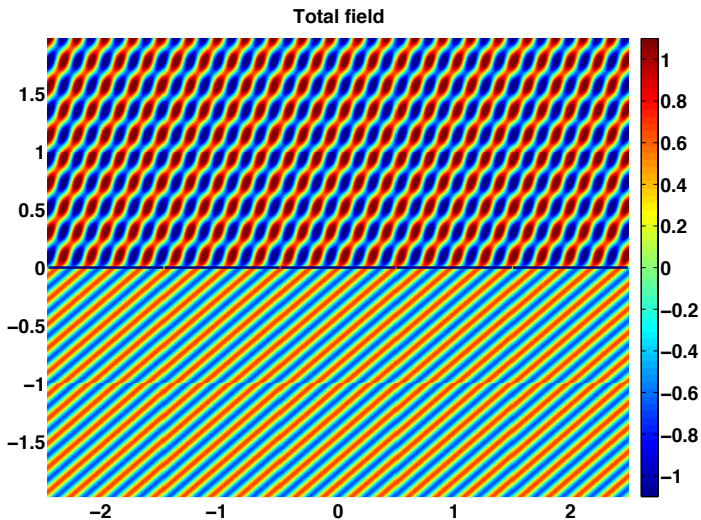
- ▶ Flat surface ($\varepsilon_1 = 1$, $\varepsilon_2 = 1.77$ (water), $\omega = 30$, Error = 2×10^{-14})



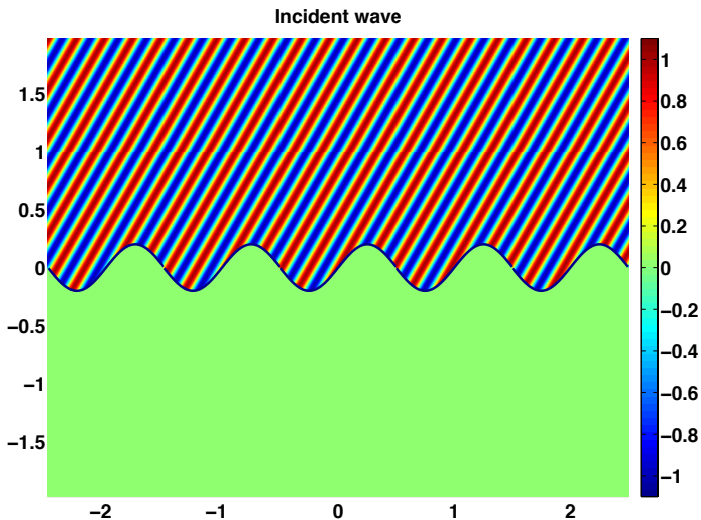
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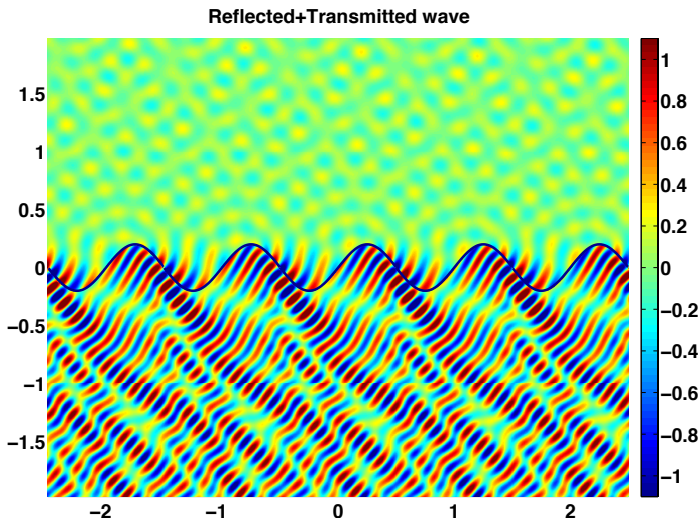
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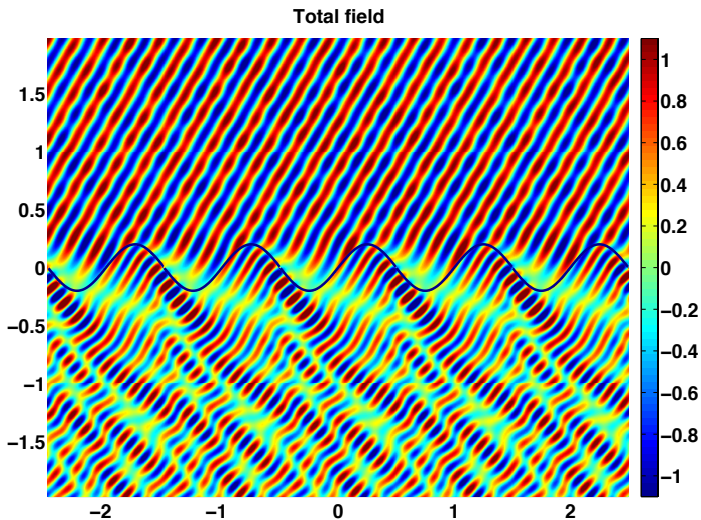
- ▶ Sine surface ($\epsilon_1 = 1$, $\epsilon_2 = 1.77$ (water), $\omega = 30$, Error = 5×10^{-13})



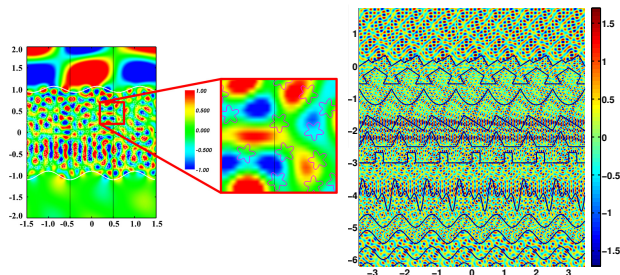
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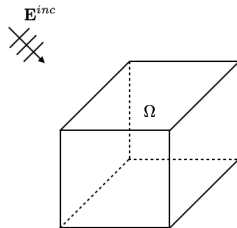
- ▶ In 2-D, boundary integral equation methods using periodizing scheme
 - Left : J. Lai, M. Kobayashi, A. Barnett, JCP 2015
 - Right : (1000 layers) M.H. Cho and A. Barnett OPEX 2015



► CPU time and memory usage

Number of interfaces	1	3	10	30	100	300	1000
Matrix Filling (sec)	0.518	1.860	4.200	5.600	12.384	32.332	103.331
Schur Complement (sec)	0.028	0.058	0.299	0.644	2.263	6.525	21.037
Block Solve (sec)	0.003	0.041	0.398	0.898	2.805	8.626	26.655
Memory (MB)	18	41	83	183	608	1753	5830
Flux Error	4.8e-12	3.1e-11	2.4e-11	4.0e-11	2.2e-11	1.3e-10	9.1e-10

- ▶ In 3-D, BIE for Maxwell's equations is challenging



- ▶ In 3-D, BIE for Maxwell's equations is challenging
 - Lippmann-Schwinger type volume integral equation (VIE) (D. Chen, W. Cai, B. Ziner, and M.H. Cho, JCP, 2016)

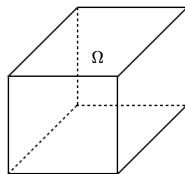
$$\mathbf{C} \cdot \mathbf{E}(\mathbf{r}) = \mathbf{E}^{inc}(\mathbf{r}) - \omega\mu(\mathbf{r}) \int_{\Omega} d\mathbf{r}' \omega\Delta\epsilon(\mathbf{r}') \cdot \bar{\mathbf{G}}_E(\mathbf{r}', \mathbf{r}),$$

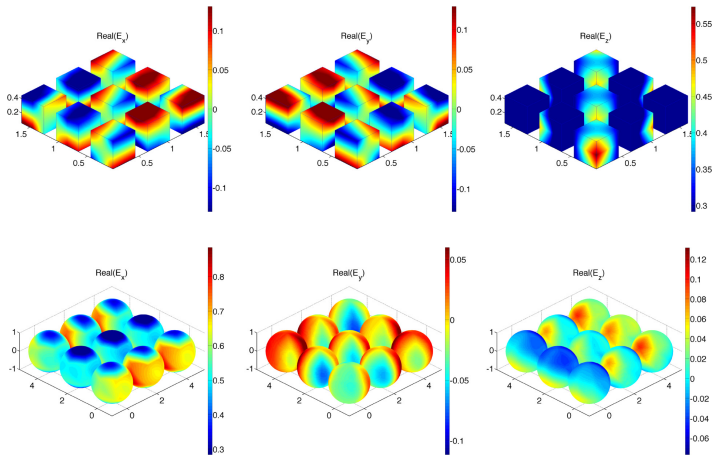
where

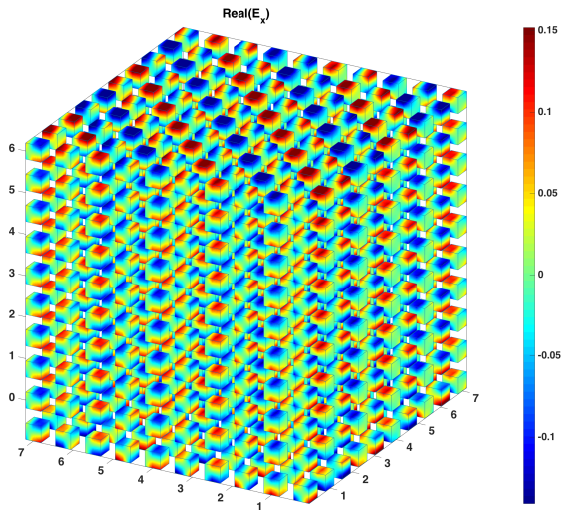
$$\mathbf{C} = \mathbf{I} + \mathbf{L}_{V\delta} \cdot \Delta\epsilon(\mathbf{r})$$

and the Dyadic Green's function

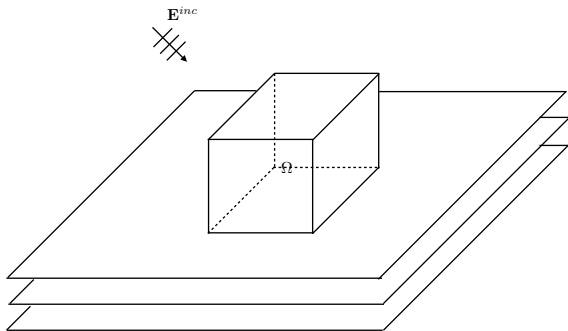
$$\bar{\mathbf{G}}_E = \frac{1}{4\pi} \left(\mathbf{I} + \frac{1}{k^2} \nabla \nabla \right) \frac{e^{-ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$



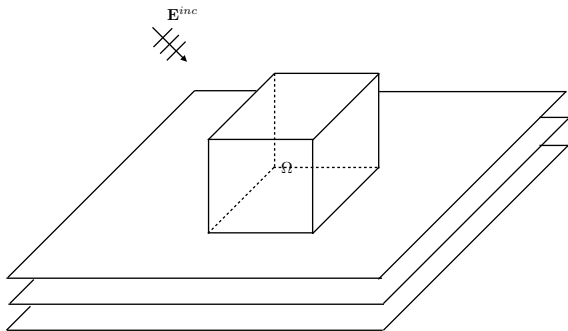




- ▶ Lippmann-Schwinger type Volume integral equation in multilayered media



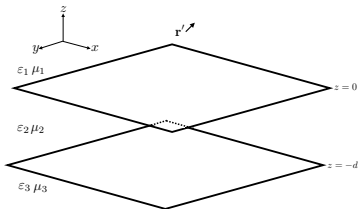
- ▶ Lippmann-Schwinger type Volume integral equation in multilayered media



- ▶ Dyadic Green's function $\bar{\mathbf{G}}_E \rightarrow$ Layered media Dyadic Green's function $\bar{\mathbf{G}}_E^L$

- ▶ Layered media Green's function using Sommerfeld integrals and Fresnel reflection coefficients (M.H. Cho and W. Cai, JSC 2017)

$$\bar{\mathbf{G}}_E^L(\mathbf{r}', \mathbf{r}) = \begin{cases} \mathbf{G}^P - \frac{1}{8\pi^2\omega\epsilon_0\epsilon_1} \mathbf{G}_1^R, & z \geq 0 \\ -\frac{1}{8\pi^2\omega\epsilon_0\epsilon_2} (\mathbf{G}_2^R + \mathbf{G}_2^T), & -d \leq z < 0 \\ -\frac{1}{8\pi^2\omega\epsilon_0\epsilon_3} \mathbf{G}_3^T, & z < -d \end{cases},$$



- ▶ Reflected parts ($j = 1, 2$)

$$G_{jxx}^R = k_j^2 g_{j,1}^R - \frac{1}{2} (g_{j,3}^R + g_{j,7}^R) + \left(\frac{1}{2} \rho^2 - (y - y')^2 \right) g_{j,2}^R$$

$$G_{jyy}^R = k_j^2 g_{j,1}^R - \frac{1}{2} (g_{j,3}^R + g_{j,7}^R) + \left(\frac{1}{2} \rho^2 - (x - x')^2 \right) g_{j,2}^R$$

$$G_{jzz}^R = -g_{j,3}^R$$

$$G_{jxy}^R = G_{jyx}^R = (x - x')(y - y') g_{j,2}^R$$

$$G_{jxz}^R = -G_{jzx}^R = -i(x - x') g_{j,6}^R, \quad G_{jyz}^R = -G_{jzy}^R = -i(y - y') g_{j,6}^R,$$

- ▶ Transmitted parts ($j = 2, 3$)

$$G_{jxx}^T = k_j^2 g_{j,1}^T - \frac{1}{2} g_{j,3}^T + \left(\frac{1}{2} \rho^2 - (y - y')^2 \right) g_{j,2}^T$$

$$G_{jyy}^T = k_j^2 g_{j,1}^T - \frac{1}{2} g_{j,3}^T + \left(\frac{1}{2} \rho^2 - (x - x')^2 \right) g_{j,2}^T,$$

$$G_{jzz}^T = g_{j,4}^T,$$

$$G_{jxy}^T = G_{jyx}^T = (x - x')(y - y') g_{j,2}^T$$

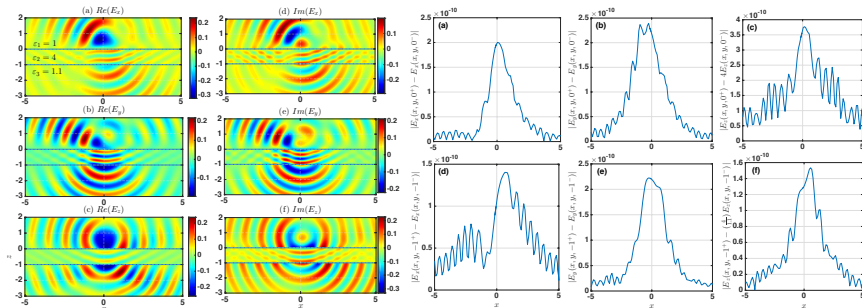
$$G_{jxz}^T = i(x - x') g_{j,6}^T, \quad G_{jyz}^T = i(y - y') g_{j,6}^T$$

$$G_{jzx}^T = i(x - x') g_{j,9}^T, \quad G_{jzy}^T = i(y - y') g_{j,9}^T,$$

where

$$g^{R,T} = 2\pi \int_0^\infty k_s^{n+1} \tilde{g} \frac{J_n(k_s \rho)}{\rho^n} e^{\pm i k_z (z+z')} dk_s \quad \text{and} \quad \tilde{g} = \tilde{g}(k_s)$$

► Electric field Green's function in a 3 layer structure



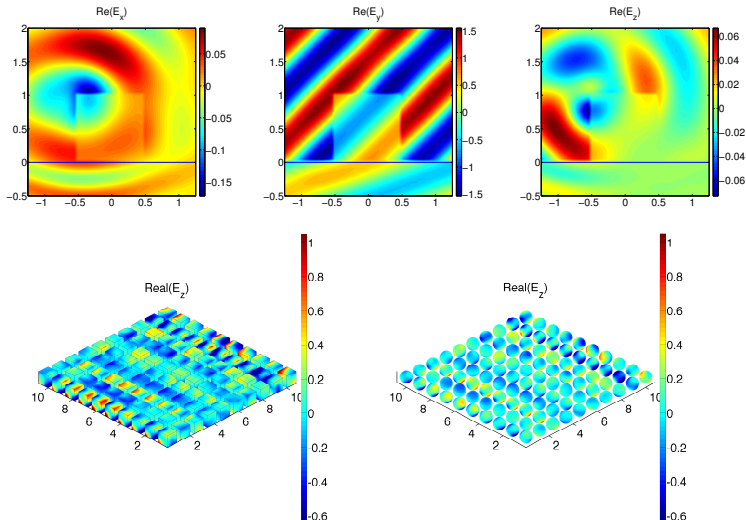
- ▶ Volume integral equation with layered media Green's function (D. Chen, M.H. Cho, and W. Cai, SISC, 2016 submitted)

$$\mathbf{C} \cdot \mathbf{E}(\mathbf{r}) = \mathbf{E}^{inc}(\mathbf{r}) - \omega\mu(\mathbf{r}) \int_{\Omega} d\mathbf{r}' \omega \Delta\epsilon(\mathbf{r}') \cdot \bar{\mathbf{G}}_E^L(\mathbf{r}', \mathbf{r}),$$

where

$$\mathbf{C} = \mathbf{I} + \mathbf{L}_{V_{\delta}} \cdot \Delta\epsilon(\mathbf{r})$$

► Volume integral equation with layered media Green's function



Fast solver - Heterogeneous Fast Multipole Method

Fast Solver

- ▶ Fast Multipole Method (FMM) by Rokhlin and Greengard

$$\sum_{i=1}^N G(x_j, x_i) q_i, \quad j = 1, 2, \dots, N$$

→ N -body problem or Matrix vector multiplication

- ▶ Direct computation: $\mathcal{O}(N^2)$
- ▶ FMM: $\mathcal{O}(N)$ or $\mathcal{O}(N \log N)$

Fast Solver

- ▶ Integral operator for Helmholtz equation in the free-space

$$u(\mathbf{x}) = \int_{\partial\Omega} g(\mathbf{x}, \mathbf{x}') q(\mathbf{x}') d\mathbf{x}' \approx \sum_{i=1}^N g(\mathbf{x}, \mathbf{x}'_i) q(\mathbf{x}'_i)$$

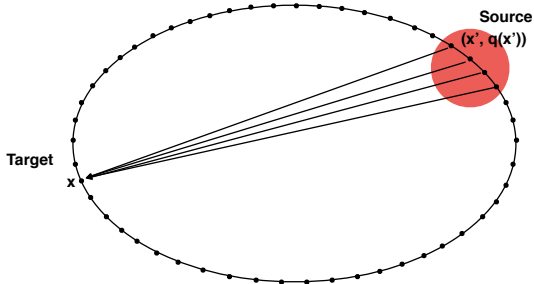
where $g(\mathbf{x}, \mathbf{x}') = \frac{i}{4} H_0^{(1)}(k|\mathbf{x} - \mathbf{x}'|)$

Fast Solver

- Integral operator for Helmholtz equation in the free-space

$$u(\mathbf{x}) = \int_{\partial\Omega} g(\mathbf{x}, \mathbf{x}') q(\mathbf{x}') d\mathbf{x}' \approx \sum_{i=1}^N g(\mathbf{x}, \mathbf{x}'_i) q(\mathbf{x}'_i)$$

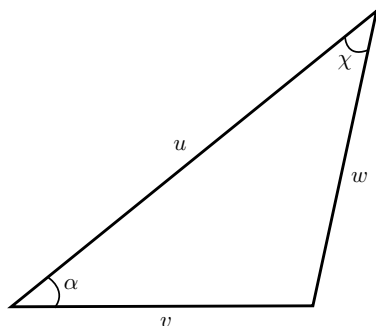
where $g(\mathbf{x}, \mathbf{x}') = \frac{i}{4} H_0^{(1)}(k|\mathbf{x} - \mathbf{x}'|)$



▶ Graf's Addition Theorem

$$C_\nu(w)e^{i\nu\chi} = \sum_{p=-\infty}^{\infty} C_{\nu+p}(u)J_p(v)e^{ip\alpha},$$

where C_ν is either $H_\nu^{(1)}$ or J_ν

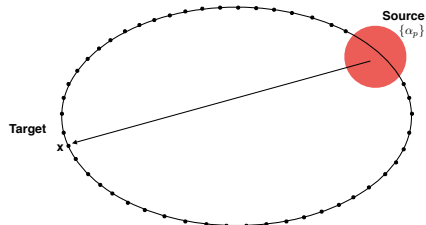


► Multipole expansion

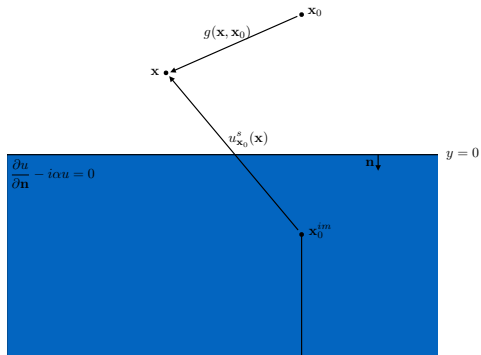
$$u(\mathbf{x}) = \sum_{i=1}^N \frac{\iota}{4} H_0^{(1)}(k|\mathbf{x} - \mathbf{x}'_i|) q(\mathbf{x}'_i) \approx \frac{\iota}{4} \sum_{p=-P}^P \alpha_p H_p(k|\mathbf{x} - \mathbf{x}_c|) e^{\iota p \theta_c},$$

where

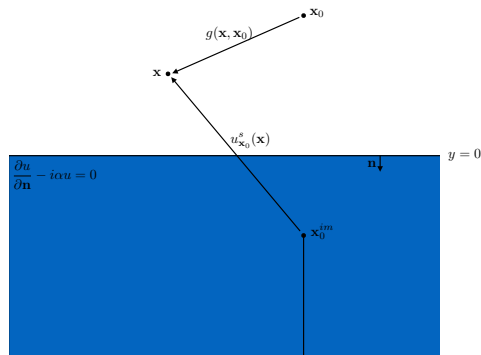
$$\alpha_p = \sum_{j=1}^N q_j e^{-\iota p \theta_j} J_p(k\rho_j)$$



- ▶ Helmholtz equation with Impedance boundary condition (method of image)

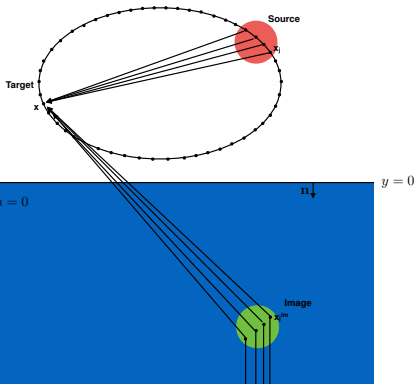


- ▶ Helmholtz equation with Impedance boundary condition (method of image)



$$\begin{aligned}
 u_{\mathbf{x}_0}(\mathbf{x}) &= g(\mathbf{x}, \mathbf{x}_0) + u_{\mathbf{x}_0}^s(\mathbf{x}) \\
 &\equiv g(\mathbf{x}, \mathbf{x}_0) + \left(g(\mathbf{x}, \mathbf{x}_0^{im}) + 2i\alpha \int_0^\infty g(\mathbf{x}, \mathbf{x}_0^{im} - s\hat{y}) e^{i\alpha s} ds \right)
 \end{aligned}$$

- ▶ N source points



$$u(\mathbf{x}) = \sum_{j=1}^N u_{\mathbf{x}_j}(\mathbf{x}) q(\mathbf{x}_j)$$

$$= \sum_{j=1}^N q_j(\mathbf{x}_j) \left(g(\mathbf{x}, \mathbf{x}_j) + g(\mathbf{x}, \mathbf{x}_j^{im}) + 2i\alpha \int_0^\infty g(\mathbf{x}, \mathbf{x}_j^{im} - s\hat{\mathbf{y}}) e^{i\alpha s} ds \right)$$

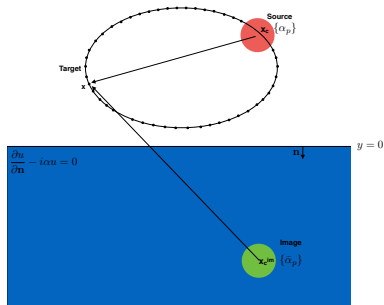
► Multipole expansion

$$u(\mathbf{x}) \approx \frac{i}{4} \sum_{p=-P}^P \alpha_p H_p(k|\mathbf{x} - \mathbf{x}_c|) e^{i p \theta_c}$$

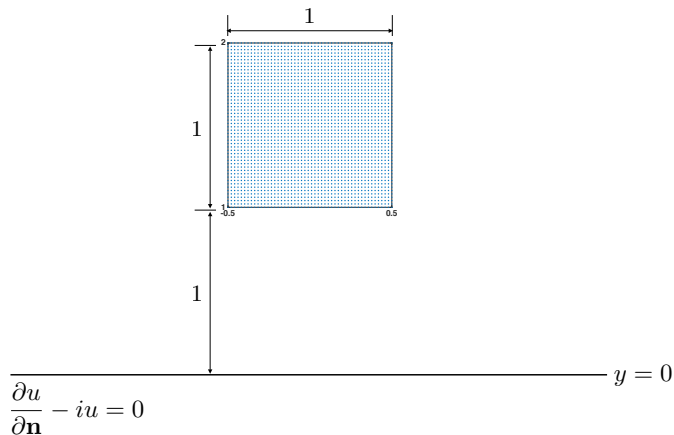
$$+ \frac{i}{4} \sum_{p=-P}^P \bar{\alpha}_p \left(H_p(k|\mathbf{x} - \mathbf{x}_c^{im}|) e^{i p \theta_{im}} \right.$$

$$\left. + 2i\alpha \int_0^\infty H_p(k|\mathbf{x} - (\mathbf{x}_c^{im} - s\hat{y})|) e^{i p \hat{\theta}_{im}} e^{i\alpha s} ds \right),$$

where $\bar{\alpha}_p$ is the complex conjugate of α_p .



- ▶ Test problem (Uniform distribution in a unit box)



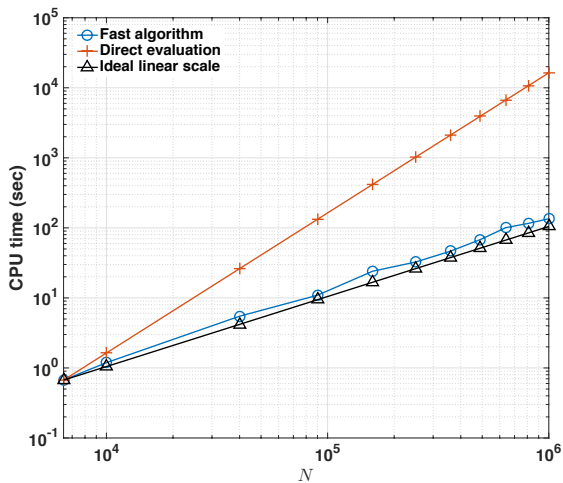
- ▶ Accuracy for $k = 0.1$ and $k = 1$ with $N = 10000$

p	Error for $k = 0.1$	Error for $k = 1$
E_5	1.23×10^{-4}	1.43×10^{-4}
E_{10}	2.73×10^{-6}	3.81×10^{-6}
E_{20}	2.06×10^{-9}	2.85×10^{-9}
E_{30}	1.19×10^{-11}	1.65×10^{-11}

- ▶ CPU time for $p = 39$ and $k = 0.1$
(Intel Xeon E5-2697 2.6Ghz with gcc, Dell 7910 workstation)

N	100	6400	10000	90000	360000	640000	810000	1000000
H-FMM time (sec)	0.01	0.67	1.19	10.92	46.58	100.85	116.03	135.05
Direct time (sec)			1.64	132.50	2199.92	6700	10732.10	16357.42

- ▶ CPU time in the log-log scale (linear scaling 😊)



Conclusions and Summary

- ▶ Boundary integral equation (BIE) method for layered media
- ▶ EM scattering problem using volume integral equation (VIE) method
- ▶ Heterogeneous fast multipole method
 - Extension to multi-layered media (on-going work)
- ▶ Stochastic methodology for meta-material design
- ▶ Some source codes
http://faculty.uml.edu/min_cho/software.html

Thank you!