Electromagnetic scattering 1: Integral-equation methods (IEMs)

Johannes Markkanen

University of Helsinki

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Volume-integral-equation (IEM)

Strengths:

- Fairly solid mathematical background
- Automatically satisfies the radiation condition
- Only the scatterer is discretized, no need for PML
- Exact propagator $->$ no numerical dispersion
- Accuracy

Weaknesses:

- Full matrix
- Accelaration techniques needed
- Singular integrals
- Complicated implementation
- Preconditioning for some problems

IEM literature

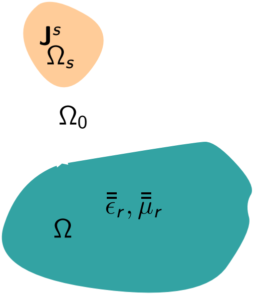
Introduction to FDTD, FEM, IEM

- Sheng Xin-Qing, Song Wei, Essentials of computational electromagnetics, IEEE,Wiley, 2012.

Some IEM books

- Volakis, J.L., Sertel, K., Integral Equation Methods for Electromagnetics, Scitech Publishing, Inc., 2012.
- Chew, W.C., Jin, J.M., Michielssen, E., Song, J., Fast and Efficient Algorithms in Computational Electromagnetics, Artech House, 2001.

Problem configuration



$$\Omega_0 = \bar{\Omega},\ \Omega_s \subset \Omega_0$$

$$\begin{aligned}
\nabla \times \mathbf{E} &= i\omega\mu_0 \mathbf{H}, & \mathbf{r} \in \Omega_0 \\
\nabla \times \mathbf{H} &= -i\omega\epsilon_0 \mathbf{E} + \mathbf{J}^s & \mathbf{r} \in \Omega_0 \\
\nabla \times \mathbf{E} &= i\omega\mu_0 \bar{\bar{\mu}}_r \cdot \mathbf{H}, & \mathbf{r} \in \Omega \\
\nabla \times \mathbf{H} &= -i\omega\epsilon_0 \bar{\bar{\epsilon}}_r \cdot \mathbf{E} & \mathbf{r} \in \Omega
\end{aligned} \tag{1}$$

Wave-equations

$$\nabla \times \nabla \times \mathbf{E} - k_0^2 \mathbf{E} = i\omega\mu_0 \mathbf{J}^s, \mathbf{r} \in \Omega_0 \tag{2}$$

$$\nabla \times \nabla \times \mathbf{E} - k_0^2 \mathbf{E} = k_0^2 (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{E} + i\omega\mu_0 \nabla \times \left[(\bar{\bar{\mu}}_r - \bar{\bar{I}}) \cdot \mathbf{H} \right], \mathbf{r} \in \Omega \tag{3}$$

Derivation of the VIE

Define equivalent electric volume current as

$$\mathbf{J} = -i\omega\epsilon_0(\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{E} \tag{4}$$

and equivalent magnetic volume current as

$$\mathbf{M} = -i\omega\mu_0(\bar{\bar{\mu}}_r - \bar{\bar{I}}) \cdot \mathbf{H}. \tag{5}$$

Hence

$$\nabla \times \nabla \times \mathbf{E} - k_0^2\mathbf{E} = i\omega\mu_0\mathbf{J}^s, \mathbf{r} \in \Omega_0 \tag{6}$$

$$\nabla \times \nabla \times \mathbf{E} - k_0^2\mathbf{E} = i\omega\mu_0\mathbf{J} - \nabla \times \mathbf{M}, \mathbf{r} \in \Omega \tag{7}$$

Recall:

$$\nabla \times \nabla \times \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0) - k_0^2\bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0) = \bar{\bar{\mathbf{I}}}\delta(\mathbf{r} - \mathbf{r}_0) \tag{8}$$

where the free-space dyadic Green's functions

$$\bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0) = \left(\bar{\bar{\mathbf{I}}} + \frac{1}{k_0^2}\nabla\nabla\right) G(\mathbf{r}, \mathbf{r}_0), \text{ with } G_0(\mathbf{r}, \mathbf{r}_o) = \frac{\exp(ik_0|\mathbf{r} - \mathbf{r}_0|)}{4\pi|\mathbf{r} - \mathbf{r}_0|} \tag{9}$$

Derivation of the VIE

Total electric field can be expressed as

$$\mathbf{E}(\mathbf{r}_0) = \int_{\Omega \cup \Omega_0} [i\omega\mu_0 \mathbf{J}(\mathbf{r}) - \nabla \times \mathbf{M}(\mathbf{r}) + \mathbf{J}^s(\mathbf{r})] \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r} \tag{10}$$

or

$$\mathbf{E}(\mathbf{r}_0) = \int_{\Omega} [i\omega\mu_0 \mathbf{J}(\mathbf{r}) - \nabla \times \mathbf{M}(\mathbf{r})] \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r} + \int_{\Omega_s} i\omega\mu_0 \mathbf{J}^s(\mathbf{r}) \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r} \tag{11}$$

Since $\mathbf{J}^s$ is the impressed source current, the incident electric field is given by

$$\mathbf{E}^{inc} = \int_{\Omega_s} i\omega\mu_0 \mathbf{J}^s(\mathbf{r}) \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r}. \tag{12}$$

Hence, the electric field volume integral equation can be written as

$$\mathbf{E}(\mathbf{r}_0) = \mathbf{E}(\mathbf{r}_0)^{inc} + \int_{\Omega} i\omega\mu_0 \mathbf{J}(\mathbf{r}) \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r} - \int_{\Omega} \nabla \times \mathbf{M}(\mathbf{r}) \cdot \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}_0)\, d\mathbf{r} \tag{13}$$

Derivation of the VIE

Since the total field is a sum of incident and scattered fields

$$\mathbf{E}^{tot} = \mathbf{E}^{inc} + \mathbf{E}^{sca} \tag{14}$$

the scattered fields, after some algebraic manipulations, can be expressed as

$$\mathbf{E}^{sca} = \frac{-1}{i\omega\epsilon_0}(\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \int_\Omega G\mathbf{J}\,\mathrm{d}\Omega - \nabla \times \int_\Omega G\mathbf{M}\,\mathrm{d}\Omega. \tag{15}$$

Analogously, for the magnetic field we can write

$$\mathbf{H}^{sca} = \frac{-1}{i\omega\mu_0}(\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \int_\Omega G\mathbf{M}\,\mathrm{d}\Omega + \nabla \times \int_\Omega G\mathbf{J}\,\mathrm{d}\Omega. \tag{16}$$

Electric current volume integral equation JVIE

Assume $\bar{\bar{\mu}}_r = \bar{\bar{I}}$:

$$\mathbf{E} = \mathbf{E}^{inc} - \frac{1}{i\omega\epsilon_0}(\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \int_\Omega G\mathbf{J}\,\mathrm{d}\Omega \tag{17}$$

Use the definition of the equivalent current

$$\mathbf{J} = -i\omega\epsilon_0(\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{E} \tag{18}$$

to derive the electric current volume integral equation JVIE

$$\mathbf{J}^{inc} = \mathbf{J} - (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot (\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \boldsymbol{\mathcal{S}}(\mathbf{J}). \tag{19}$$

Here the volume potential operator is defined as

$$\boldsymbol{\mathcal{S}}(\mathbf{f}) = \int_\Omega G\mathbf{f}\,\mathrm{d}\Omega \tag{20}$$

Other formulations

We can write formulations also for the electric field or flux density

JVIE:

$$\mathbf{J}^{inc} = \mathbf{J} - (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot (\nabla\nabla + k_0^2 \bar{\bar{I}}) \cdot \boldsymbol{\mathcal{S}}(\mathbf{J}). \tag{21}$$

DVIE:

$$\mathbf{D}^{inc} = \bar{\bar{\epsilon}}_r^{-1} \cdot \mathbf{D} - (\nabla\nabla + k_0^2 \bar{\bar{I}}) \cdot \boldsymbol{\mathcal{S}} \left((\bar{\bar{I}} - \bar{\bar{\epsilon}}_r^{-1}) \cdot \mathbf{D} \right) \tag{22}$$

EVIE:

$$\mathbf{E}^{inc} = \bar{\bar{\epsilon}}_r \cdot \mathbf{E} - \nabla \times \nabla \times \boldsymbol{\mathcal{S}} \left((\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{E} \right) \tag{23}$$

Mapping properties

$$\begin{aligned} \text{JVIE} : &\quad L^2(\Omega) \to L^2(\Omega) \\ \text{DVIE} : &\quad H_{div}(\Omega) \to H_{curl}(\mathbb{R}^3) \\ \text{EVIE} : &\quad H_{curl}(\Omega) \to H_{div}(\mathbb{R}^3) \end{aligned}$$

Discretizations

Projection method can be used for discretizing the equations

- JVIE with L^2-conforming basis and testing functions e.g. piecewise constant functions
- DVIE with div-conforming basis and testing functions (L^2-dual space of H_{curl} is H_{div})
- EVIE with curl-conforming basis and testing functions (L^2-dual space of H_{div} is H_{curl})

Possible issues:
In source free region $\nabla \cdot \mathbf{D} = 0$ and $\nabla \cdot \mathbf{B} = 0$

- In DVIE, there is no guarantee that the solution satisfies $\nabla \cdot \mathbf{D} = 0$
- The EVIE equation is force to be valid in the space in which $\nabla \cdot \mathbf{D} = 0$ might not hold

Projection method

Solve linear problem of the form

$$Lu = f, \quad L : U \rightarrow F, f \in F$$

U and F are some Hilbert spaces, and the unknown $u \in U$
Expand the unknown with a set of basis functions b_n span $B_N \subset U$

$$u \approx \tilde{u}_N = \sum_{n=1}^{N} c_n b_n$$

Require the residual

$$R_N = L\tilde{u}_N - f,$$

to be orthogonal to the space $T_M \subset F$ spanned by testing functions t_m

$$< t_m, R_N >_F = 0, \forall m = 1, 2, ..., M$$

Weak formulation for JVIE

Discretization of JVIE:

$$\mathbf{J}^{inc} = \mathbf{J} - (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot (\nabla\nabla + k_0^2 \bar{\bar{I}}) \cdot \mathcal{S}(\mathbf{J}). \tag{24}$$

Expand $\mathbf{J}$ with piecewise constant functions as

$$\mathbf{J} \approx \sum_{n}^{N_t} (c_n^x \hat{\mathbf{x}} + c_n^y \hat{\mathbf{y}} + c_n^z \hat{\mathbf{z}}) / \sqrt{V_k} = \sum_{i=1}^{3} \sum_{n=1}^{N_t} c_n^i \mathbf{b}_n^i \tag{25}$$

Use Galerkin's technique for testing the equation i.e. $\mathbf{t}_m^j = \mathbf{b}_n^i$

$$\left\langle \mathbf{t}_m^j, \mathbf{J}^{inc} \right\rangle = \sum_{i,n} \left\langle \mathbf{t}_m^j, \mathbf{b}_n^j - (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot (\nabla\nabla + k_0^2 \bar{\bar{I}}) \cdot \mathcal{S}(\mathbf{b}_n^i) \right\rangle c_n^i \tag{26}$$

for all $m = 1, ..., N_t, j = 1, 2, 3$

Matrix equation JVIE

Matrix form:

$$A^{ji}_{mn} c^i_n = f^j_m \tag{27}$$

Elements of the system matrix

$$\begin{aligned} A^{ji}_{mn} &= \int_{T_m} \mathbf{t}^j_m \cdot \mathbf{b}^i_n \, \mathrm{d}V \\ + \int_{\partial T_m} \mathbf{n} \cdot (\bar{\bar{\tau}}^T_m \cdot \mathbf{t}^j_m) \cdot &\int_{\partial T_n} G \, \mathbf{n}' \cdot \mathbf{b}^i_n \, \mathrm{d}S' \, \mathrm{d}S \\ - \int_{T_m} \mathbf{t}^j_m \cdot \bar{\bar{\tau}}_m \cdot k_0^2 \bar{\bar{I}} \cdot &\int_{T_n} G \mathbf{b}^i_n \, \mathrm{d}V' \mathrm{d}V, \end{aligned}$$

Weakly singular integrals!

$$f^j_m = \int_{T_m} \mathbf{t}^j_m \cdot \mathbf{J}^{inc} \tag{28}$$

Weak formulation for DVIE

Discretization of DVIE:

$$\mathbf{D}^{inc} = \bar{\bar{\epsilon}}_r^{-1}\mathbf{D} - (\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \boldsymbol{\mathcal{S}}\left((\bar{\bar{I}} - \bar{\bar{\epsilon}}_r^{-1}) \cdot \mathbf{D}\right). \tag{29}$$

Expand $\mathbf{D}$ with div-conforming functions (SWG) as

$$\mathbf{D} \approx \sum_n^{N_f} c_n \mathbf{b}_n^{div} \tag{30}$$

Use Galerkin's technique for testing the equation i.e. $\mathbf{t}_m^{div} = \mathbf{b}_n^{div}$

$$\left\langle \mathbf{t}_m^{div}, \mathbf{D}^{inc} \right\rangle = \sum_i \left\langle \mathbf{t}_m^{div}, \bar{\bar{\epsilon}}_r^{-1} \cdot \mathbf{b}_n^{div} - (\nabla\nabla + k_0^2\bar{\bar{I}}) \cdot \boldsymbol{\mathcal{S}}\left((\bar{\bar{I}} - \bar{\bar{\epsilon}}_r^{-1}) \cdot \mathbf{b}_n^{div}\right) \right\rangle c_n \tag{31}$$

for all $m = 1, ..., N_f$

Matrix equation DVIE

Matrix form:

$$A_{mn} c_n = f_m \tag{32}$$

Elements of the system matrix

$$\begin{aligned} A_{mn} = \int_{T_m} \mathbf{t}_m^{div} \cdot \bar{\bar{\epsilon}}_r^{-1} \cdot \mathbf{b}_n^{div} \,\mathrm{d}V \\ - \int_{T_m} \nabla \cdot \mathbf{t}_m^{div} \int_{T_n} \nabla G \cdot (\bar{\bar{I}} - \bar{\bar{\epsilon}}_r^{-1}) \cdot \mathbf{b}_n^{div} \,\mathrm{d}V' \mathrm{d}V \\ - \int_{\partial T_m} \mathbf{n} \cdot \mathbf{t}_m^{div} \int_{T_n} \nabla G \cdot (\bar{\bar{I}} - \bar{\bar{\epsilon}}_r^{-1}) \cdot \mathbf{b}_n^{div} \,\mathrm{d}V' \mathrm{d}S \\ - \int_{T_m} \mathbf{t}_m^{div} \cdot k_0^2 \bar{\bar{I}} \cdot \int_{T_n} G \mathbf{b}_n^{div} \,\mathrm{d}V' \mathrm{d}V, \end{aligned}$$

Surface integrals cancel out on each element boundaries except on the outer boundary!

$$f_m = \int_{T_m} \mathbf{t}_m^{div} \cdot \mathbf{D}^{inc} \tag{33}$$

Weak formulation for EVIE

Discretization of EVIE:

$$\mathbf{E}^{inc} = \bar{\bar{\epsilon}}_r \cdot \mathbf{E} - \nabla \times \nabla \times \boldsymbol{\mathcal{S}} \left((\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{E} \right). \tag{34}$$

Expand $\mathbf{E}$ with curl-conforming functions edge-elements as

$$\mathbf{E} \approx \sum_{n}^{N_e} c_n \mathbf{b}_n^{curl} \tag{35}$$

Use Galerkin's technique for testing the equation i.e. $\mathbf{t}_m^{curl} = \mathbf{b}_n^{curl}$

$$\left\langle \mathbf{t}_m^{curl}, \mathbf{E}^{inc} \right\rangle = \sum_i \left\langle \mathbf{t}_m^{curl}, \bar{\bar{\epsilon}}_r \cdot \mathbf{b}_n^{curl} - \nabla \times \nabla \times \boldsymbol{\mathcal{S}} \left((\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{b}_n^{curl} \right) \right\rangle c_n \tag{36}$$

for all $m = 1, \ldots, N_f$

Matrix equation EVIE

Matrix form:

$$A_{mn} c_n = f_m \tag{37}$$

Elements of the system matrix

$$A_{mn} = \int_{T_m} \mathbf{t}_m^{div} \cdot \bar{\bar{\epsilon}}_r \cdot \mathbf{b}_n^{curl} \, \mathrm{d}V$$
$$- \int_{T_m} \nabla \times \mathbf{t}_m^{curl} \cdot \int_{T_n} \nabla G \times (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{b}_n^{curl} \, \mathrm{d}V' \mathrm{d}V$$
$$- \int_{\partial T_m} \mathbf{n} \times \mathbf{t}_m^{curl} \cdot \int_{T_n} \nabla G \times (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot \mathbf{b}_n^{curl} \, \mathrm{d}S' \mathrm{d}V$$

Surface integrals cancel out on each element boundaries except on the outer boundary!

$$f_m = \int_{T_m} \mathbf{t}_m^{curl} \cdot \mathbf{E}^{inc} \tag{38}$$

Computation of matrix elements

Singular Green's function:

$$G(\mathbf{r},\mathbf{r}') = \frac{\exp(ik_0|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|} \tag{39}$$

The Green's function is singular at $\mathbf{r} = \mathbf{r}'$

We want to compute integrals of the form

$$\begin{gathered} \int_{T_m} G(\mathbf{r},\mathbf{r}') N_i \,\mathrm{d}V \\ \int_{\partial T_m} G(\mathbf{r},\mathbf{r}') N_i \,\mathrm{d}S \end{gathered} \tag{40}$$

Standard numerical integration schemes do not work efficiently when $\mathbf{r}$ is close to $\mathbf{r}'$

Singularity extraction, singularity cancelletion, direct evaluation method,...

Singularity extraction technique

Extract singular terms and compute them analytically. Remaininng part is smooth and can be computed with e.g. Gaussian quadrature

$$\int_\Omega G \, \mathrm{d}\Omega = \int_\Omega \frac{e^{ikR}}{4\pi R} - \frac{1}{4\pi} \sum_{n=0,2,\ldots}^{N} \frac{(ik)^n}{n!} R^{n-1} \, \mathrm{d}\Omega + \frac{1}{4\pi} \sum_{n=0,2,\ldots}^{N} \frac{(ik)^n}{n!} \int_\Omega R^{n-1} \, \mathrm{d}\Omega$$

- First term: sufficiently smooth (integrate numerically)
- Second term: singular or discontinuous derivative (integrate analytically)
- Analytical formulae exist for linear triangles and tetrahedra

Pre-corrected FFT algorithm (pFFT)

FFT-based acceleration technique

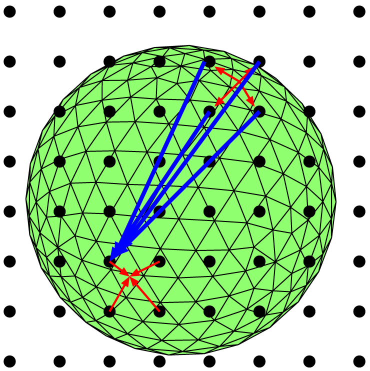
Integral equations $\Rightarrow$ full matrix A: storage $\mathcal{O}(N^2)$, matrix-vector multiplication $\mathcal{O}(N^2)$

Iterative solution

- $r_n = Ax_n - b$
- $x_{n+1} = x_n + Rr_n$

Acceleration

- Uniform grid
- Anterpolation
- Propagation
- Interpolation
- Near zone corrections



FFT-based acceleration technique: Inter- and Anterpolation

Near-field matching scheme (pFFT)

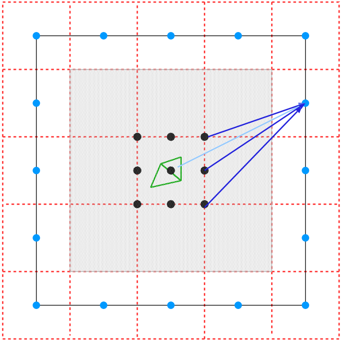
Find the grid coefficients by matching near fields produced by original sources and auxiliary sources

$$P^{gt}\hat{b} = P^{qt} b$$

$$P^{gt}_{ij} = \frac{e^{ik|\mathbf{r}^t - \mathbf{r}^g|}}{4\pi|\mathbf{r}^t - \mathbf{r}^g|}$$

$$P^{qt}_{ij} = \int_{spt(b_j)} \mathbf{b}_j(\mathbf{r}) \frac{e^{ik|\mathbf{r}^t - \mathbf{r}|}}{4\pi|\mathbf{r}^t - \mathbf{r}|} \, \mathrm{d}V$$

$$dP^{qt}_{ij} = \int_{spt(b_j)} \nabla \cdot \mathbf{b}_j(\mathbf{r}) \frac{e^{ik|\mathbf{r}^t - \mathbf{r}|}}{4\pi|\mathbf{r}^t - \mathbf{r}|} \, \mathrm{d}V$$



Transformation matrices (sparse)

$$\Lambda(k,j) = [P^{gt}]^{\dagger} P^{qt,j}, \Gamma(k,j) = [dP^{gt}]^{\dagger} P^{qt,j}$$

FFT-based acceleration technique: Propagation 1D case

1D example: Consider 1D uniform grid

$$G_{mn} = \frac{\exp(ik|\mathbf{r}_m - \mathbf{r}_n|)}{4\pi|\mathbf{r}_m - \mathbf{r}_n|} = G_{m-n} \tag{41}$$

hence

$$\mathbf{G} = \begin{pmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \\ G_{31} & G_{32} & G_{33} & G_{34} \\ G_{41} & G_{42} & G_{43} & G_{44} \end{pmatrix} = \begin{pmatrix} G_0 & G_{-1} & G_{-2} & G_{-3} \\ G_1 & G_0 & G_{-1} & G_{-2} \\ G_2 & G_1 & G_0 & G_{-1} \\ G_3 & G_2 & G_1 & G_0 \end{pmatrix} \tag{42}$$

level-one block Toeplitz! We only need to store vector

$$\mathbf{g} = \begin{bmatrix} G_0 & G_1 & G_2 & G_3 & 0 & G_3 & G_2 & G_1 \end{bmatrix} \tag{43}$$

FFT-based acceleration technique: Propagation 1D case

Next we want to compute matrix vector product

$$\mathbf{y} = \mathbf{G}\mathbf{x} \tag{44}$$

where $\mathbf{x} = [x_1, x_2, x_3, x_4]^T$. By zero-padding $\mathbf{x}$ vector $\mathbf{x} = [x_1, x_2, x_3, x_4, 0, 0, 0, 0]^T$, the matrix vector multiplication can be calculated by convolution

$$\mathbf{y} = \mathbf{g} * \mathbf{x}, \tag{45}$$

which is evaluated in Fourier domain via FFT

$$\mathbf{y} = \mathcal{F}^{-1}(\mathcal{F}(\mathbf{g}) \cdot \mathcal{F}(\mathbf{x})) \tag{46}$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ denote Fourier and inverse Fourier transforms, and $\cdot$ represents the element-wise multiplication

FFT-based acceleration technique: Matrix vector multiplication

In 3D we obtain level-three Block-Toeplitz $G -> $ Storage $\mathcal{O}(N_{grid})$

- Matrix vector product becomes convolution
- Can be efficiently evaluated with the FFT $\mathcal{O}(N_{grid} log N_{grid})$

JVIE (isotropic case):

$$\begin{aligned} A_{mn}^{ji} = \int_{\partial T_m} \mathbf{n} \cdot \mathbf{t}_m^j (\epsilon_r - 1) \int_{\partial T_n} G\, \mathbf{n}' \cdot \mathbf{b}_n^i \, \mathrm{d}S' \, \mathrm{d}S \\ - \int_{T_m} \mathbf{t}_m^j \cdot (\epsilon_r - 1) k_0^2 \bar{\bar{I}} \cdot \int_{T_n} G \mathbf{b}_n^i \, \mathrm{d}V' \mathrm{d}V, \end{aligned} \tag{47}$$

The matrix-vector multiplication can be approximated as

$$\begin{aligned} A^{FFT} x = (\epsilon_r - 1) \Gamma^T \mathcal{F}^{-1} \mathcal{F}(G) \mathcal{F}(\Gamma x)) \\ -(\epsilon_r - 1) k^2 \Lambda^T \mathcal{F}^{-1} \mathcal{F}(G) \mathcal{F}(\Lambda x)) \end{aligned} \tag{48}$$

FFT-based acceleration technique: Matrix vector multiplication

In 3D we obtain level-three Block-Toeplitz $G -> $ Storage $\mathcal{O}(N_{grid})$

- Matrix vector product becomes convolution
- Can be efficiently evaluated with the FFT $\mathcal{O}(N_{grid} log N_{grid})$

JVIE (isotropic case):

$$\begin{aligned} A^{ji}_{mn} = & \int_{\partial T_m} \mathbf{n} \cdot \mathbf{t}^j_m (\epsilon_r - 1) \int_{\partial T_n} G\, \mathbf{n}' \cdot \mathbf{b}^i_n \, \mathrm{d}S' \, \mathrm{d}S \\ & - \int_{T_m} \mathbf{t}^j_m \cdot (\epsilon_r - 1) k_0^2 \overline{\overline{I}} \cdot \int_{T_n} G \mathbf{b}^i_n \, \mathrm{d}V' \mathrm{d}V, \end{aligned} \tag{47}$$

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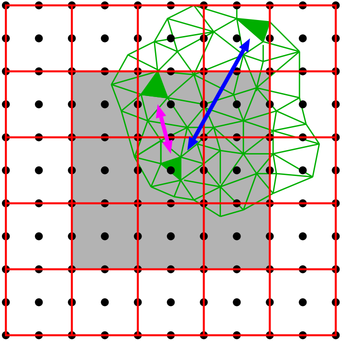
- Six 3-D FFTs and IFFTs / iteration $\mathcal{O}(N_{grid} log(N_{grid}))$
- Six sparse matrix-vector multiplication / iteration $\mathcal{O}(N_{tet})$

FFT-based acceleration technique: Near-zone correction

- Inter/anterpolations are not accurate when **r** and **r**′ are close to each other
- Compute near zone interactions directly



- $Ax = A^{FFT}x + A^{corr}x$
- $A^{corr} = A^{dir} - A^{FFT}$
- A^{corr} is sparse $->$ storage $\mathcal{O}(N)$
- matrix-vector multiplication $\mathcal{O}(N)$ operations

FFT-JVIE algorithm

- Create auxiliary grid $\mathcal{O}(N_{grid})$
- Compute $\mathcal{F}(G)$ $\mathcal{O}(N_{grid} log(N_{grid}))$
- Construct inter/anterpolators Γ, Λ $\mathcal{O}(N_{tet})$
- Compute near-zone corrections A^{corr} $\mathcal{O}(N_{tet})$
- Compute excitation vector b $\mathcal{O}(N_{tet})$
- Start GMRES
- Compute matrix vector product in each iteration step
  $Ax = A^{corr}x + k^2\Gamma^T\mathcal{F}^{-1}(\mathcal{F}(G)\mathcal{F}(\Gamma x)) - \Lambda^T\mathcal{F}^{-1}(\mathcal{F}(G)\mathcal{F}(\Lambda x))$

  $N_{iter}(\mathcal{O}(N_{grid} log N_{grid}) + \mathcal{O}(N_{tet})$
- Compute scattering quantities
- Total complexity:
  time: $N_{iter}\mathcal{O}(N_{grid} log(N_{grid}) + N_{tet})$
  memory: $\mathcal{O}(N_{grid} + N_{tet})$

Multilevel fast multipole algorithm (MLFMA)

Addition theorem for the Green's function

Addition theorem for the Green's function

$$\frac{\exp(ik|\mathbf{d}+\mathbf{D}|)}{|\mathbf{d}+\mathbf{D}|} = ik\sum_{n=0}^{\infty}(-1)^n(2n+1)j_n(k|\mathbf{d}|)h_n^{(2)}(k|\mathbf{D}|)P_n(\hat{\mathbf{d}}\cdot\hat{\mathbf{D}}) \quad (49)$$

valid when $|\mathbf{D}| > |\mathbf{d}|$ and where

j_n = spherical Bessel function
$h_n^{(2)}$ = spherical Hankel function
P_n = Legendre polynomial

Plane-wave expansion

$$4\pi i^n j_n(k|\mathbf{d}|)P_n(\hat{\mathbf{d}}\cdot\hat{\mathbf{D}}) = \int_{S^2}\exp(ik\hat{\mathbf{k}}\cdot\mathbf{d})P_n(\hat{\mathbf{k}}\cdot\hat{\mathbf{D}})\,\mathrm{d}\hat{\mathbf{k}} \quad (50)$$

"change of basis" from spherical to plane-wave

Plane-wave expansion of the Green's function

Plane-wave expansion of the Green's function

$$G(\mathbf{D}+\mathbf{d}) = \frac{\exp(ik|\mathbf{d}+\mathbf{D}|)}{4\pi|\mathbf{d}+\mathbf{D}|} \approx \int_{S^2} T(\mathbf{k},\mathbf{D})\exp(i\mathbf{k}\cdot\mathbf{d})\,\mathrm{d}\hat{\mathbf{k}} \qquad (51)$$

when $|\mathbf{D}| > |\mathbf{d}|$. Integration is over the surface of unit sphere S^2 The Rokhlin's translation function is defined as

$$T_L = \frac{ik}{(4\pi)^2}\sum_{n=0}^{L} i^n(2n+1)h_n^{(1)}(kD)P_n\left(\frac{\mathbf{k}\cdot\mathbf{D}}{kD}\right). \qquad (52)$$

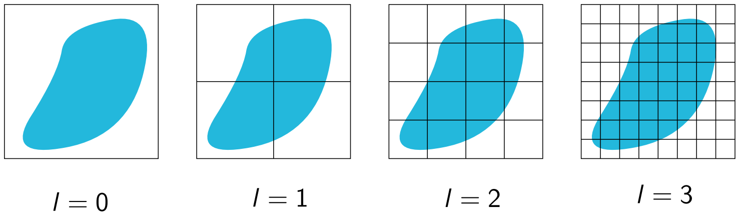
Truncate L as

$$L = k|\mathbf{d}| + 1.8\left(log_{10}\frac{1}{\varepsilon}\right)^{2/3}(k|\mathbf{d}|)^{1/3} \qquad (53)$$

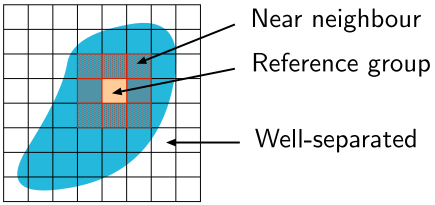
where ε is desired digits of accuracy

Oct-tree decomposition

Decomposition in subdomains by an oct-tree

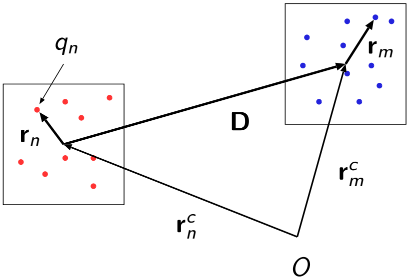


Two groups are called near neighbours if they share a common vertex



Translation

Consider two well-separated cubes source points $\mathbf{r}_n$ and field points $\mathbf{r}_m$



Field due to charges q_n at point $\mathbf{r}_m^c + \mathbf{r}_m$ can be computed as

$$F(\mathbf{r}_m^c + \mathbf{r}_m) = \int_{S^2} \left(\sum_n -q_n \exp(i\mathbf{k} \cdot \mathbf{r}_n) \right) T_L(\mathbf{k}, \mathbf{D}) \exp(i\mathbf{k} \cdot \mathbf{r}_m) \, \mathrm{d}\hat{\mathbf{k}} \quad (54)$$

JVIE case

Recall:

$$A_{pq}^{ij} = \int_{T_p} \mathbf{t}_p^j \cdot (\bar{\bar{\epsilon}}_r - \bar{\bar{I}}) \cdot (\nabla\nabla + k_0^2 \bar{\bar{I}}) \cdot \int_{T_q} G \mathbf{b}_q^i \, \mathrm{d}V' \mathrm{d}V \tag{55}$$

This can be written as

$$A_{pq}^{ij} = \int_{S^2} (\mathbf{v}(p, \mathbf{k}, n))^* \; T_L(\mathbf{k}, \mathbf{D}) \, \mathbf{v}(q, \mathbf{k}, m) \, \mathrm{d}\hat{\mathbf{k}} \tag{56}$$

where

$$\mathbf{v}(q, \mathbf{k}, n) = (k\bar{\bar{I}} - \mathbf{k}\mathbf{k}) \cdot \int_{T_q} \mathbf{b}_q^i \exp(i\mathbf{k} \cdot \mathbf{r}_n) \, \mathrm{d}V \tag{57}$$

Single level algorithm

Setup

1. Subdivide the scatterer in subdomains by an oct-tree
2. Compute interaction matrix directly for elements that belongs to neighbour groups $A = A^{far} + A^{near}$
3. Compute and store radiation patterns $\mathbf{v}(q, \mathbf{k}, n)$
4. Compute and store translators $T_L(\mathbf{k}, \mathbf{D}_{mn})$ for all well-separated groups

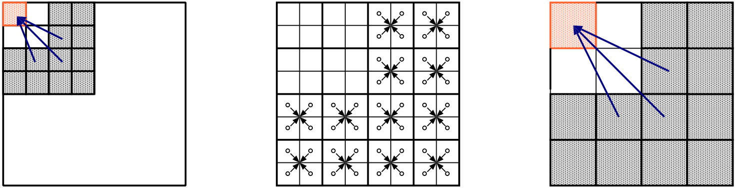
Iterative solver: matrix vector multiplication

1. Compute sparse matrix vector product $y^{near} = A^{near}x$
2. Aggregation $\mathbf{a}_{i,n} = \sum_q \mathbf{v}(q, \mathbf{k}_i, n)\mathbf{x}_q$
3. Translation $\mathbf{t}_{i,m} = \sum_n T_L(\mathbf{k}_i, \mathbf{D}_{mn})\mathbf{a}_{i,n}$
4. Dissaggregation $y_p^{far} = \sum_i (\mathbf{v}(p, \mathbf{k}_i, m))^* w_i \cdot \mathbf{t}_{i,m}$
5. $y = y^{near} + y^{far}$

Computational Complexity $\mathcal{O}(N^{1.5})$

Multilevel algorithm

based on hierarchical oct-tree structure



Translation $l = 3$ Interpolation from level 3 to 2 Translation $l = 2$

Inter- and anterpolation operators for moving between levels

Translations performed only between interacting groups in levels $l = 2, 3, \ldots, l_{max}$

Interacting groups: Well-separated groups whose parent groups are neighbours

Computational complexity $\mathcal{O}(NlogN)$