Implicit handling of multilayered material substrates in full-wave SCUFF-EM calculations

Homer Reid

August 16, 2017

Contents

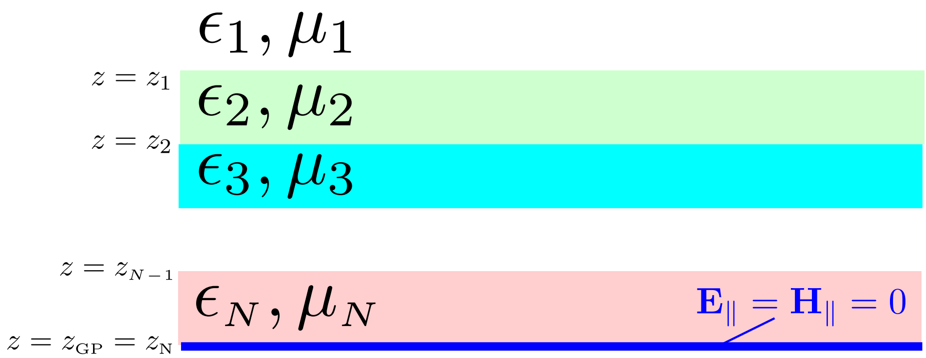

Figure 1: Geometry of the layered substrate. The nth layer has relative permittivity and permeability ϵ_n, μ_n, and its lower surface lies at $z = z_n$. The ground plane, if present, lies at $z = z_{\rm GP}$.

1 Overview

In a previous memo[1] I considered SCUFF-STATIC electrostatics calculations in the presence of a multilayered dielectric substrate. In this memo I extend that discussion to the case of *full-wave* (i.e. nonzero frequencies beyond the quasistatic regime) scattering calculations in the SCUFF-EM core library.

Substrate geometry

As shown in Figure 1, I consider a multilayered substrate consisting of N material layers possibly terminated by a perfectly-conducting ground plane. The uppermost layer (layer 1) is the infinite half-space above the substrate. The nth layer has relative permittivity and permeability ϵ_n, μ_n, and its lower surface lies at $z = z_n$. The ground plane, if present, lies at $z \equiv z_{\rm N} \equiv z_{\rm GP}$. If the ground plane is absent, layer N is an infinite half-space[2] ($z_{\rm N} = -\infty$).

Definition of the substrate DGF

I will use the symbol $\mathbf{\Gamma}(\omega, \mathbf{x}_{\rm D}, \mathbf{x}_{\rm S})$ for the *total* 6×6 dyadic Green's function relating time-harmonic fields at $\mathbf{x}_{\rm D}$ to sources at $\mathbf{x}_{\rm S}$:

$$\mathbf{\Gamma} = \left(\begin{array}{cc} \mathbf{\Gamma}^{\rm EE} & \mathbf{\Gamma}^{\rm EM} \\ \mathbf{\Gamma}^{\rm ME} & \mathbf{\Gamma}^{\rm MM} \end{array} \right) \tag{1a}$$

[1] "Implicit handling of multilayered dielectric substrates in SCUFF-STATIC"

[2] As in the electrostatic case, this means that a finite-thickness substrate consisting of N material layers is described as a stack of $N+1$ layers in which the bottommost layer is an infinite vacuum half-space.

with the 3×3 subblocks defined by

$$\Gamma_{ij}^{\text{PQ}}(\omega, \mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = \begin{pmatrix} i\text{-component of P-type field at } \mathbf{x}_{\text{D}} \text{ due to } j\text{-} \\ \text{directed Q-type source at } \mathbf{x}_{\text{S}}, \text{ all fields and} \\ \text{sources having time dependence} \sim e^{-i\omega t} \end{pmatrix} \tag{1b}$$

Homogeneous DGF In an infinite *homogeneous* medium with relative permittivity and permeability $\{\epsilon^r, \mu^r\}$, $\mathbf{\Gamma}$ reduces to its homogeneous form, for which I will use the symbol $\mathbf{\Gamma}^{0r}$ (where the r index labels the medium, which in this case will be one of the layers in Figure 1, i.e. $r \in \{1, 2, \cdots, N\}$):

$$\mathbf{\Gamma}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = \mathbf{\Gamma}^{0r}(\mathbf{x}_{\text{D}} - \mathbf{x}_{\text{S}}), \qquad \Big(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}} \in \text{infinite homogeneous medium } r\Big)$$

$$\mathbf{\Gamma}^{0r}(\mathbf{r}) \equiv \begin{pmatrix} ik_r Z_0 Z^r \mathbf{G}(k_r, \mathbf{r}) & ik_r \mathbf{C}(k_r, \mathbf{r}) \\ -ik_r \mathbf{C}(k_r, \mathbf{r}) & \frac{ik_r}{Z_0 Z^r} \mathbf{G}(k_r, \mathbf{r}) \end{pmatrix} \tag{2}$$

Inhomogeneous DGF On the other hand, in the presence of the multilayered substrate the full DGF $\mathbf{\Gamma}$ receives corrections, which may be thought of as the fields radiated by surface currents induced on the interfacial surfaces of the substrate, and which I will denote by the symbol $\boldsymbol{\mathcal{G}}$:

$$\mathbf{\Gamma}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = \boldsymbol{\mathcal{G}}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) + \begin{cases} \mathbf{\Gamma}^{0r}(\mathbf{x}_{\text{D}} - \mathbf{x}_{\text{S}}), & \mathbf{x}_{\text{S}} \in \text{layer r} \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

Like $\mathbf{\Gamma}$, $\boldsymbol{\mathcal{G}}$ is a 6×6 matrix with a 2×2 block structure:

$$\boldsymbol{\mathcal{G}}(\omega; \mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = \begin{pmatrix} \boldsymbol{\mathcal{G}}^{\text{EE}} & \boldsymbol{\mathcal{G}}^{\text{EM}} \\ \boldsymbol{\mathcal{G}}^{\text{ME}} & \boldsymbol{\mathcal{G}}^{\text{MM}} \end{pmatrix} \tag{4a}$$

with the 3×3 subblocks defined by

$$\mathcal{G}_{ij}^{\text{PQ}} = \begin{pmatrix} \text{P-type field at } \mathbf{x}_{\text{D}} \text{ due to surface currents on} \\ \text{substrate interface layers induced by } j\text{-directed} \\ \text{Q-type source at } \mathbf{x}_{\text{S}} \end{pmatrix} \tag{4b}$$

LIBSUBSTRATE is a code for numerical computation of $\boldsymbol{\mathcal{G}}$.

Organization of SCUFF-EM implementation and this memo

The full-wave substrate implementation in SCUFF-EM consists of multiple working parts that fit together in a somewhat modular fashion.

Roughly speaking, the computational problem may be divided into two parts:

(a) For given source and evaluation (or "destination") points $\{\mathbf{x}_{\text{S}}, \mathbf{x}_{\text{D}}\}$ at a given angular frequency ω in the presence of a multilayer substrate, numerically compute the substrate DGF correction $\boldsymbol{\mathcal{G}}(\omega, \mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}})$. This task is independent of SCUFF-EM and is implemented by a standalone library called LIBSUBSTRATE, described in Section 2 of this memo.

(b) For a SCUFF-EM geometry in the presence of a substrate, compute the substrate corrections to the BEM system matrix $\mathbf{M}$ and RHS vector $\mathbf{v}$, as well as the substrate corrections to post-processing quantities such as scattered fields. This is done by the file `Substrate.cc` in LIBSCUFF and is described in Section **??** of this memo.

2 LIBSUBSTRATE: Numerical computation of substrate Green's functions

Numerical evaluation of substrate contributions to dyadic Green's functions is handled by a C++ library called LIBSUBSTRATE. Although this library is packaged and distributed with SCUFF-EM and depends on other support libraries in the SCUFF-EM distribution, it is independent of the particular integral-equation formulation implemented by LIBSCUFF, and thus should be of general utility beyond SCUFF-EM.

2.1 Overview of computational strategy

LIBSUBSTRATE decomposes the problem of computing $\boldsymbol{\mathcal{G}}$ into several logical steps, as follows:

1. Solve a linear system to obtain the Fourier-space representation $\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q})$. Here $\mathbf{q} = (q_x, q_y)$ is a 2D Fourier variable. (Section 2.2.)

2. Reduce the two-dimensional integral over $\mathbf{q}$ to a one-dimensional integral over $|\mathbf{q}| \equiv q$. (Section 2.3.)

3. Evaluate the q integral using established methods for evaluating Sommerfeld integrals. (Section **??**.)

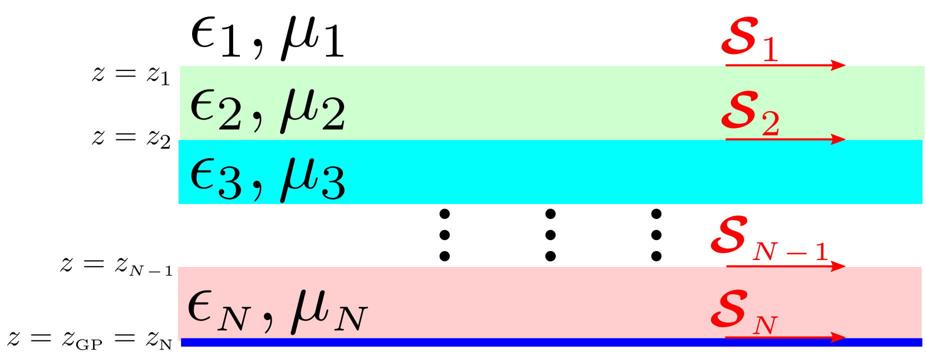

Figure 2: Effective surface-current approach to treatment of multilayer substrate. External field sources induce a distribution of electric and magnetic surface currents $\boldsymbol{\mathcal{S}}_n = \binom{\mathbf{K}_n}{\mathbf{N}_n}$ on the nth material interface, and the fields radiated by these effective currents account for the disturbance presented by the substrate.

2.2 Computation of Fourier-space DGF $\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q})$

To compute the substrate correction to the fields of external sources, I consider the effective tangential electric and magnetic surface currents $\mathbf{K}$ and $\mathbf{N}$ induced on the interfacial layers by the external field sources (Figure 2). This is the direct extension to full-wave problems of the formalism I used in the electrostatic case, and it comports well with the spirit of surface-integral-equation methods.

More specifically, on the material interface layer at $z = z_n$ I have a four-vector surface-current density $\boldsymbol{\mathcal{S}}_n(\boldsymbol{\rho})$, where $\boldsymbol{\rho} = (x, y)$ and the components of $\boldsymbol{\mathcal{S}}$ are

$$\boldsymbol{\mathcal{S}}_n(\boldsymbol{\rho}) = \left(\begin{array}{c} K_x(\boldsymbol{\rho}) \\ K_y(\boldsymbol{\rho}) \\ N_x(\boldsymbol{\rho}) \\ N_y(\boldsymbol{\rho}) \end{array}\right). \tag{5}$$

Fields in layer interiors. I will adopt the convention that the lower (upper) bounding surface for each region is the positive (negative) bounding surface for that region in the usual sense of SCUFF-EM regions and surfaces (in which the sign of a {surface,region} pair $\{\mathcal{S}, \mathcal{R}\}$ is the sign with which surface currents on $\mathcal{S}$ contribute to fields in $\mathcal{R}$). Thus, at a point $\mathbf{x} = (\boldsymbol{\rho}, z)$ in the interior of layer n ($z_{n-1} > z > z_n$), the six-vector of total fields $\boldsymbol{\mathcal{F}} = \left(\begin{array}{c} \mathbf{E} \\ \mathbf{H} \end{array}\right)$ reads

$$\boldsymbol{\mathcal{F}}_n(\boldsymbol{\rho}, z) = -\boldsymbol{\Gamma}^{0n}(z_{n-1}) \star \boldsymbol{\mathcal{S}}_{n-1} + \boldsymbol{\Gamma}^{0n}(z_n) \star \boldsymbol{\mathcal{S}}_n + \boldsymbol{\mathcal{F}}_n^{\rm ext}(\boldsymbol{\rho}, z) \tag{6}$$

where $\boldsymbol{\mathcal{F}}_n^{\rm ext}$ are the externally-sourced (incident) fields due to sources in layer n, $\boldsymbol{\Gamma}^{0n}$ is the 6×6 homogeneous dyadic Green's function for material layer n, and $\star$ is shorthand for the convolution operation

$$\text{“}\boldsymbol{\mathcal{F}}(\boldsymbol{\rho},z)\equiv\boldsymbol{\Gamma}(z')\star\boldsymbol{\mathcal{S}}\text{''}\qquad\Longrightarrow\qquad\boldsymbol{\mathcal{F}}(\boldsymbol{\rho},z)=\int\boldsymbol{\Gamma}(\boldsymbol{\rho}-\boldsymbol{\rho}',z-z')\cdot\boldsymbol{\mathcal{S}}(\boldsymbol{\rho}')d\boldsymbol{\rho}'\tag{7}$$

where the integral extends over the entire interfacial plane. I will evaluate convolutions of this form using the 2D Fourier representation of $\boldsymbol{\Gamma}^{0n}$:

$$\boldsymbol{\Gamma}^{0n}(\boldsymbol{\rho},z)=\int\frac{d^2\mathbf{q}}{(2\pi)^2}\widetilde{\boldsymbol{\Gamma}^{0n}}(\mathbf{q},z)e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\tag{8a}$$

$$\widetilde{\boldsymbol{\Gamma}^{0n}}(\mathbf{q},z)=\frac{1}{2}\left(\begin{array}{cc}-\frac{\omega\mu_0\mu_n}{q_{zn}}\widetilde{\mathbf{G}}^{\pm} & +\widetilde{\mathbf{C}}^{\pm}\\ -\widetilde{\mathbf{C}}^{\pm} & -\frac{\omega\epsilon_0\epsilon_n}{q_{zn}}\widetilde{\mathbf{G}}^{\pm}\end{array}\right)e^{iq_z|z|}\tag{8b}$$

$$\widetilde{\mathbf{G}}^{\pm}(\mathbf{q},k)=\left(\begin{array}{ccc}1&0&0\\0&1&0\\0&0&1\end{array}\right)-\frac{1}{k^2}\left(\begin{array}{ccc}q_x^2 & q_xq_y & \pm q_xq_z\\ q_yq_x & q_y^2 & \pm q_yq_z\\ \pm q_zq_x & \pm q_zq_y & q_z^2\end{array}\right)\tag{8c}$$

$$\widetilde{\mathbf{C}}^{\pm}(\mathbf{q},k)=\left(\begin{array}{ccc}0 & \mp 1 & +q_y/q_z\\ \pm 1 & 0 & -q_x/q_z\\ -q_y/q_z & +q_x/q_z & 0\end{array}\right)\tag{8d}$$

$$k_n\equiv\sqrt{\epsilon_0\epsilon_n\mu_0\mu_n}\cdot\omega,\qquad q_z\equiv\sqrt{k^2-|\mathbf{q}|^2},\qquad \pm=\text{sign }z.\tag{8e}$$

With this representation, convolutions like (7) become products in Fourier space:

$$\boldsymbol{\Gamma}(z')\star\boldsymbol{\mathcal{S}}=\boldsymbol{\mathcal{F}}(\boldsymbol{\rho},z)=\int\frac{d^2\mathbf{q}}{(2\pi)^2}\widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q},z)e^{i\mathbf{q}\cdot\boldsymbol{\rho}},\quad\text{with}\quad\widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q},z)=\widetilde{\boldsymbol{\Gamma}}(\mathbf{q},z-z')\widetilde{\boldsymbol{\mathcal{S}}}(\mathbf{q})$$

Surface currents from incident fields. To determine the surface currents induced by given incident-field sources, I apply boundary conditions. The boundary condition at $z=z_n$ is that the tangential $\mathbf{E},\mathbf{H}$ fields be continuous: in Fourier space, we have

$$\widetilde{\boldsymbol{\mathcal{F}}}_{\parallel}(\mathbf{q},z=z_n^+)=\widetilde{\boldsymbol{\mathcal{F}}}_{\parallel}(\mathbf{q},z=z_n^-)\tag{9}$$

The fields just **above** the interface ($z\to z_n^+$) receive contributions from three sources:

- Surface currents at $z=z_{n-1}$, which contribute with a minus sign and via the Green's function for region n;
- Surface currents at $z=z_n$, which contribute with a plus sign and via the Green's function for region n; and
- external field sources in region n.

The fields just **below** the interface ($z=z_n^-$) receive contributions from three sources:

- Surface currents at $z=z_n$, which contribute with a minus sign and via the Green's function for region $n+1$;
- Surface currents at $z=z_{n+1}$, which contribute with a plus sign and via the Green's function for region $n+1$; and
- external field sources in region $n+1$.

Then equation (9) reads (temporarily omitting $\mathbf{q}$ arguments)

$$\begin{aligned}
&-\widetilde{\mathbf{\Gamma}^{0n}}_{\parallel}(z_n-z_{n-1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n-1}+\widetilde{\mathbf{\Gamma}^{0n}}_{\parallel}(0^+)\cdot\widetilde{\boldsymbol{\mathcal{S}}}_n+\widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n\parallel}(z_n)\\
&\qquad=-\widetilde{\mathbf{\Gamma}^{0,n+1}}\|(0^-)\cdot\widetilde{\boldsymbol{\mathcal{S}}}_n+\widetilde{\mathbf{\Gamma}^{0,n+1}}\|(z_n-z_{n+1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n+1}+\widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n+1\|}(z_n)
\end{aligned}$$

or

$$\mathbf{M}_{n,n-1}\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n-1}+\mathbf{M}_{n,n}\cdot\widetilde{\boldsymbol{\mathcal{S}}}_n+\mathbf{M}_{n,n+1}\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n+1}=\widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n+1\|}(z_n)-\widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n\|}(z_n) \tag{10}$$

with the 4×4 matrix blocks[3]

$$\mathbf{M}_{n,n-1}=-\widetilde{\mathbf{\Gamma}^{0n}}_{\parallel}(z_n-z_{n-1}) \tag{13a}$$

$$\mathbf{M}_{n,n}=+\widetilde{\mathbf{\Gamma}^{0n}}_{\parallel}(0^+)+\widetilde{\mathbf{\Gamma}^{0,n+1}}_{\parallel}(0^-) \tag{13b}$$

$$\mathbf{M}_{n,n+1}=-\widetilde{\mathbf{\Gamma}^{0,n+1}}_{\parallel}(z_n-z_{n+1}) \tag{13c}$$

Writing down equation (10) equation for all N dielectric interfaces yields a $4N\times4N$ system of linear equations, with triadiagonal 4×4 block form, relating the surface currents on all layers to the external fields due to sources in all regions:

$$\mathbf{M}\cdot\mathbf{s}=\mathbf{f} \tag{14}$$

[3]The 4×4 $\mathbf{M}$ blocks here have 2×2 block structure:

$$\mathbf{M}_{n,n}=\sum_{r\in\{n,n+1\}}\frac{1}{2}\left(\begin{array}{cc}-\frac{\omega\epsilon_r}{Z_0q_{zr}}\mathbf{g}(k_r,\mathbf{q}) & 0\\ 0 & -\frac{\omega\mu_rZ_0}{q_{zr}}\mathbf{g}(k_r,\mathbf{q})\end{array}\right) \tag{11}$$

$$\mathbf{M}_{n,n\pm1}=\frac{1}{2}\left(\begin{array}{cc}-\frac{\omega\epsilon_r}{Z_0q_{zr}}\mathbf{g}(k_r,\mathbf{q}) & \mathbf{c}^{\pm}\\ -\mathbf{c}^{\pm} & -\frac{\omega\mu_rZ_0}{q_{zn^*}}\mathbf{g}(k_r,\mathbf{q})\end{array}\right)e^{iq_{zr}|z_n-z_{n\pm1}|} \tag{12}$$

where I put $r\equiv\begin{cases}n, & \text{for } \mathbf{M}_{n,n-1}\\ n+1, & \text{for } \mathbf{M}_{n,n+1}\end{cases}$. and

$$\mathbf{g}(k;\mathbf{q})=\mathbf{1}-\frac{\mathbf{q}\mathbf{q}^\dagger}{k^2},\qquad \mathbf{c}^{\pm}=\left(\begin{array}{cc}0 & \mp1\\ \pm1 & 0\end{array}\right)$$

where $\mathbf{M}$ is the $4N\times 4N$ block-tridiagonal matrix (13) and where the $4N$-vectors $\mathbf{s}$, $\mathbf{f}$ read

$$\mathbf{s}=\left(\begin{array}{c}\widetilde{\boldsymbol{\mathcal{S}}}_1\\ \widetilde{\boldsymbol{\mathcal{S}}}_2\\ \widetilde{\boldsymbol{\mathcal{S}}}_3\\ \vdots\\ \widetilde{\boldsymbol{\mathcal{S}}}_N\end{array}\right),\qquad \mathbf{f}=\left(\begin{array}{c}-\widetilde{\boldsymbol{\mathcal{F}}}_{1\parallel}(z_1)+\widetilde{\boldsymbol{\mathcal{F}}}_{2\parallel}(z_1)\\ -\widetilde{\boldsymbol{\mathcal{F}}}_{2\parallel}(z_2)+\widetilde{\boldsymbol{\mathcal{F}}}_{3\parallel}(z_2)\\ -\widetilde{\boldsymbol{\mathcal{F}}}_{3\parallel}(z_3)+\widetilde{\boldsymbol{\mathcal{F}}}_{3\parallel}(z_4)\\ \vdots\\ -\widetilde{\boldsymbol{\mathcal{F}}}_{N-1,\parallel}(z_{N-1})+\widetilde{\boldsymbol{\mathcal{F}}}_{N\parallel}(z_{N-1})\end{array}\right).$$

Solving (14) yields the induced surface currents on all layers in terms of the incident fields:

$$\mathbf{s}=\mathbf{W}\cdot\mathbf{f}\quad\text{where}\quad \mathbf{W}\equiv\mathbf{M}^{-1}$$

or, more explicitly,

$$\widetilde{\boldsymbol{\mathcal{S}}}_n=\sum_m W_{nm}\mathbf{f}_m \tag{15}$$

Surface currents induced by point sources

For DGF computations the incident fields arise from a single point source—say, a j-directed source in region s. Then the only nonzero length-4 blocks of the RHS vector in (14) are $\mathbf{f}_{s-1},\mathbf{f}_{\text{S}}$ with components ($\ell=\{1,2,4,5\}$)

$$\Big(\mathbf{f}_{s-1}\Big)_\ell=-\widetilde{\Gamma}^{0s}_{\ell j}(z_{s-1}-z_{\text{S}}),\qquad \Big(\mathbf{f}_{s}\Big)_\ell=+\widetilde{\Gamma}^{0s}_{\ell j}(z_{\text{S}}-z_{\text{S}}) \tag{16}$$

and the surface currents on interface layer n are obtained by solving (15):

$$\begin{aligned}\widetilde{\boldsymbol{\mathcal{S}}}_n&=\mathbf{W}_{n,s-1}\,\mathbf{f}_{s-1}+\mathbf{W}_{n,s}\,\mathbf{f}_s\\ &=\sum_{p=0}^{1}(-1)^{p+1}\mathbf{W}_{n,s-1+p}\cdot\widetilde{\mathbf{\Gamma}^{0s}}_{\parallel,j}(z_{\text{S}}-z_{s-1+p})\end{aligned} \tag{17}$$

Fields due to surface currents

Given the surface currents induced by a j-directed point source at $\mathbf{x}_{\text{S}}$, I evaluate the fields due to these currents to get the substrate DGF contribution $\boldsymbol{\mathcal{G}}$. If the evaluation point $\mathbf{x}_{\text{D}}$ lies in region d, then the fields receive contributions from the surface currents at z_{d-1} and z_{D}, propagated by the homogeneous DGF for region d:

$$\begin{aligned}\widetilde{\boldsymbol{\mathcal{F}}}(z_{\text{D}})&=-\widetilde{\mathbf{\Gamma}^{0d}}(z_{\text{D}}-z_{d-1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{d-1}+\widetilde{\mathbf{\Gamma}^{0d}}(z_{\text{D}}-z_{\text{D}})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_d\\ &=\sum_{q=0}^{1}(-1)^{q+1}\widetilde{\mathbf{\Gamma}^{0d}}(z_{\text{D}}-z_{d+q-1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{d+q-1}\end{aligned}$$

(The minus sign in the first term arises because, in my convention, surface currents on the upper surface of a region contribute to the fields in that region with a minus sign). Inserting (17), the i component here—which is the ij component of the substrate DGF—is

$$\widetilde{\mathcal{G}}_{ij}(z_{\mathrm{D}}, z_{\mathrm{S}}) = \sum_{p,q=0}^{1} (-1)^{p+q} \widetilde{\mathbf{\Gamma}^{0d}}_{i,\parallel}(z_{\mathrm{D}} - z_{d-1+q}) \mathbf{W}_{d-1+q,s-1+p} \widetilde{\mathbf{\Gamma}^{0s}}_{\parallel,j}(z_{s-1+p} - z_{\mathrm{S}}). \tag{18}$$

The calculation of equation (18) is carried out by the routine `GetGTwiddle` in LIBSUBSTRATE.

2.3 Reduction of 2D integrals over q to 1D (Sommerfeld) integrals over q

The real-space DGF correction is the inverse Fourier transform of (18):

$$\boldsymbol{\mathcal{G}}(\boldsymbol{\rho}, z_{\text{D}}, z_{\text{S}}) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}; z_{\text{D}}; z_{\text{S}}) e^{i\mathbf{q}\cdot\boldsymbol{\rho}}$$

or, in polar coordinates $(q_x, q_y) = (q\cos\theta_{\mathbf{q}}, q\sin\theta_{\mathbf{q}})$,

$$= \int_0^\infty \frac{q\,dq}{2\pi} \int_0^{2\pi} \frac{d\theta_q}{2\pi} \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}; z_{\text{D}}; z_{\text{S}}) e^{iq\rho\cos(\theta_q - \theta_\rho)}.$$

The goal of this section is to integrate out the angular variable θ_q to reduce the 2D integral over $\mathbf{q}$ to a 1D integral over $q = |\mathbf{q}|$.

Scalar×matrix structure of $\widetilde{\boldsymbol{\mathcal{G}}}$ I begin by noting that $\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q})$ may be decomposed as a sum of scalar functions of $q = |\mathbf{q}|$ times q-independent matrix-valued functions of $\theta_{\mathbf{q}}$:

$$\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}) = \sum_{n=1}^{18} \widetilde{g}^{(n)}(q) \boldsymbol{\Lambda}^{(n)}(\theta_{\mathbf{q}}) \tag{19}$$

For example, the upper two quadrants read

$$\widetilde{\mathcal{G}}^{\text{EE}}(\mathbf{q}) = \widetilde{g}^{\text{EE}0\parallel}(q)\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{0\parallel}} + \widetilde{g}^{\text{EE}0z}(q)\underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\mathbf{\Lambda}^{0z}}$$

$$+ \widetilde{g}^{\text{EE1A}}(q)\underbrace{\begin{pmatrix} 0 & 0 & \cos\theta_{\mathbf{q}} \\ 0 & 0 & \sin\theta_{\mathbf{q}} \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{1}(\theta_{\mathbf{q}})} + \widetilde{g}^{\text{EE1B}}(q)\underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \cos\theta_{\mathbf{q}} & \sin\theta_{\mathbf{q}} & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{1\dagger}(\theta_{\mathbf{q}})}$$

$$+ \widetilde{g}^{\text{EE2}}(q)\underbrace{\begin{pmatrix} \cos^2\theta_{\mathbf{q}} & \cos\theta_{\mathbf{q}}\sin\theta_{\mathbf{q}} & 0 \\ \cos\theta_{\mathbf{q}}\sin\theta_{\mathbf{q}} & \sin^2\theta_{\mathbf{q}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{2A}(\theta_{\mathbf{q}})}$$

$$\widetilde{\mathcal{G}}^{\text{EM}}(\mathbf{q}) = g^{\text{EM}0\parallel}(q)\underbrace{\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{0\times}} + g^{\text{EM2}}(q)\underbrace{\begin{pmatrix} \cos\theta_{\mathbf{q}}\sin\theta_{\mathbf{q}} & \sin^2\theta_{\mathbf{q}} & 0 \\ -\cos^2\theta_{\mathbf{q}} & -\cos\theta_{\mathbf{q}}\sin\theta_{\mathbf{q}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbf{\Lambda}^{2\times}}$$

$$+ g^{\text{EM1A}}(q)\underbrace{\begin{pmatrix} 0 & 0 & -\sin\theta_{\mathbf{q}} \\ 0 & 0 & +\cos\theta_{\mathbf{q}} \\ 0 & 0 & 1 \end{pmatrix}}_{\mathbf{\Lambda}^{1\times}} + g^{\text{EM1B}}(q)\underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\sin\theta_{\mathbf{q}} & \cos\theta_{\mathbf{q}} & 1 \end{pmatrix}}_{\mathbf{\Lambda}^{1\times\dagger}}$$

and the expressions for $\widetilde{\mathcal{G}}^{\text{ME}}$ and $\widetilde{\mathcal{G}}^{\text{MM}}$ are similar, involving the same Λ matrices with different $\widetilde{g}$ prefactors.

The real-space substrate DGF reads

$$\mathcal{G}(\boldsymbol{\rho}, z_{\text{D}}, z_{\text{S}}) = \int_0^\infty \frac{q\,dq}{2\pi}\int_0^{2\pi}\frac{d\theta_q}{2\pi}\widetilde{\mathcal{G}}(\mathbf{q}; z_{\text{D}}; z_{\text{S}})e^{iq\rho\cos(\theta_q-\theta_\rho)}.$$

Insert (19):

$$= \sum_n \int_0^\infty \frac{q\,dq}{2\pi}\widetilde{g}^{(n)}(q)\int_0^{2\pi}\frac{d\theta_q}{2\pi}\mathbf{\Lambda}^{(n)}(\theta_q)e^{iq\rho(\theta_q-\theta_\rho)}$$

Evaluate θ_q integrals using Table **??**:

$$= \sum_m \mathbf{\Lambda}^{(m)}(\theta_\rho)\int_0^\infty \widetilde{\mathfrak{g}}^{(m)}(q)\,dq$$

$$\frac{1}{2\pi}\int_0^{2\pi} e^{iq\rho\cos(\theta_q-\theta_\rho)}\left\{\begin{array}{c} 1 \\ \cos\theta_q \\ \sin\theta_q \\ \cos^2\theta_q \\ \cos\theta_q\sin\theta_q \\ \sin^2\theta_q \end{array}\right\} d\theta_q = \left\{\begin{array}{l} J_0(q\rho) \\ iJ_1(q\rho)\cos\theta_\rho \\ iJ_1(q\rho)\sin\theta_\rho \\ -J_2(q\rho)\cos^2\theta_\rho + \frac{J_1(q\rho)}{q\rho} \\ -J_2(q\rho)\cos\theta_\rho\sin\theta_\rho \\ -J_2(q\rho)\sin^2\theta_\rho + \frac{J_1(q\rho)}{q\rho} \end{array}\right\},$$

Figure 3: Table of integrals used to reduce 2D integrals over $\mathbf{q}$ to 1D integrals over $|q|$.

$$\widetilde{\mathfrak{g}}^{\text{EE0}\parallel}(q) = \frac{q}{2\pi}\left[\widetilde{g}^{\text{EE0}\parallel}(q)J_0(q\rho) + \widetilde{g}^{\text{EE2}}(q)\frac{J_1(q\rho)}{q\rho}\right]$$

2.4 Evaluation of Sommerfeld integrals

3 SCUFF-EM integration: Substrate contributions to BEM matrix and RHS vector

$$\begin{aligned}\boldsymbol{\mathcal{G}}^{\text{PQ}}(\rho,\theta,z_{\text{D}},z_{\text{S}}) &= \sum_{\nu p} g^{\text{PQ}\nu p}(\rho,z_{\text{D}},z_{\text{S}})\boldsymbol{\Lambda}^{\text{PQ}\nu p}(\theta) \\ g^{\text{PQ}\nu p}(\rho) &= \int \frac{qdq}{(2\pi)}\widetilde{g}^{\text{PQ}\nu p}(q)J_\nu(q\rho)e^{i\alpha(q,z_{\text{D}},z_{\text{S}})}\boldsymbol{\Lambda}^{\text{PQ}\nu p}(\theta)\end{aligned}$$

$$M^{\text{PQ}}_{\alpha\beta}\Big\langle \mathbf{b}_\alpha \Big| \boldsymbol{\mathcal{G}}^{\text{PQ}} \Big| \mathbf{b}_\beta \Big\rangle$$

4 Unit-test framework

The LIBSUBSTRATE standalone library comes with a unit-test suite to test core functionality related to calculation of substrate DGFs. Separately, the unit-test suite for LIBSCUFF includes tests to check the integration of LIBSUBSTRATE into LIBSCUFF.

4.1 LIBSUBSTRATE unit tests

4.1.1 `tGTwiddle`

The unit-test code `tGTwiddle.cc` tests that the full Fourier-space DGF $\widetilde{\mathbf{\Gamma}}(\mathbf{q}, z_{\text{D}}, z_{\text{S}})$ satisfies the appropriate boundary conditions at each layer of the layered substrate, namely

$$C^{+}(\mathrm{P}, i, \ell)\widetilde{\Gamma}^{\text{PQ}}_{ij}(\mathbf{q}, z_\ell + \eta, z_{\text{S}})C^{-}(\mathrm{P}, i, \ell)\widetilde{\Gamma}^{\text{PQ}}_{ij}(\mathbf{q}, z_\ell - \eta, z_{\text{S}}) \tag{20}$$

where

$$C^{\pm}(P, i, \ell) = \begin{cases} 1, & i \in \{x, y\} \\ \epsilon^{\pm}_{\ell}, & i = z, P = E \\ \mu^{\pm}_{\ell}, & i = z, P = H \end{cases}$$

where $\{\epsilon, \mu\}^{\pm}_{\ell}$ are the material properties for the layer above/below z_ℓ, i.e. (Figure **??**)

$$\{\epsilon_\ell, \mu_\ell\}^{+} = \{\epsilon_\ell, \mu_\ell\}, \qquad \{\epsilon_\ell, \mu_\ell\}^{-} = \{\epsilon_{\ell+1}, \mu_{\ell+1}\}.$$

If a ground plane is present, we have the additional condition

$$\widetilde{\Gamma}^{\text{PQ}}_{ij}(q, z_{\text{GP}}, z_{\text{S}}) = 0 \quad \text{for} \quad i \in \{x, y\}. \tag{21}$$

Conditions (**??**) and (**??**) must hold *independently* of the indices $\mathrm{Q} \in \{\mathrm{E}, \mathrm{H}\}$ and $j \in \{1, 2, 3\}$ and of the values of $\mathbf{q}$ and z_{S}.