Implicit handling of multilayered dielectric substrates in SCUFF-STATIC

Homer Reid

April 3, 2017

Contents

1	Overview			2
2.2 Including implicit substrates in Scuff-em electrostatic			Running SCUFF-EM calculations with implicit substrates rate definition file	s 3 3
3	Theory: How it works			5
	3.1	Electr	ostatic Green's function in the presence of dielectric substrate	5
		3.1.1	Basic strategy	5
		3.1.2	Expressing G in terms of σ	6
		3.1.3	Applying boundary conditions to determine σ	7
		3.1.4	Evaluating Bessel-function integrals	8
		3.1.5	Special handling for source and evaluation points on di-	
			electric interface layer	8
		3.1.6	Example	10
	3.2 Assembling the modified BEM system		abling the modified BEM system	13
A	Pot	ential	due to surface-charge layer	14

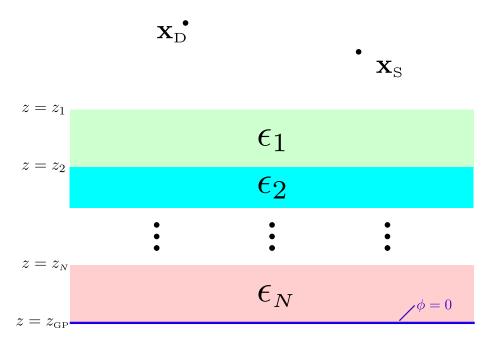


Figure 1: Geometry of the layered dielectric substrate. The *n*th layer has relative DC permittivity ϵ_n , and its upper surface lies at $z=z_n$. The ground plane, if present, lies at $z=z_{\rm GP}$.

1 Overview

In this memo I describe an extension to the SCUFF-EM electrostatics module to allow implicit treatment of layered substrates consisting of multiple dielectric layers, of arbitrary thicknesses and permittivities, with an optional perfectly conducting ground plane (Figure 1).¹

Proceeding in reverse order from theory to practice, the structure of this memo is as follows:

- In Section 2 I discuss the usage of this new feature in SCUFF-EM electrostatics calculations.
- In Section 3 I discuss the physics and mathematics of the underlying method and some technical details regarding its implementation in SCUFF-EM.

¹Note that, if there is no ground plane, then the bottommost layer in Figure 1 (layer N) is assumed to be infinitely thick (it has no lower surface). Thus, a physical substrate consisting of M finite-thickness dielectric layers with no ground plane is treated here as a stack of N=M+1 layers in which the bottommost layer is vacuum, i.e. $\epsilon_N=1$.

2 Practice: Running Scuff-em calculations with implicit substrates

2.1 Substrate definition file

Referring to Figure 1, a substrate geometry is specified by

- the z-coordinate of the upper surface of each dielectric layer
- the permittivity of each layer
- the z-coordinate of the optional ground plane.

This data is specified to SCUFF-EM in the form of a simple text file (conventionally given file extension .substrate) consisting of one line for each dielelectric layer plus an optional line specifying the ground plane, of the form

```
z1 Material1
z2 Material2
...
zN MaterialN
zGP GROUNDPLANE
```

where e.g.

- **z1** is the z-coordinate of the upper surface of layer 1
- Material1 is a SCUFF-EM material designation describing the material of layer 1
- The optional final line, which invokes the fixed keyword GROUNDPLANE, specifies that a perfectly-conducting ground plane lives at coordinate z=zGP.

Note that, because of the scale invariance of electrostatics, there is no intrinsic length unit here; instead, numerical values specified for z_n refer to the same length units—be they microns, millimeters, or what have you— used in mesh files and --EPFiles.

Here are some examples of .substrate files:

• An infinite-thickness dielectric slab with $\epsilon_r = 4$ filling the lower half-space:

```
0 CONST_EPS_4
```

• A finite-thickness dielectric slab with $\epsilon_r = 4$ and thickness 1 whose upper surface is the xy plane:

```
O CONST_EPS_4
-1 VACUUM
```

• The same finite-thickness slab as before, but now lying atop a ground plane:

```
O CONST_EPS_4
-1 GROUNDPLANE
```

• A unit-thickness layer of $\epsilon_r = 4$ atop an infinite-thickness slab of silicon:

```
O CONST_EPS_4
-1 SILICON
```

• A unit-thickness layer of $\epsilon_r = 4$ atop a thickness-2 layer of silicon:

```
O CONST_EPS_4
-1 SILICON
-3 VACUUM
```

• Same as previous item, but now with a ground plane beneath the silicon layer:

```
O CONST_EPS_4
-1 SILICON
-3 GROUNDPLANE
```

2.2 Including implicit substrates in SCUFF-EM electrostatics calculations

To run SCUFF-EM electrostatics calculations with an implicit substrate described by a file MySubstrate.substrate, there are two ways to proceed.

• You can include the line

```
SUBSTRATE MySubstrate.substrate
```

to the <code>.scuffgeo</code> file defining the meshed geometry. Then the substrate will be present for all calculations—including both API calculations and command-line calculations—involving that geometry file.

• For command-line calculations, you can add the option

```
--SubstrateFile MySubstrate.substrate
```

to the SCUFF-STATIC command line. The substrate file specified in this way will override any SUBSTRATE specification that may be present in the .scuffgeo file.

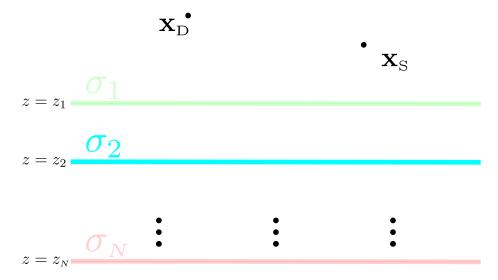


Figure 2: In the surface-integral-equation picture of the geometry of Figure 1, the effect of the dielectric substrate is represented by a collection of surface-charge layers $\{\sigma_n(\boldsymbol{\rho})\}$, where σ_n lives at the upper surface of dielectric layer n, i.e. at $z=z_n$.

3 Theory: How it works

This discussion consists of two parts:

- I first derive a mathematical expression for the electrostatic Green's function in the presence of the multilayered dielectric substrate—that is, the function $G(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}})$ giving the electrostatic potential at \mathbf{x}_{D} due to a unitstrength point source at \mathbf{x}_{S} in the presence of the substrate (Figure 1). (The subscripts "D" and "S" stand for "destination" and "source.")
- Then I discuss how the discretized surface-integral-equation system assembled by SCUFF-EM is modified to accommodate this modified Green's function.

3.1 Electrostatic Green's function in the presence of dielectric substrate

3.1.1 Basic strategy

In keeping with the spirit of the surface-integral-equation method, I will proceed by determining the effective surface-charge densities induced at each dielectric interface by the point source (Figure 2). For an N-layer substrate there are N such layers, with the surface-charge density at the interface between layers n-1

and n denoted by $\sigma_n(\rho)$. Note that I do not include a surface-charge layer for the ground plane, whose effect I capture implicitly via the method of images.

3.1.2 Expressing G in terms of σ

I write the full Green's function $G(\mathbf{x}_{D}, \mathbf{x}_{S})$ —the potential at $\mathbf{x}_{D} = (\boldsymbol{\rho}_{D}, z_{D})$ due to a unit-strength² point charge at $\mathbf{x}_{S} = (\boldsymbol{\rho}_{S}, z_{S})$ —as a sum of contributions from (a) the point source itself, (b) the image charge of the point source (if a ground plane is present), and (c) the surface-charge layers:

$$G(\mathbf{x}_{\mathrm{D}}, \mathbf{x}_{\mathrm{S}}) = G_{0}(\mathbf{x}_{\mathrm{D}}, \mathbf{x}_{\mathrm{S}}) - \delta_{\mathrm{GP}}G_{0}(\mathbf{x}_{\mathrm{D}}, \mathbf{x}_{\mathrm{S}}^{*}) + \sum_{n} \mathcal{G}^{\sigma_{n}}(\mathbf{x}_{\mathrm{D}})$$

$$\mathcal{G}(\mathbf{x}_{\mathrm{D}}, \mathbf{x}_{\mathrm{S}})$$

$$(1)$$

where

$$G_0(\mathbf{x}_{ ext{ iny D}}, \mathbf{x}_{ ext{ iny S}}) = rac{1}{4\pi |\mathbf{x}_{ ext{ iny D}} - \mathbf{x}_{ ext{ iny S}}|}$$

is the bare vacuum Green's function [and $\mathcal{G}(\mathbf{x}_D, \mathbf{x}_S)$ is the correction due to the substrate],

$$\mathbf{x}_{S}^{*} = (x_{S}, y_{S}, z_{S}^{*}), \quad z_{S}^{*} \equiv 2z_{GP} - z_{S}$$

are the coordinates of the image charge due to the ground plane at $z=z_{\text{GP}}$,

$$\delta_{GP} = \begin{cases} 0, & \text{no ground plane} \\ 1, & \text{ground plane} \end{cases}$$

and $\phi(\mathbf{x}; \sigma, z)$ is the potential at \mathbf{x} due to a surface-charge layer $\sigma(\boldsymbol{\rho})$ at z. Putting $\boldsymbol{\rho} \equiv (\boldsymbol{\rho}_{\mathrm{D}} - \boldsymbol{\rho}_{\mathrm{S}})$ and $\boldsymbol{\rho} \equiv |\boldsymbol{\rho}|$ and using the results of Appendix A, we have

$$G(\rho; z_{\rm D}, z_{\rm S}) = G_0(\rho; z_{\rm D}, z_{\rm S}) - \delta_{\rm GP} G_0(\rho; z_{\rm D}, z_{\rm S}^*) + \sum_n \int \frac{dq}{4\pi} \tilde{\sigma}_n(q) J_0(q\rho) \zeta(z_{\rm D}, z_n)$$

and the z-directed electric field $E_z = -\frac{\partial G}{\partial z}$ reads

$$E_{z}(\rho; z_{\rm D}, z_{\rm S}) = E_{z0}(\rho; z_{\rm D}, z_{\rm S}) - \delta_{\rm GP} E_{z0}(\rho; z_{\rm D}, z_{\rm S}^{*}) + \sum_{n} \int \frac{q dq}{4\pi} \widetilde{\sigma}_{n}(q) J_{0}(q\rho) \xi(z_{\rm D}, z_{n})$$

with

$$E_{z0}(\rho, z, z') \equiv \frac{(z - z')}{4\pi[\rho^2 + (z - z')^2]^{3/2}}.$$

The functions ζ and ξ are defined in Appendix A.

 $^{^2}$ I assume that charge is measured in units of $\frac{1}{\epsilon_0}$ (the inverse vacuum permittivity), so that there is no factor of ϵ_0 in the denominators of expressions like (1). In this memo, ϵ_0 refers to the relative permittivity of the uppermost medium in Figure 1.

3.1.3 Applying boundary conditions to determine σ

The boundary condition at the interface between dielectric layers m-1 and m reads

$$\epsilon_{m-1}E_z(\rho; z_m^+; z_s) = \epsilon_m E_z(\rho; z_m^-; z_s)$$

with z_m^\pm denoting points lying just above or just below z_m and with the convention $\epsilon_0=1$. Using the above results, we have

$$\int \frac{qdq}{4\pi} J_0(q\rho) \sum_n \left[\epsilon_{m-1} \xi(q; z_m^+; z_n) - \epsilon_m \xi(q; z_m^-; z_n) \right] \widetilde{\sigma}_n(q)$$

$$= \left(\epsilon_m - \epsilon_{m-1} \right) \left[E_{z0}(\rho; z_m; z_s) - \delta_{GP} E_{z0}(\rho; z_m, z_s^*) \right]$$

or, inverse Bessel-transforming³ and rearranging slightly,

$$\sum_{n} \underbrace{\left[\frac{\epsilon_{m-1}\xi(q; z_{m}^{+}; z_{n}) - \epsilon_{m}\xi(q; z_{m}^{-}; z_{n})}{\epsilon_{m-1} - \epsilon_{m}}\right]}_{M_{mn}} \widetilde{\sigma}_{n}(q) = -\underbrace{4\pi \left[\widetilde{E}_{z0}(q, z_{m}, z_{s}) - \delta_{GP}\widetilde{E}_{z0}(q, z_{m}, z_{s}^{*})\right]}_{\epsilon_{m}}$$
(2)

with

$$4\pi \widetilde{E_{z0}}(q, z, z') = 4\pi \int_0^\infty \rho J_0(q\rho) E_{z0}(\rho, z, z') d\rho$$
$$= \operatorname{sign}(z - z') e^{-q|z - z'|}.$$

Equation (2) is an $N \times N$ linear system of the form

$$\mathcal{M}\widetilde{\boldsymbol{\sigma}}(q) = \mathbf{e} \tag{3}$$

that we may solve to compute the Fourier transforms $\widetilde{\sigma_n}(q)$ of the surface-charge densities at each dielectric interface. The elements of the \mathcal{M} matrix and \mathbf{e} vector read

$$\mathcal{M}_{mn} = \begin{cases} \xi(q; z_m; z_n), & m \neq n \\ \frac{\epsilon_{m-1} \xi(q; z_m^+; z_m) - \epsilon_m \xi(q; z_m^-; z_m)}{\epsilon_{m-1} - \epsilon_m}, & m = n \end{cases}$$
(4a)

$$e_m = -\xi(q; z_m; z_s). \tag{4b}$$

$$\int_0^\infty \rho J_0(q\rho)J_0(q'\rho)d\rho = \frac{1}{q}\delta(q-q').$$

³Multiply both sides by $\rho J_0(q'\rho)$, integrate over all ρ , and use

3.1.4 Evaluating Bessel-function integrals

The contributions of the surface-charge layers to the Green's function and its derivatives are given by

$$\begin{pmatrix} \mathcal{G}^{\sigma} \\ -\partial_{x}\mathcal{G}^{\sigma} \\ -\partial_{y}\mathcal{G}^{\sigma} \\ -\partial_{z}\mathcal{G}^{\sigma} \end{pmatrix} = \int \sum_{n} \frac{dq}{4\pi} \widetilde{\sigma}_{n}(q) \underbrace{\begin{pmatrix} J_{0}(q\rho)\zeta(q; z_{D}; z_{n}) \\ qxJ_{1}(q\rho)\zeta(q; z_{D}; z_{n})/\rho \\ qyJ_{1}(q\rho)\zeta(q; z_{D}; z_{n})/\rho \\ qJ_{0}(q\rho)\xi(q; z_{D}; z_{n}) \end{pmatrix}}_{\mathcal{J}(q,\rho,z_{D},z_{n})}.$$
(5)

The q integral here may be evaluated by numerical quadrature, with values of $\sigma_n(q)$ at each quadrature point determined by solving the system (3).

3.1.5 Special handling for source and evaluation points on dielectric interface layer

The convergence of the integrals (5) is generally speeded by factors like $e^{-q|z_{\rm S,D}-z_p|}$, which cause the integrand to decay exponentially as $q\to\infty$. However, when $z_{\rm S}=z_{\rm D}=z_p$ (source and destination point both lie on the pth dielectric interface) the integrand is undamped and numerical quadrature converges slowly due to the oscillatory nature of the Bessel-function integrands. To remedy this, I subtract the undamped contributions from the integrands in (5) and evaluate these analytically, leaving behind integrands that decay rapidly with q and yield convergent numerical quadrature.

Case A: Infinite dielectric slab

I first consider the special case in which the substrate consists of an infinite-thickness slab with permittivity ϵ_1 , so that there is only a single dielectric interface layer at z_1 . If $z_s = z_D = z_1^+$ (both source and evaluation point approach interface layer from above), then equation (3) becomes simply⁴

$$\widetilde{\sigma}(q) = -\left(\frac{\epsilon_1 - \epsilon_0}{\epsilon_1 + \epsilon_0}\right)$$
 (independent of q) (6)

and the integrals (5) may be evaluated in closed form to read

$$\begin{cases}
\mathcal{G}^{\sigma}(\boldsymbol{\rho}) \\
-\partial_{x}\mathcal{G}^{\sigma}(\boldsymbol{\rho}) \\
-\partial_{y}\mathcal{G}^{\sigma}(\boldsymbol{\rho}) \\
-\partial_{z}\mathcal{G}^{\sigma}(\boldsymbol{\rho})
\end{cases} = -\frac{1}{4\pi} \begin{pmatrix} \epsilon_{1} - \epsilon_{0} \\
\epsilon_{1} + \epsilon_{0} \end{pmatrix} \begin{pmatrix} 1/\rho \\ x/\rho^{3} \\ y/\rho^{3} \\
\pm \delta(\rho) \end{pmatrix} \tag{7}$$

Equation (7) gives just the contribution to the potential from the induced surface charge at the dielectric interface. The *total* potential is the sum of this plus the

⁴Note that for $\epsilon_1 > \epsilon_0$ the surface-charge density induced by a positive point source is negative, as expected.

free-space contribution of the point source, equation (1):

$$G(\boldsymbol{\rho}) = G_0(\boldsymbol{\rho}) + \mathcal{G}^{\sigma}(\boldsymbol{\rho})$$

$$= \frac{1}{4\pi |\boldsymbol{\rho}|} \left[1 - \frac{\epsilon_1 - \epsilon_0}{\epsilon_1 + \epsilon_0} \right]$$

$$= \frac{1}{4\pi \epsilon^{\text{effective}} |\boldsymbol{\rho}|} \quad \text{where} \quad \epsilon^{\text{effective}} \equiv \frac{\epsilon_1 + \epsilon_0}{2\epsilon_0}$$

$$= \frac{1}{\epsilon^{\text{effective}}} G_0(\boldsymbol{\rho}) \quad \text{(exactly.)}$$
(9)

Thus, the electrostatics of e.g. planar conductors confined to the surface of an infinite-thickness dielectric slab is *exactly* equivalent to their electrostatics in vacuum, but with the vacuum permittivity replaced by the average of the permittivities above and below the slab.

Case B: Multiple dielectric interfaces

Next I consider the general case in which the source and evaluation points both lie on one of multiple dielectric interfaces (call it the pth interface, so we have $z_{\rm S}=z_{\rm D}=z_p$.) In this case the (Fourier transform of the) surface charge on the pth interface is not exactly given by (6), but does tend to the constant value (6) in the $q\to\infty$ limit. Thus I can substract that constant term from the integrand in (5)—restoring the exponential decay of the integrand as $q\to\infty$ —and account for its contributions exactly in the form of (7). In equations, I go like this:

$$\int \frac{dq}{4\pi} R(q) \widetilde{\sigma}_p(q) Z_p(q) = \int \frac{dq}{4\pi} R(q) \underbrace{\left[\widetilde{\sigma}_p(q) Z_p(q) - \widetilde{\sigma}_p(\infty) Z_p(\infty)\right]}_{\to 0 \text{ as } q \to \infty} + \widetilde{\sigma}_p(\infty) Z_p(\infty) \int \frac{dq}{4\pi} R(q) \tag{10}$$

where R(q) and $Z_p(q)$ are the radial and z-factors in the integrand of (5):

$$R(q) = \left\{ \begin{array}{l} J_0(q\rho) \\ qxJ_1(q\rho)/\rho \\ qyJ_1(q\rho)/\rho \\ qJ_0(q\rho) \end{array} \right\}, \qquad Z_p(q) = \left\{ \begin{array}{l} \zeta(q;z_{\mathrm{D}};z_{\mathrm{p}}) \\ \zeta(q;z_{\mathrm{D}};z_{\mathrm{p}}) \\ \zeta(q;z_{\mathrm{D}};z_{\mathrm{p}}) \\ \xi(q;z_{\mathrm{D}};z_{\mathrm{p}}) \end{array} \right\}.$$

The integral in the second term of (10) may be evaluated in closed form:

$$\widetilde{\sigma}_p(\infty)Z_p(\infty)\int \frac{dq}{4\pi}R(q) = -\frac{1}{4\pi} \begin{pmatrix} \epsilon_p - \epsilon_{p-1} \\ \epsilon_p + \epsilon_{p+1} \end{pmatrix} \begin{cases} 1/\rho \\ x/\rho^3 \\ y/\rho^3 \\ 2\pi\delta(\rho) \end{cases}$$

3.1.6 Example

Figure 3 shows the potential $\phi(\mathbf{x}_D)$ and z-directed electric field $E_z(\mathbf{x}_D)$ for points $\mathbf{x}_D = (0.1, 0.2, z)$ due to a unit-strength point source at $\mathbf{x}_S = (0, 0, 1)$ in the presence of a two-layer substrate. The substrate consists of an upper layer of silicon $(\epsilon_r = 12)$ filling the range $z \in [-1, 0]$ lying atop a lower layer with $\epsilon_r = 2$. The lower layer is of infinite thickness (purple curves in upper and lower plots) or of thickness 1 any lying atop a ground plane (green curve in upper plot).

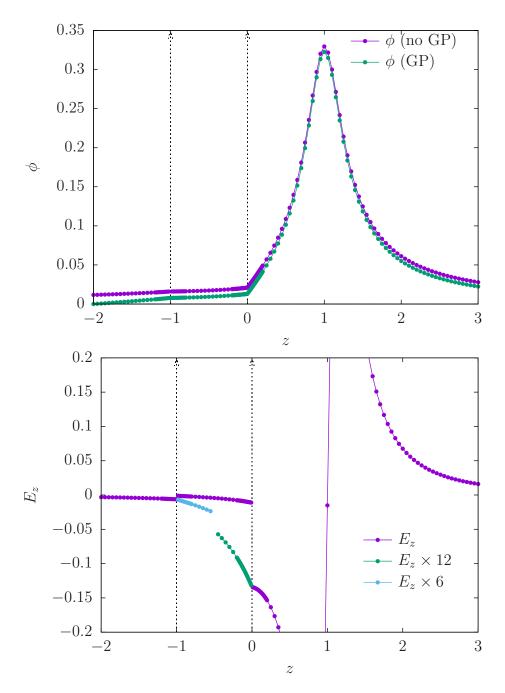


Figure 3: Potential (top) and z-directed electric field (bottom) at $\mathbf{x}_{\mathrm{D}} = (0.1, 0.2, z)$ due to a unit-strength point source at $\mathbf{x}_{\mathrm{S}} = (0, 0, 1)$ in the presence of a substrate consisting of an upper layer of silicon ($\epsilon_r = 12$) and a lower layer of $\epsilon_r = 2$. The lower layer is of infinite thickness (purple curves in upper and lower plots) or of thickness 1 lying atop a ground plane at $z_{\mathrm{GP}} = -2$ (green curve in upper plot). Dashed vertical lines indicate the locations of the dielectric interface layers. For reference, in the interior of the silicon layer in the lower plot we have plotted the quantities $\frac{\epsilon_1}{\epsilon_0} E_z$ (green curve) and $\frac{\epsilon_1}{\epsilon_2} E_z$ (cyan curve) to indicate that these quantities properly match the values of E_z on the other sides of the upper and lower dielectric interfaces.

The take-home messages of Figure 3 are

- The potential is continuous with discontinuous derivative at dielectric-interface layers and properly vanishes at the ground plane (green curve in upper plot).
- The E_z field properly exhibits jumps of magnitude $\frac{\epsilon_1}{\epsilon_0}=12$ at the upper dielectric interface (z=0) and $\frac{\epsilon_1}{\epsilon_2}=6$ at the lower dielectric interface (z=1).

3.2 Assembling the modified BEM system

In the boundary-element-method (BEM) implemented by the SCUFF-EM electrostatics module, we solve a linear system of the form 5

$$\mathbf{M}^{(0)} \cdot \boldsymbol{\sigma} = \mathbf{v}$$

where entries of the M matrix are linear combinations of integrals over basis functions involving the vacuum electrostatic Green's function; for example, the matrix element for two basis functions lying atop conducting surfaces reads

$$M_{mn}^{(0)} = \left\langle b_m(\mathbf{x}_m) \middle| G_0(\mathbf{x}_m, \mathbf{x}_n) \middle| b_n(\mathbf{x}_n) \right\rangle. \tag{11}$$

In the presence of a multilayer substrate, (11) is augmented by additional terms describing the contributions of the substrate:

$$\mathbf{M}^{(0)} \to \mathbf{M}^{(0)} + \mathbf{M}^{GP} + \mathbf{M}^{\sigma}$$

where $\mathbf{M}^{(0)}$ is the vacuum contribution (11) and

$$M_{mn}^{GP} = \left\langle b_{\alpha}(\mathbf{x}_{\alpha}) \middle| \mathcal{G}^{GP}(\mathbf{x}_{\alpha}, \mathbf{x}_{\beta}) \middle| b_{\beta}(\mathbf{x}_{\beta}) \right\rangle$$
$$M_{mn}^{\sigma} = \left\langle b_{\alpha}(\mathbf{x}_{\alpha}) \middle| \mathcal{G}^{\sigma}(\mathbf{x}_{\alpha}, \mathbf{x}_{\beta}) \middle| b_{\beta}(\mathbf{x}_{\beta}) \right\rangle$$

where \mathcal{G}^{GP} and \mathcal{G}^{σ} are the contributions of the ground plane and the surface-charge layers to the substrate Green's function correction \mathcal{G} .

 $^{^5{}m This}$ is equation (11) in the memo "SCUFF-STATIC: Pure Electrostatics in SCUFF-EM," available here: http://homerreid.github.io/scuff-em-documentation/tex/scuff-static.pdf

A Potential due to surface-charge layer

In this appendix I derive an expression for the potential due to a 2D layer of surface charge $\sigma(x, y)$ parallel to the xy plane and lying a fixed distance above or below that plane.

2D Fourier representation of free-space Green's function

The 3D Fourier representation of the free-space Green's function—the potential at $\mathbf{x}_{\mathrm{D}} = (\boldsymbol{\rho}_{\mathrm{D}}, z_{\mathrm{D}})$ due to a point charge at $\mathbf{x}_{\mathrm{S}} = (\boldsymbol{\rho}_{\mathrm{S}}, z_{\mathrm{S}})$ (where the "D" and "S" subscripts label the "destination" and "source" points respectively)—is

$$G_0(\mathbf{x}_{\scriptscriptstyle D}, \mathbf{x}_{\scriptscriptstyle S}) = \frac{1}{4\pi |\mathbf{x}_{\scriptscriptstyle D} - \mathbf{x}_{\scriptscriptstyle S}|}$$
$$= \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x} - \mathbf{x}')}}{|\mathbf{k}|^2}$$

Evaluating the k_z integral yields the 2D Fourier representation:

$$= \frac{1}{2} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \frac{e^{i\mathbf{q}\cdot(\boldsymbol{\rho}_{\mathrm{D}} - \boldsymbol{\rho}_{\mathrm{S}}) - q|z_{\mathrm{D}} - z_{\mathrm{S}}|}}{q}, \qquad \mathbf{q} \equiv \mathbf{k}_{\parallel}, \quad q \equiv |\mathbf{q}|.$$
 (12)

Potential due to surface-charge layer at $z=z_{\rm s}$

Using (12), the potential at $\mathbf{x}_{D} = (\boldsymbol{\rho}_{D}, z_{D})$ due to a surface-charge layer $\sigma(\boldsymbol{\rho}_{S})$ at $z = z_{S}$ is

$$\phi(\boldsymbol{\rho}_{D}, z_{D}) = \int G_{0}(\boldsymbol{\rho}_{D}, z_{D}; \boldsymbol{\rho}_{S}, z_{S}) \sigma(\boldsymbol{\rho}_{S}) d\boldsymbol{\rho}_{S}$$

$$= \frac{1}{2} \int \frac{d\mathbf{q}}{(2\pi)^{2}} \frac{e^{i\mathbf{q}\cdot\boldsymbol{\rho}_{D} - q|z_{D} - z_{S}|}}{q} \underbrace{\int d\boldsymbol{\rho}_{S} \sigma(\boldsymbol{\rho}_{S}) e^{-i\mathbf{q}\cdot\boldsymbol{\rho}_{S}}}_{\widetilde{\sigma}(\mathbf{q})}$$

$$= \int \frac{d\mathbf{q}}{(2\pi)^{2}} \frac{\widetilde{\sigma}(\mathbf{q}) e^{i\mathbf{q}\cdot\boldsymbol{\rho}_{D} - q|z_{D} - z_{S}|}}{2q}$$
(13)

where $\tilde{\sigma}$ is the Fourier transform of σ . For circularly-symmetric cases in which $\tilde{\sigma}$ depends only on the magnitude of \mathbf{q} , as will be the case here, this can be simplified to read

$$\phi(\boldsymbol{\rho}_{\mathrm{D}}, z_{\mathrm{D}}) = \int \frac{dq}{4\pi} \widetilde{\sigma}(q) J_0(q \rho_{\mathrm{D}}) e^{-q|z_{\mathrm{D}} - z_{\mathrm{S}}|}$$
(14)

with $\rho_{\rm D} = |\boldsymbol{\rho}_{\rm D}|$.

Potential due to surface-charge layer in presence of ground plane

In the presence of an infinitely conducting ground plane at $z=z_{\rm GP}< z_{\rm S}$, the contribution of each infinitesimal surface-charge element at $z=z_{\rm S}$ is augmented

by an image-charge element of the opposite sign at $z=z_{\rm GP}-\overline{z_{\rm S}}$, where I defined $\overline{z_{\rm S}}\equiv z_{\rm S}-z_{\rm GP}$. The form of the potential due to the surface-charge layer plus ground plane now depends on whether the evaluation point lies above or below the surface-charge layer:

$$\phi(\boldsymbol{\rho}_{\mathrm{D}}, z_{\mathrm{D}}) = \int \frac{dq}{4\pi} \widetilde{\sigma}(q) J_{0}(q \rho_{\mathrm{D}}) \begin{cases} 2e^{-q\overline{z}_{\mathrm{D}}} \sinh q\overline{z}_{\mathrm{S}}, & z_{\mathrm{D}} > z_{\mathrm{S}} \\ 2e^{-q\overline{z}_{\mathrm{S}}} \sinh q\overline{z}_{\mathrm{D}}, & z_{\mathrm{GP}} < z_{\mathrm{D}} < z_{\mathrm{S}} \end{cases}$$
(15)

where $\overline{z_D} \equiv z_D - z_{GP}$. I will write (14) and (15) in the common form

$$\phi(\boldsymbol{\rho}_{\mathrm{D}}, z_{\mathrm{D}}) = \int \frac{dq}{4\pi} \widetilde{\sigma}(q) J_{0}(q \rho_{\mathrm{D}}) \zeta(q; z_{\mathrm{D}}; z_{\mathrm{S}})$$
(16)

where

$$\zeta(q;z_{\scriptscriptstyle \rm D};z_{\scriptscriptstyle \rm S}) \equiv \begin{cases} \zeta_{\scriptscriptstyle \rm NGP}(q;z_{\scriptscriptstyle \rm D};z_{\scriptscriptstyle \rm S}) \equiv e^{-q|z_{\scriptscriptstyle \rm D}-z_{\scriptscriptstyle \rm S}|}, & \text{no ground plane} \\ \\ \zeta_{\scriptscriptstyle \rm GP}(q;z_{\scriptscriptstyle \rm D};z_{\scriptscriptstyle \rm S}), \equiv 2e^{-q\overline{z_{\scriptscriptstyle \rm S}}} \sinh q\overline{z_{\scriptscriptstyle <}} & \text{ground plane} \end{cases}$$

with $\overline{z} \equiv z - z_{\rm GP}$ and $z_{>}(z_{<})$ the greater (lesser) of $z_{\rm D}, z_{\rm S}$. I will also define a function ξ according to

$$\frac{d}{dz_{\scriptscriptstyle \mathrm{D}}}\zeta(q;z_{\scriptscriptstyle \mathrm{D}};z_{\scriptscriptstyle \mathrm{S}}) \equiv -q\xi(q;z_{\scriptscriptstyle \mathrm{D}};z_{\scriptscriptstyle \mathrm{S}}).$$

Then one finds

$$\begin{split} \xi_{\text{\tiny NGP}}(q;z_{\text{\tiny D}};z_{\text{\tiny S}}) &\equiv \text{sgn}(z_{\text{\tiny D}} - z_{\text{\tiny S}}) e^{-q|z_{\text{\tiny D}} - z_{\text{\tiny S}}|} \\ \xi_{\text{\tiny GP}}(q;z_{\text{\tiny D}};z_{\text{\tiny S}}) &\equiv \begin{cases} +2e^{-q\overline{z_{\text{\tiny D}}}} \sinh q\overline{z_{\text{\tiny S}}}, \\ -2e^{-q\overline{z_{\text{\tiny S}}}} \cosh q\overline{z_{\text{\tiny D}}}, \end{cases} & z_{\text{\tiny D}} < z_{\text{\tiny S}} \end{split}$$

E-field components

Taking derivatives of (16) yields

$$\begin{split} E_{x} &= -\frac{\partial \phi}{\partial x} = \frac{x_{\mathrm{D}}}{\rho_{\mathrm{D}}} \int \frac{q dq}{4\pi} \widetilde{\sigma}(q) J_{1}(q \rho_{\mathrm{D}}) \zeta(q; z_{\mathrm{D}}; z_{\mathrm{S}}) \\ E_{y} &= -\frac{\partial \phi}{\partial y} = \frac{y_{\mathrm{D}}}{\rho_{\mathrm{D}}} \int \frac{q dq}{4\pi} \widetilde{\sigma}(q) J_{1}(q \rho_{\mathrm{D}}) \zeta(q; z_{\mathrm{D}}; z_{\mathrm{S}}) \\ E_{z} &= -\frac{\partial \phi}{\partial z} = \int \frac{q dq}{4\pi} \widetilde{\sigma}(q) J_{0}(q \rho_{\mathrm{D}}) \xi(q; z_{\mathrm{D}}; z_{\mathrm{S}}). \end{split}$$