# Evaluation of four-dimensional integrals for matrix elements in SCUFF-EM

Homer Reid

November 24, 2015

## Contents

# 1 BEM Matrix Elements

## 1.1 Edges, basis functions, and surface-current expansions

SCUFF-EM approximates the electric and magnetic surface currents $\mathbf{K}, \mathbf{N}$ on each surface in a geometry as an expansion in a set of $N_{\text{BF}}$ basis functions. In six-vector notation we have

$$\begin{pmatrix} \mathbf{K}(\mathbf{x}) \\ \mathbf{N}(\mathbf{x}) \end{pmatrix} = \sum_{\alpha=1}^{N_{\text{BF}}} c_\alpha \boldsymbol{\mathcal{B}}_\alpha(\mathbf{x})$$

$$\boldsymbol{\mathcal{B}}_{2a}(\mathbf{x}) = \begin{pmatrix} \mathbf{b}_a(\mathbf{x}) \\ 0 \end{pmatrix}, \qquad \boldsymbol{\mathcal{B}}_{2a+1}(\mathbf{x}) = \begin{pmatrix} 0 \\ \mathbf{b}_a(\mathbf{x}) \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{K}(\mathbf{x}) \\ \mathbf{N}(\mathbf{x}) \end{pmatrix} = \sum_{a=1}^{N_{\text{E}}} \begin{pmatrix} k_a \mathbf{b}_a(\mathbf{x}) \\ n_a \mathbf{b}_a(\mathbf{x}) \end{pmatrix}$$

(The actual coefficients computed by SCUFF-EM are $\hat{n}_a \equiv -Z_0 n_a$.)

Here $\alpha$ runs over all basis functions in the SCUFF-EM calculation (of which there are $N_{\text{BF}}$ in total), $a$ runs over all internal edges on all surfaces (of which there are $N_{\text{E}}$ in total), and $\mathbf{b}_a(\mathbf{x})$ is the RWG basis function associated with the $a$th interior edge.

## 1.2 BEM Matrix Elements

If two basis functions $\boldsymbol{\mathcal{B}}_\alpha, \boldsymbol{\mathcal{B}}_\beta$ lie on the same surface and this surface is a dielectric interface, then the $(\alpha, \beta)$ element of the BEM matrix receives contributions from both the media exterior and interior to the surface. Otherwise ($\boldsymbol{\mathcal{B}}_\alpha, \boldsymbol{\mathcal{B}}_\beta$ on the same PEC surface or on different surfaces) there is only a contribution from the exterior medium:[1]

$$M_{\alpha\beta}(\omega) = \begin{cases} M^{\text{ext}}_{\alpha\beta}(\omega) + M^{\text{int}}_{\alpha\beta}(\omega), & \boldsymbol{\mathcal{B}}_\alpha, \boldsymbol{\mathcal{B}}_\beta \quad \text{on same (dielectric) surface} \\ M^{\text{ext}}_{\alpha\beta}(\omega) & \boldsymbol{\mathcal{B}}_\alpha, \boldsymbol{\mathcal{B}}_\beta \quad \text{on same (PEC) surface or different surfaces} \end{cases}$$

Each pair of interior edges $(E_a, E_b)$ contributes a $2 \times 2$ block of matrix elements to the BEM matrix for medium $r$:

$$M^r_{ab}(\omega) = i\frac{\omega}{c_0} \begin{pmatrix} \mu_r \mathbb{G}_{ab}(k_r) & -n_r \mathbb{C}_{ab}(k_r) \\ -n_r \mathbb{C}_{ab}(k_r) & -\epsilon_r \mathbb{G}_{ab}(k_r) \end{pmatrix} \tag{1}$$

Here $c_0$ is the vacuum speed of light, $\{\epsilon_r, \mu_r\}$ are the relative permittivity and permeability of medium $r$ at frequency $\omega$, and

$$n_r = \sqrt{\epsilon_r \mu_r}, \qquad k_r = n_r \frac{\omega}{c_0}.$$

[1] More accurately, there is only a contribution from the medium common to the surfaces on which $\boldsymbol{\mathcal{B}}_\alpha, \boldsymbol{\mathcal{B}}_\beta$ lie. In the case of nested surfaces this will be the interior medium for one of the surfaces.

The $\mathbb{G}, \mathbb{C}$ matrix elements and their $k$ derivatives are

$$\mathbb{G}_{ab}(k) = \int \left( \mathbf{b}_a \cdot \mathbf{b}_b - \frac{[\nabla \cdot \mathbf{b}_a]\,[\nabla \cdot \mathbf{b}_b]}{k^2} \right) G_0(k, \mathbf{r}) d^4\mathbf{r} \tag{2a}$$

$$\mathbb{C}_{ab}(k) = \frac{1}{ik} \int (\mathbf{b}_a \times \mathbf{b}_b) \cdot \nabla G_0(k, \mathbf{r})\, d^4\mathbf{r} \tag{2b}$$

In these equations, I have

$$G_0(k, \mathbf{r}) = \begin{cases} \dfrac{e^{ikr}}{4\pi r}, & \text{non-periodic} \\ \\ \displaystyle\sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}} \cdot \mathbf{L}} \frac{e^{ik|\mathbf{r}+\mathbf{L}|}}{4\pi|\mathbf{r}+\mathbf{L}|} & \text{Bloch-periodic with Bloch vector } \mathbf{k}_{\mathrm{B}} \end{cases} \tag{3}$$

## Alternative notation

Equations (1) and (2) are the way I have always defined things in SCUFF-EM; among their advantages is the fact that $\mathbb{C}$ has the same units as $\mathbb{G}$ (namely, inverse length). However, for present purposes it is actually convenient to write (1) in the slightly different form

$$M^r_{ab}(\omega) = \begin{pmatrix} \frac{i\omega\mu_r}{c} \mathbb{G}_{ab}(k_r) & -\widehat{\mathbb{C}}_{ab}(k_r) \\ -\widehat{\mathbb{C}}_{ab}(k_r) & -\frac{i\omega\epsilon_r}{c} \mathbb{G}_{ab}(k_r) \end{pmatrix} \tag{4}$$

where

$$\widehat{\mathbb{C}}(k) \equiv ik\mathbb{C}(k), \qquad \widehat{\mathbb{C}}_{ab} = \int (\mathbf{b}_a \times \mathbf{b}_b) \cdot \nabla G_0(k, \mathbf{r})\, d^4\mathbf{r}. \tag{5}$$

# 2 Force and torque integrals

## 2.1 Force

$$
\begin{aligned}
F_i &= \frac{1}{2\omega}\mathrm{Im}\int \left(\begin{array}{c}\mathbf{K}(\mathbf{x})\\ \mathbf{N}(\mathbf{x})\end{array}\right)^\dagger \left(\begin{array}{c}\partial_i\mathbf{E}(\mathbf{x})\\ \partial_i\mathbf{H}(\mathbf{x})\end{array}\right) d\mathbf{x}\\
&= \frac{1}{2\omega}\mathrm{Im}\int \left(\begin{array}{c}\mathbf{K}(\mathbf{x})\\ \mathbf{N}(\mathbf{x})\end{array}\right)^\dagger \left(\begin{array}{cc} i\omega\mu_r\partial_i\mathbb{G}(\mathbf{x},\mathbf{x}') & \partial_i\widehat{\mathbb{C}}(\mathbf{x},\mathbf{x}')\\ -\partial_i\widehat{\mathbb{C}}(\mathbf{x},\mathbf{x}') & i\omega\epsilon_r\partial_i\mathbb{G}(\mathbf{x},\mathbf{x}')\end{array}\right)\left(\begin{array}{c}\mathbf{K}(\mathbf{x}')\\ \mathbf{N}(\mathbf{x}')\end{array}\right) d\mathbf{x}\,d\mathbf{x}'\\
&= \frac{1}{2\omega}\mathrm{Im}\sum_{ab}\left(\begin{array}{c}k_a\\ n_a\end{array}\right)^\dagger\left(\begin{array}{cc} i\omega\mu_r\partial_i\mathbb{G}_{ab} & \partial_i\widehat{\mathbb{C}}_{ab}\\ -\partial_i\widehat{\mathbb{C}}_{ab} & i\omega\epsilon_r\partial_i\mathbb{G}_{ab}\end{array}\right)\left(\begin{array}{c}k_b\\ n_b\end{array}\right)\\
&= -\sum_{b>a}\Bigg\{\frac{Z_0}{c}\Big[\mathrm{Im}\,\Big(k_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\mu_r\partial_i\mathbb{G}_{ab}\Big)\Big] + \frac{1}{cZ_0}\Big[\mathrm{Im}\,\Big(n_a^*n_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\epsilon_r\partial_i\mathbb{G}_{ab}\Big)\Big]\\
&\qquad + \frac{1}{\omega}\Big[\mathrm{Re}\,\Big(k_a^*n_b - n_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\partial_i\widehat{\mathbb{C}}_{ab}\Big)\Big]\Bigg\}
\end{aligned}
$$

## 2.2 Torque

$$
\begin{aligned}
\mathcal{T}_i &= \mathcal{T}_i^{(1)} + \mathcal{T}_i^{(2)}\\
\mathcal{T}_i^{(1)} &= \frac{1}{2\omega}\mathrm{Im}\int \left(\begin{array}{c}\mathbf{K}(\mathbf{x})\\ \mathbf{N}(\mathbf{x})\end{array}\right)^\dagger \left(\begin{array}{c}\partial_{\theta_i}\mathbf{E}(\mathbf{x})\\ \partial_{\theta_i}\mathbf{H}(\mathbf{x})\end{array}\right) d\mathbf{x}\\
&= -\sum_{b>a}\Bigg\{\frac{Z_0}{c}\Big[\mathrm{Im}\,\Big(k_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\mu_r\partial_{\theta_i}\mathbb{G}_{ab}\Big)\Big] + \frac{1}{cZ_0}\Big[\mathrm{Im}\,\Big(n_a^*n_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\epsilon_r\partial_{\theta_i}\mathbb{G}_{ab}\Big)\Big]\\
&\qquad - \frac{1}{\omega}\Big[\mathrm{Re}\,\Big(k_a^*n_b - n_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\partial_{\theta_i}\widehat{\mathbb{C}}_{ab}\Big)\Big]\Bigg\}
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{T}_i^{(2)} &= \frac{1}{2\omega}\mathrm{Im}\int\Big\{\mathbf{K}^*\times\mathbf{E} + \mathbf{N}^*\times\mathbf{H}\Big\}_i\,d\mathbf{x}\\
&= \frac{1}{2\omega}\varepsilon_{ijk}\mathrm{Im}\iint\Big\{K_j^*\Big[i\omega\mu_r\mathbb{G}_{k\ell}\Big]K_\ell + K_j^*\Big[\widehat{\mathbb{C}}_{k\ell}\Big]N_\ell\\
&\qquad - N_j^*\Big[\widehat{\mathbb{C}}_{k\ell}\Big]K_\ell + N_j^*\Big[i\omega\epsilon_r\mathbb{G}_{k\ell}\Big]N_\ell\Big\}\,d^4\mathbf{x}\\
&= -\sum_{b>a}\Bigg\{\frac{Z_0}{c}\Big[\mathrm{Im}\,\Big(k_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\mu_r\widetilde{\mathbb{G}}_{i;ab}\Big)\Big] + \frac{1}{cZ_0}\Big[\mathrm{Im}\,\Big(n_a^*n_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\epsilon_r\widetilde{\mathbb{G}}_{i;ab}\Big)\Big]\\
&\qquad - \frac{1}{2\omega}\Big[\mathrm{Re}\,\Big(k_a^*n_b - n_a^*k_b\Big)\Big]\Big[\mathrm{Im}\,\Big(\widetilde{\mathbb{C}}_{i;ab}\Big)\Big]\Bigg\}
\end{aligned}
$$

$$\widetilde{\mathbb{G}}_{i;ab} \equiv \varepsilon_{ijk} \iint b_{aj} \mathbb{G}_{k\ell} b_{b\ell} \, d\mathbf{r}, \qquad \widetilde{\mathbb{C}}_{i;ab} \equiv \varepsilon_{ijk} \iint b_{aj} \widehat{\mathbb{C}}_{k\ell} b_{b\ell} \, d\mathbf{r}$$

## 3 Frequency derivatives

The $\omega$ derivative of (4) reads

$$\frac{d}{d\omega}M^r_{ab} = \frac{i}{c}\left(\begin{array}{cc} (\omega\mu_r)'\mathbb{G}_{ab}(k_r) & 0 \\ 0 & (\omega\epsilon_r)'\mathbb{G}_{ab}(k_r) \end{array}\right) + \left(\begin{array}{cc} \frac{i\omega\mu_r}{c}\mathbb{G}'_{ab}(k_r) & -\widehat{\mathbb{C}}'_{ab}(k_r) \\ -\widehat{\mathbb{C}}'_{ab}(k_r) & -\frac{i\omega\epsilon_r}{c}\mathbb{G}_{ab}(k_r) \end{array}\right)$$

where

$$(\omega\mu_r)' = \mu_r + \omega\frac{d\mu_r}{d\omega}, \qquad (\omega\epsilon_r)' = \epsilon_r + \omega\frac{d\epsilon_r}{d\omega},$$

and primes on $\mathbb{G}$ and $\widehat{\mathbb{C}}$ denote differentiation with respect to $k$.

The $k$ derivatives of the $\mathbb{G}, \widehat{\mathbb{C}}$ matrix elements are

$$\mathbb{G}'_{ab}(k) = \frac{2}{k^3}\int \left[\nabla\cdot\mathbf{b}_a\right]\left[\nabla\cdot\mathbf{b}_b\right] G_0(k,\mathbf{r})\,d^4\mathbf{r} \tag{6a}$$

$$+\int\left(\mathbf{b}_a\cdot\mathbf{b}_b - \frac{\left[\nabla\cdot\mathbf{b}_a\right]\left[\nabla\cdot\mathbf{b}_b\right]}{k^2}\right) G'_0(k,\mathbf{r})\,d^4\mathbf{r} \tag{6b}$$

$$\mathbb{C}'_{ab}(k) = \int (\mathbf{b}_a\times\mathbf{b}_b)\cdot\nabla G'_0(k,\mathbf{r})\,d^4\mathbf{r} \tag{6c}$$

In both the periodic and non-periodic cases, $k$ derivatives of $G_0$ may be related to spatial derivatives according to

$$\frac{\partial}{\partial k}G_0 = -i|\mathbf{r}|^2\left(\frac{\mathbf{r}\cdot\nabla G_0}{|\mathbf{r}|} - ikG_0\right) \tag{7}$$

$$\frac{\partial}{\partial k}\nabla G_0 = -k\mathbf{r}G_0 \tag{8}$$

Importantly, the kernels defined by (8) are both *nonsingular* at $\mathbf{r}=0$, allowing the use of simple numerical cubature to evaluate matrix elements.

# 4 Computation of matrix elements

## 4.1 BEM matrix elements

$$\mathbb{G}_{ab} = \iint \left(\mathbf{b}_a \cdot \mathbf{b}_b - \frac{4}{k^2}\right) G_0(r)\, d^4\mathbf{r} \tag{9}$$

$$= \mathbb{C}_{ab} \qquad = \frac{1}{ik}\varepsilon_{ijk} \iint b_{ai} b_{bj} \partial_k G_0(r)\, d^4\mathbf{r} \tag{10}$$

## 4.2 Force integrals

$$\partial_i \mathbb{G}_{ab} = \iint \underbrace{\left(\mathbf{b}_a \cdot \mathbf{b}_b - \frac{4}{k^2}\right)}_{P^{\text{EFIE}}} \partial_i G_0(r)\, d^4\mathbf{r} \tag{11}$$

$$= \sum_p \overline{\psi}_p \iint P^{\text{EFIE}} r_i r^p \, d\mathbf{r} + \iint P^{\text{EFIE}} r_i \psi^{\text{DS}}(r)\, d^4\mathbf{r} \tag{12}$$

$$\text{Im }\partial_i \widehat{\mathbb{C}}_{ab} = \varepsilon_{jk\ell} \iint b_{aj} b_{bk} \Big[\text{Im }\partial_i \partial_\ell G_0(r)\Big]\, d\mathbf{r} \tag{13}$$

## 4.3 Torque integrals

$$\partial_{\theta_i} \mathbb{G}_{ab} = \varepsilon_{ijk} \iint \left(\mathbf{b}_a \cdot \mathbf{b}_b - \frac{4}{k^2}\right) (\mathbf{x}_a - \mathbf{x}_0)_j \partial_k G_0(r)\, d^4\mathbf{r} \tag{14}$$

$$\partial_{\theta_i} \mathbb{C}_{ab} = \frac{1}{ik}\varepsilon_{ijk}\varepsilon_{jk\ell} \iint b_{aj} b_{bk} (\mathbf{x}_a - \mathbf{x}_0)_j \partial_i \partial_\ell G_0(r)\, d^4\mathbf{r} \tag{15}$$

$$\begin{aligned}
\widetilde{\mathbb{G}}_{i;ab} &\equiv \varepsilon_{ijk} \int b_{aj}(\mathbf{x}) \underbrace{\mathbb{G}_{k\ell}(\mathbf{x},\mathbf{x}')}_{\left(\delta_{k\ell} + \frac{1}{k^2}\partial_k\partial_\ell\right)G_0} b_{b\ell}(\mathbf{x}')\, d\mathbf{x}\, d\mathbf{x}' \\
&= \int \left\{ (\mathbf{b}_a \times \mathbf{b}_b)_i \left(G_0 + \frac{1}{k^2}\psi\right) + \Big[(\mathbf{b}_a \times \mathbf{r})_i (\mathbf{b}_b \cdot \mathbf{r})\Big]\zeta(r) \right\} d\mathbf{x}\, d\mathbf{x}' \\
\widetilde{\mathbb{C}}_{i;ab} &\equiv \varepsilon_{ijk} \int b_{aj}(\mathbf{x}) \underbrace{\widehat{\mathbb{C}}_{k\ell}(\mathbf{x},\mathbf{x}')}_{\epsilon_{k\ell m} r_m \psi(r)} b_{b\ell}(\mathbf{x}')\, d\mathbf{x}\, d\mathbf{x}' \\
&= \int \left\{ \Big(\mathbf{b}_a \cdot \mathbf{r}\Big) b_{bi} - \Big(\mathbf{b}_a \cdot \mathbf{b}_b\Big) r_i \right\} \psi(r)\, d\mathbf{x}\, d\mathbf{x}'
\end{aligned}$$

$$\partial_i G_0(r) = r_i \psi(r)$$

$$\partial_i \partial_j G_0(r) = \delta_{ij} \psi(r) + r_i r_j \zeta(r)$$

$$\psi(r) = (ikr - 1)\frac{e^{ikr}}{4\pi r^3}$$

$$\zeta(r) = \Big[(ikr)^2 - 3ikr + 3\Big]\frac{e^{ikr}}{4\pi r^5}$$

# A Scalar and dyadic Green's functions and their most singular terms

## A.1 Scalar GF

$$\begin{aligned}
G_0(r) &= \frac{e^{ikr}}{4\pi r} \\
\partial_i G_0(r) &= r_i \psi(r), \qquad \psi(r) \equiv (ikr-1)\frac{e^{ikr}}{4\pi r^3} \\
\partial_i \partial_j G_0(r) &= \delta_{ij}\psi(r) + r_i r_j \zeta(r), \qquad \zeta(r) \equiv \frac{e^{ikr}}{4\pi r^5}\Big[3 - 3ikr + (ikr)^2\Big]
\end{aligned}$$

## A.2 Desingularized scalar GF

$$G_0(r) = \frac{1}{4\pi r} + \frac{\texttt{ExpRel}(ikr,1)}{4\pi r}$$

$$\begin{aligned}
\partial_i G_0(r) &= r_i \psi^{\mathrm{S}}(r) + r_i \psi^{\mathrm{DS}}(r), \\
\psi^{\mathrm{DS}}(r) &= \frac{\texttt{ExpRel}(ikr,3)}{4\pi r^3} \\
\psi^{\mathrm{S}}(r) &= \sum_p C_p r^p, \qquad C_{-3} = -\frac{1}{4\pi}, \qquad C_{-1} = -\frac{k^2}{8\pi}, \qquad C_0 = -\frac{ik^3}{8\pi}
\end{aligned}$$

$$\mathrm{Im}\ \partial_i \partial_j G_0(r) = \text{nonsingular}$$

## A.3 Dyadic GFs

$$\mathbb{G}_{ij}(\mathbf{r}) = \frac{e^{ikr}}{4\pi(ik)^2 r^3}\left[F_1(ikr)\delta_{ij} + F_2(ikr)\frac{r_i r_j}{r^2}\right], \qquad C_{ij}(k,\mathbf{r}) = \frac{e^{ikr}}{4\pi(ik)r^3}\varepsilon_{ijk} r_k F_3(ikr),$$
$$F_1(x) = 1 - x + x^2, \qquad F_2(x) = -3 + 3x - x^2, \qquad F_3(x) = -1 + x. \tag{16}$$

## Desingularized DGFs

$$\mathbb{G}_{ij}(\mathbf{r}) = \mathbb{G}^{\mathrm{S}}_{ij}(\mathbf{r}) + \mathbb{G}^{\mathrm{DS}}_{ij}(\mathbf{r})$$

$$\mathbb{G}^{\mathrm{DS}}_{ij}(\mathbf{r}) = \frac{\texttt{ExpRel}(ikr,3)}{4\pi(ik)^2 r^3}\left[F_1(ikr)\delta_{ij} + F_2(ikr)\frac{r_i r_j}{r^2}\right], \qquad \mathbb{C}^{\mathrm{DS}}_{ij}(\mathbf{r}) = \frac{\texttt{ExpRel}(ikr,3)}{4\pi(ik)r^3}\varepsilon_{ijk} r_k$$

$$\mathbb{G}^{\mathrm{S}}_{ij}(\mathbf{r}) = \Big[\sum_p \Upsilon^1_p r^p\Big]\delta_{ij} + \Big[\sum_p \Upsilon^2_p r^p\Big]\frac{r_i r_j}{r^2}$$

$$\mathbb{C}^{\mathrm{s}}_{ij}(\mathbf{r}) = \Big[\sum_p \Upsilon^3_p r^p\Big]\varepsilon_{ijk} r_k$$

$$\Upsilon^1_{-3} = -\frac{1}{4\pi k^2}, \qquad \Upsilon^1_{-1} = +\frac{1}{8\pi}, \qquad \Upsilon^1_0 = +\frac{ik}{8\pi}, \qquad \Upsilon^1_1 = -\frac{k^2}{8\pi},$$

$$\Upsilon^2_{-3} = +\frac{3}{4\pi k^2}, \qquad \Upsilon^2_{-1} = +\frac{1}{8\pi}, \qquad \Upsilon^2_0 = +\frac{ik}{8\pi}, \qquad \Upsilon^2_1 = +\frac{k^2}{8\pi},$$

$$\Upsilon^3_{-3} = +\frac{i}{4\pi k}, \qquad \Upsilon^3_{-1} = +\frac{ik}{8\pi}, \qquad \Upsilon^3_0 = -\frac{k^2}{8\pi}, \qquad \Upsilon^3_1 = 0.$$