Efficient Computation of the 2D Green's Function for 1D Periodic Layered Structures Using the Ewald Method

F. Capolino¹, D. R. Wilton¹, and W. A. Johnson²

¹Dept. of Electrical and Computer Engineering
University of Houston
Houston, TX 77204-4005 USA
capolino@uh.edu, wilton@uh.edu

²Electromagnetics and Plasma Physics
Analysis Dept.
Sandia National Laboratories
Albuquerque, NM 87123-1152 USA
waloul@sandia.gov

1. Introduction

In applying numerical full wave methods to periodic structures, fast and accurate means to evaluate the periodic Green's function are often needed. The free space Green's function for three dimensional (3D) problems with 2D periodicity has been efficiently accelerated via the Ewald method in [1], and has been extended for the evaluation of the Green's function in multilayered media in [2]. In [3] the extension of the Ewald method to 2D problems with 1D periodicity was given for the case of coplanar source and observation points. An extension of the approach to the non coplanar case was also briefly summarized in [3], in which a formula for non coplanar source and observation was obtained by integrating in closed form the results in [1]. Here, we present an alternative direct procedure for applying the Ewald approach to obtain the Green's function for an array of line sources with 1D periodicity. The approach is the 2D analog of that of [1]. Furthermore, we derive an algorithm for choosing the Ewald splitting parameter E that extends the efficiency of the method when the periodicity is somewhat larger than a wavelength. The case of periodic 2D multilayered media is also treated analogously as in [2] for the 3D case. In particular, the dyadic Green's function formalism of [4], which yields mixed potential integral equations for layered media, is combined with the Ewald method. An analogous formulation, to be reported in the future, has also been successfully applied to accelerate the Green's function for a periodic linear array of point sources (1D periodicity).

2. Green's Function Transformation

Consider the element-by-element superposition of the fields radiated by an infinite array of progressively phased line sources:

\[ G(x, x') = \sum_{n=-\infty}^{\infty} e^{-ik_{eq}nd} H_0^{(2)}(k R_n) \frac{1}{4j} \]

where \( k_{eq} = k \sin \Theta_0 \) is the phase gradient along the z direction with equivalent scan angle \( \Theta_0 \) and \( R_n = [(z - z')^2 + (x - x')^2 + (z - z')^2]^{1/2} \) is the distance between the observation point \( x = (x, z) \) and the nth source point \( x_n = (x + nd, z') \) (see Fig. 1). For simplicity the homogeneous medium is supposed to have small losses; hence \( k = k_e + j k_i = |k| e^{j \phi}, k_i < 0, \phi < 0 \). By integrating in the fundamental identity for the Ewald transformation for an array of point sources [1], one obtains

\[ \frac{1}{4j} H_0^{(2)}(k R) = \frac{1}{2 \pi} \int_0^{\infty} \frac{e^{-R s + i \pi/2}}{s} ds, \]

with convergence assured by the integration path shown in Fig. 2. If the contour in (2) is split into two parts, \( \int_0^{\infty} = \left( \int_0^{\infty} + \int_E \right) \), then the Green's function in (1) is decomposed as

W. A. Johnson's contribution to this work was performed under the auspices of the US Department of Energy by Sandia National Labs., a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, under contract No. DE-AC04-94AL85000.
\[ G(r, r') = G_1(r, r') + G_2(r, r') \]  
(3)

with

\[
G_1(r, r') = \sum_{n=-\infty}^{\infty} e^{-j\beta_n r} \int_{0}^{E} \frac{e^{-R_n^2 s^2} x^2(s, r')}{s} \, ds,
\]
\[
G_2(r, r') = \sum_{n=-\infty}^{\infty} e^{-j\beta_n r} \int_{0}^{E} \frac{e^{-R_n^2 s^2} x^2(s, r')}{s} \, ds,
\]
(4)

One notes that the series \( G_1 \) does not decay exponentially, while the series \( G_2 \) has Gaussian convergence because \( \Re(s) > E \) on the path of integration.

**Transformation of \( G_1(r, r') \).** Since the series in (4) does not decay exponentially, it is transformed using the Poisson summation formula

\[
\sum_{n=-\infty}^{\infty} f(n) = d^{-1} \sum_{q=-\infty}^{\infty} \int_{0}^{\infty} f(2\pi q/d) \, dq,
\]

with \( f(k) = \int_{0}^{\infty} f(s) \exp(-2\pi i s k) \, ds \), and \( f(n) \) identified with terms of (4a). Then, the order of integration in \( \xi \) and \( s \) is interchanged and the \( \xi \)-integral is evaluated using \( \int_{0}^{\infty} e^{-\xi^2} \, d\xi = \sqrt{\pi} e^{\xi^2/4} \) to obtain

\[
f \left( \frac{2\pi q}{d} \right) = e^{-\frac{j\pi s (s-q)}{2\pi}} \int_{0}^{E} \frac{e^{-R_\xi^2 s^2 + k_\xi^2/(4\xi^2)}}{s^2} \, ds,
\]

with \( k_\xi \) and \( k_s \) denoting the Floquet wave numbers along \( z \) and \( \xi \), respectively. The substitution \( s' = 1/s \) maps the domain of integration \((0, E)\) shown in Fig. 2 onto \((1/E, \infty)\), and transforms (5) into a "standard" form (see [1]) which is manipulated as shown therein into the numerically efficient representation

\[
G_1(r, r') = \frac{1}{4d} \sum_{n=-\infty}^{\infty} e^{-\frac{j\pi n (s-q)}{2}} \left[ \exp \left( \frac{j\pi k_\xi}{2E} |z - z'| \right) + e^{-\frac{j\pi n (s-q)}{2}} \exp \left( \frac{j\pi k_\xi}{2E} |z - z'| \right) \right],
\]
(6)

in which \( \text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} \exp(-t^2) \, dt \) is the complementary error function.

**Transformation of \( G_2(r, r') \).** Efficient evaluation of \( G_2 \) is based on the evaluation of the integral

\[ I = \int_{0}^{E} e^{-R_\xi^2 s^2 + k_\xi^2/(4\xi^2)} \, ds. \]

First performing the change of variable \( u = s^2 \), leading to \( I = \frac{1}{2} \int_{0}^{\infty} u^{-1} \exp(-R_\xi^2 u + k_\xi^2/(4u)) \, du \), then employing the Taylor expansion \( \exp[k_\xi^2/(4u)] = \sum_{n=0}^{\infty} (k_\xi^2/2)^n / n! \), followed by the change of variable \( t = u/E^2 \), leads to

\[
G_2(r, r') = \frac{1}{4\pi} \sum_{n=-\infty}^{\infty} e^{-\frac{j\pi n (s-q)}{2}} \sum_{p=0}^{\infty} \frac{1}{2E} \exp \left( \frac{j\pi k_s}{2E} \right),
\]
(7)

in which \( E_p \) is the \( p \)-th order exponential integral, \( E_p(z) = \int_{0}^{\infty} \exp(-t^p) / t \, dt \) [5, p. 228]. \( E_1(z) \) may be evaluated numerically using the algorithm of [5, p. 231], and the higher
order integrals may be evaluated by the recurrence relation $E_{n+1}(z) = \frac{1}{n} \left[ e^{-z} - z E_n(z) \right]$, $p = 1, 2, 3, \ldots$

Asymptotic Convergence of Series $G_1$ and $G_2$. Since $k_0 \approx 2\pi q/d$, $k_2 \approx -j(2\pi q/d)$ for large $q$ and $R_0 \approx n$ for large $n$, large argument expansions of the complementary error function and exponential integrals lead to asymptotic behaviors of $\exp\left[ -\frac{(2\pi q)}{d} \right] / (2\pi q)^{1/2}$ and $\exp\left[ -\frac{(2\pi q)}{d} \right] / (2\pi q)^{1/2}$ for terms of $G_1$ and $G_2$, respectively. Hence the two series both exhibit Gaussian convergence.

Choice of Splitting Parameter $E$. The optimum value of the splitting parameter $E_o$ is obtained by minimizing an estimate of the total time required to compute both series to a given number of significant figures. It results in making the two series for $G_1$ and $G_2$ converge at the same asymptotic rate and leads to $E_o = \frac{k_0}{2M}$. However, for rapid convergence of the $p$-sum in (7), $(k/2p^2)^{1/2} / p!$ must be negligible for $p \approx \frac{k}{2}\pi$, i.e., $\frac{k}{2p^2} < \frac{k}{2}\pi$. With $E$ the desired error and $P$ the desired number of $p$-terms to achieve convergence (typically 10 to 15), this implies that $E > E_1 \equiv \frac{k}{2}(P/2)^{1/2}$.

For simplicity, we deal here only with electric currents and their radiated magnetic vector potential dyads and scalar potentials. We choose the representation of “Formulation C” of [4]. There, the scattered electric field $E_s(r)$ produced by a periodic current $J(r')$ is represented as $E_s(r) = -j\omega A - \nabla \phi$, with $A(r) = \int J(r') \hat{V}_A(r, r') \, dS'$, $\phi(r) = -j\omega \nabla \cdot A(r) = \int \nabla \cdot J(r') \, dS'$, $k^2(r, r') = \int k^2(r') \, dS' + \int s_{ii} J(r') \hat{P}_z(r, r') \, dS'$. For numerical convenience, the vector potential dyadic Green’s function $\hat{G}^A$ is expressed as

$$
\hat{G}^A(r, r') = \frac{1}{d} \int \sum_{q = -\infty}^{\infty} \hat{G}_q^A(z, z') - \hat{G}_q^{A\omega}(z, z') e^{-j\omega u(x-x')} + \frac{1}{d} \sum_{q = -\infty}^{\infty} \hat{G}_q^{A\omega}(z, z') e^{-j\omega u(x-x')} + \frac{1}{d} \sum_{q = -\infty}^{\infty} \hat{G}_q^{A\omega}(z, z') e^{-j\omega u(x-x')} (9)
$$

where $\hat{G}_q^A = (\hat{\omega} + \hat{\phi})(\hat{\omega} + \hat{\phi}) \hat{G}_{q\omega}^A + \hat{\omega} \hat{\omega} \hat{G}_{q\omega}^A + \hat{\phi} \hat{\phi} \hat{G}_{q\omega}^A$, in which $\hat{G}_{q\omega}^A = (j\omega)^{-1} \hat{V}_A^q(z, z')$, $\hat{G}_{q\omega}^A = \mu(j\omega)^{-1} H_0^1(z, z')$, $\hat{G}_{q\omega}^A = \mu(j\omega)^{-1} H_0^1(z, z')$. A similar representation applies to the scalar potentials $\hat{K}^q(r, r')$ and $P_{q}(r, r')$. The terms $V_{q\omega}^A(z, z')$ and $P_{q}(z, z')$ are the voltage and current, respectively, at a unit current source (denoted by the subscript $i$) located at $z'$ on the equivalent transmission line representing the $q$th Floquet wave of polarization $\alpha = e$ or $h$ in the multilayered medium. $T_{q\omega}^A(z, z')$ is similarly defined, but its subscript $u$ denotes a unit voltage source. We also find that $V_{q\omega}^A(z, z') = j\mu \omega g_{q\omega}^{A\omega}(z, z')$ and $T_{q\omega}^A(z, z') = j\omega g_{q\omega}^{A\omega}(z, z')$ where $g_{q\omega}^{A\omega}(z, z')$ and $g_{q\omega}^{A\omega}(z, z')$ are the scalar longitudinal Green’s functions developed in [6, pp. 446, 455]. Indeed, using reciprocity and the argument in [5, pp. 194, 195], all the voltages and currents for all combinations of polarizations and unit source types may be expressed in terms of these two characteristic scalar Green’s functions and their derivatives.

Extraction of the Asymptotic Form of Series. In (9), for numerical convenience terms $\hat{G}_q^{A\omega}(z, z')$, asymptotic for large $q$ to the terms $\hat{G}_q^A(z, z')$ of the spectral dyadic Green’s function, are subtracted term by term from the original series and their sum is added back as a separate series. Removing the asymptotic form of each term from the spectral sum

$$
E = \max\{E_0, E_1, E_2\} = \max\left\{ E_0 \right\}
$$

(8)

II. Field Representation for Multi-Layered Periodic Media

For simplicity, we deal here only with electric currents and their radiated magnetic vector potential dyads and scalar potentials. We choose the representation of “Formulation C” of [4]. There, the scattered electric field $E_s(r)$ produced by a periodic current $J(r')$ is represented as $E_s(r) = -j\omega A - \nabla \phi$, with $A(r) = \int J(r') \hat{V}_A(r, r') \, dS'$, $\phi(r) = -j\omega \nabla \cdot A(r) = \int \nabla \cdot J(r') \, dS'$, $k^2(r, r') = \int k^2(r') \, dS' + \int s_{ii} J(r') \hat{P}_z(r, r') \, dS'$. For numerical convenience, the vector potential dyadic Green’s function $\hat{G}^A$ is expressed as

$$
\hat{G}^A(r, r') = \frac{1}{d} \int \sum_{q = -\infty}^{\infty} \hat{G}_q^A(z, z') - \hat{G}_q^{A\omega}(z, z') e^{-j\omega u(x-x')} + \frac{1}{d} \sum_{q = -\infty}^{\infty} \hat{G}_q^{A\omega}(z, z') e^{-j\omega u(x-x')} (9)
$$

where $\hat{G}_q^A = (\hat{\omega} + \hat{\phi})(\hat{\omega} + \hat{\phi}) \hat{G}_{q\omega}^A + \hat{\omega} \hat{\omega} \hat{G}_{q\omega}^A + \hat{\phi} \hat{\phi} \hat{G}_{q\omega}^A$, in which $\hat{G}_{q\omega}^A = (j\omega)^{-1} \hat{V}_A^q(z, z')$, $\hat{G}_{q\omega}^A = \mu(j\omega)^{-1} H_0^1(z, z')$, $\hat{G}_{q\omega}^A = \mu(j\omega)^{-1} H_0^1(z, z')$. A similar representation applies to the scalar potentials $\hat{K}^q(r, r')$ and $P_{q}(r, r')$. The terms $V_{q\omega}^A(z, z')$ and $P_{q}(z, z')$ are the voltage and current, respectively, at a unit current source (denoted by the subscript $i$) located at $z'$ on the equivalent transmission line representing the $q$th Floquet wave of polarization $\alpha = e$ or $h$ in the multilayered medium. $T_{q\omega}^A(z, z')$ is similarly defined, but its subscript $u$ denotes a unit voltage source. We also find that $V_{q\omega}^A(z, z') = j\mu \omega g_{q\omega}^{A\omega}(z, z')$ and $T_{q\omega}^A(z, z') = j\omega g_{q\omega}^{A\omega}(z, z')$ where $g_{q\omega}^{A\omega}(z, z')$ and $g_{q\omega}^{A\omega}(z, z')$ are the scalar longitudinal Green’s functions developed in [6, pp. 446, 455]. Indeed, using reciprocity and the argument in [5, pp. 194, 195], all the voltages and currents for all combinations of polarizations and unit source types may be expressed in terms of these two characteristic scalar Green’s functions and their derivatives.

Extraction of the Asymptotic Form of Series. In (9), for numerical convenience terms $\hat{G}_q^{A\omega}(z, z')$, asymptotic for large $q$ to the terms $\hat{G}_q^A(z, z')$ of the spectral dyadic Green’s function, are subtracted term by term from the original series and their sum is added back as a separate series. Removing the asymptotic form of each term from the spectral sum
accelerates its convergence. The remaining sum in (9) may then be accelerated via the Ewald method. Each of these terms, in turn, is an asymptotic form of the various transmission line voltages and currents, and consists of up to three terms of the form $F_{\ell m} \exp[-j(k_\ell x + k_m z - z' - 2\pi q)/\lambda_{\ell m}], \ell = 1, 2, 3$. For the first term, $F_{1m} = 1$ and $z_2 = 0$, and the term is readily recognized as the direct contribution from the original array of line sources radiating in a homogeneous medium. For the remaining terms, the constant $F_{\ell m}$ represents the asymptotic layer boundary reflection coefficient for large $q$ and with $n = s$ or $h$. These terms represent reflections appearing to arise from (quasi-) images located at $z' + z_2$ in layers above or below the original source layer as shown in Fig. 3a. All three terms result in series having the spectral form of homogeneous medium periodic Green's functions; the Ewald method may thus be used to sum them. The potentials $K_0$ and $P_1$ may be treated the same way.

Numerical Example: Convergence. The test problem shown in Figure 3b consists of two periodic strip gratings (period $d = 1.3m$) on top ($z = 0$) and in the middle ($z = -1m$) of a dielectric layer (relative dielectric permeability $\epsilon = 2.3$), which resides in the region $-2m < z < 0$. Each strip is 1m wide. The periodic structure is illuminated from above by a plane wave with unitary magnetic field $H$ directed along $y$, and frequency equal to 100MHz. The current on both top and bottom strips, shown in Fig.3c, is evaluated by the method of moments defined on a single array cell, using the periodic Green's function developed in the previous sections. The solution is compared with a reference solution constructed with the corresponding three dimensional (3D) problem of an infinite 2D array of metallic patches with dimensions $1 \times 1$ m, and periodicities $d_1 = 1.3m$ and $d_2 = 1m$. In the 2D problem, the evaluation of the Green's function requires only a few terms to achieve accuracy to four significant digits: the first spectral sum in (9) is over indices $-5 < q < +5$, while the second spectral sum in (9) transformed according to the Ewald method, as explained in the previous sections, is over indices from $-1$ to $+1$. The bottom strip current is larger than the top one since the bottom strip is $5.06$ wavelengths long.

References

[1] K. E. Jordan, G. R. Richter, and P. Sheng, "An efficient numerical evaluation of the Green's function for the Helmholtz operator on periodic structures," J. Comp. Physics, vol. 63, pp. 222-235, 1986.
[2] D. R. Jackson, D. R. Jackson, and N. J. Champagne, "Efficient computation of periodic and nonperiodic Green's function in layered media using the MPFE," in URSI Int. Symp. on Electrom. Theory, Thessaloniki, Greece, May 25-28 1998.
[3] A. W. Madani and A. F. Peterson, "A comparison of acceleration procedures for the two-dimensional periodic Green's function," IEEE Trans. Antennas Propagat., vol. 44, no. 4, pp. 567-571, April 1996.
[4] K. A. Michalski, "Electromagnetic scattering and radiation by surfaces of arbitrary shape in layered media," part 1: Theory. IEEE Trans. Antennas Propagat., vol. 38, no. 3, pp. 335-344, 1990.
[5] J. A. Stratton, Handbook of Mathematical Functions, Dover, New York, 1970.
[6] L. D. Landau and E. M. Lifshitz, Electrodynamics of Continuous Media, Pergamon Press, New York, 1960.