Scattering of Electromagnetic Waves

Numerical Simulations

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SCATTERING OF ELECTROMAGNETIC WAVES
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To my family, Hannah, Clarisse, and Kaleb for their love.

— L. Tsang

To our families.

— J. A. Kong, K. H. Ding, C. O. Ao
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Scattering of Electromagnetic Waves

Volume I: Theories and Applications (Tsang, Kong, and Ding)
Volume II: Numerical Simulations (Tsang, Kong, Ding, and Ao)
Volume III: Advanced Topics (Tsang and Kong)
Electromagnetic wave scattering is an active, interdisciplinary area of research with myriad practical applications in fields ranging from atomic physics to medical imaging to geoscience and remote sensing. In particular, the subject of wave scattering by random discrete scatterers and rough surfaces presents great theoretical challenges due to the large degrees of freedom in these systems and the need to include multiple scattering effects accurately. In the past three decades, considerable theoretical progress has been made in elucidating and understanding the scattering processes involved in such problems. Diagrammatic techniques and effective medium theories remain essential for analytical studies; however, rapid advances in computer technology have opened new doors for researchers with the full power of Monte Carlo simulations in the numerical analysis of random media scattering. Numerical simulations allow us to solve the Maxwell equations exactly without the limitations of analytical approximations, whose regimes of validity are often difficult to assess. Thus it is our aim to present in these three volumes a balanced picture of both theoretical and numerical methods that are commonly used for tackling electromagnetic wave scattering problems. While our book places an emphasis on remote sensing applications, the materials covered here should be useful for students and researchers from a variety of backgrounds as in, for example, composite materials, photonic devices, optical thin films, lasers, optical tomography, and X-ray lithography. Introductory chapters and sections are also added so that the materials can be readily understood by graduate students. We hope that our book would help stimulate new ideas and innovative approaches to electromagnetic wave scattering in the years to come.

The increasingly important role of numerical simulations in solving electromagnetic wave scattering problems has motivated us to host a companion web site that contains computer codes on topics relevant to the book. These computer codes are written in the MATLAB programming language and are available for download from our web site at www.emwave.com. They are provided to serve two main purposes. The first is to supply our readers a hands-on laboratory for performing numerical experiments, through which the concepts in the book can be more dynamically relayed. The second is to give new researchers a set of basic tools with which they could quickly build on projects of their own. The fluid nature of the web site would also allow us to regularly update the contents and keep pace with new research developments.
The present volume covers numerical simulation techniques and results for electromagnetic wave scattering in random media and rough surfaces. Due to the large degree of freedom associated with these systems, especially for 3-D scattering problems, fast computational methods are essential for maximizing returns from limited computational resources. Indeed, the subject of numerical electromagnetics has seen explosive growth in recent years. For lack of space, we choose to focus here on methods and techniques which are more directly related to our own research.

We begin in Chapter 1 with Monte Carlo simulations of a simple one-dimensional random medium — a layered medium characterized by permittivity fluctuations. Simulation results are used to explain passive remote sensing measurements of the Antarctic firn. For two- and three-dimensional scattering, it is advantageous to formulate the problem in terms of surface integral equations where the unknowns are confined to a lower dimensionality. Numerical solutions of surface integral equations are often obtained through the method of moments (MoM). We also discuss a useful technique known as the discrete dipole approximation (DDA) for solving volume integral equation. The DDA can be used to model inhomogeneous, irregularly shaped object by discretizing it as a collection of point dipoles. In MoM and DDA, numerical solutions are obtained by approximating the integral equations with a set of linear equations. Thus matrix computation is an essential aspect of numerical electromagnetics. When the size of the system becomes very large, direct matrix inversion becomes inefficient, and iterative methods such as the conjugate gradient methods are often used instead. Iterative methods usually require repeated computations of matrix-vector multiplication, and for problems with translational invariance, it is possible to utilize fast Fourier transform (FFT) to speed up this operation. The use of FFT in conjunction with iterative solvers is the cornerstone of fast computational methods introduced later in this book. Therefore we discuss these topics at some length in Chapter 2.

The remainder of the book is divided into two main parts. Chapters 3–6 deal with simulations of rough surface scattering, while volume scattering simulations involving random discrete scatterers are studied in Chapters 7–13 (except Chapter 11 — which contains aspects of both rough surface and volume scattering). The topic of electromagnetic wave interactions with rough surfaces has important applications in microwave remote sensing of ocean surface, geophysical terrain, and agricultural fields as well as in the design and manufacturing of optical systems and X-ray lithography. In Chapter 3, we discuss scattering and emission by periodic rough surfaces. Two
solution methods are used to solve this problem. The first is the T-matrix method, which makes use of Floquet mode expansions and the extended boundary condition. The T-matrix formulation is exact, but the resulting equations become ill-conditioned when the surface is very rough. The second method uses a surface integral equation approach with MoM. Although computationally more intensive than the T-matrix method, the surface integral equation approach is applicable to surfaces with deep corrugation. We also describe Ewald’s method for speeding up calculations of the Green’s function in periodic medium. This has applications in active research areas such as frequency selective surfaces and photonic bandgap materials.

In Chapter 4, we discuss one-dimensional random rough surface scattering. The core ideas behind rough surface scattering simulations are introduced here. We describe in details the discretization procedure for the surface integral equations in the Dirichlet, Neumann, and two-media problems. Numerical methods for generating Gaussian and fractal rough surface profiles are described. The issue of truncating the rough surface and limiting the computational domain is also an important one. We discuss two popular approaches. The first approach uses a tapered incident wave that illuminates only a part of the entire rough surface, while the second approach uses a periodic boundary condition. As described in Volume I, random rough surfaces are often characterized by their power spectra. This is convenient for theoretical work, but how well does it model reality? We include discussion of wave scattering from real-life rough surface profiles. In addition to simulating bistatic scattering from rough surfaces, we also take an in-depth look at emissivity calculations based on rough surface simulations, which impose much more stringent energy conservation requirement.

Chapters 5 and 6 are devoted respectively to fast computational methods in 1-D and 2-D rough surface scattering simulations. The development of fast computational methods is particularly important in scattering by 2-D rough surfaces (3-D scattering problem) where the number of unknowns can quickly escalate as we increase the surface size. Since real-life surfaces are 2-D, we emphasize in this book fast computational methods that can be applied to scattering by both 1-D and 2-D rough surfaces. We introduce the sparse matrix iterative approach with canonical grid (SMCG). In this method, the impedance matrix is split into a strong part that consists of near-neighbor interactions and a weak part that consists of all the rest. An iterative scheme such as the conjugate gradient method is adopted to solve the matrix equation. The strong matrix is sparse and can be easily handled. However, the weak interactions require the multiplication of the dense weak
matrix with successive iterates and could therefore present a major computational bottleneck. To speed up such calculations, the concept of canonical grid (CG) is introduced. The essential nature of CG is that it is translationally invariant. In rough surface scattering problems, the CG is usually taken to be the mean flat surface. By translating the unknowns to the CG, the weak interactions can be performed simultaneously for all unknowns using FFT. This reduces memory requirements from $O(N^2)$ to $O(N)$ and operation counts from $O(N^2)$ to $O(N \log N)$. We also introduce the physics-based two-grid (PBTG) method for dealing with lossy dielectric surfaces. In this method, a dense grid suitable for the lower half-space and a coarse grid suitable for the upper half-space are chosen. By taking advantage of the attenuative nature of the Green's function in the lower half-space and the slowly varying nature of the Green's function in the upper half-space with respect to the dense grid, one can achieve the accuracy of a single dense grid with the computational efficiency of a single coarse grid. Other fast methods discussed and illustrated in Chapter 5 include the steepest descent fast multipoles method (SDFMM) and the method of ordered multiple interactions (MOMI).

In contrast to rough surface scattering, volume scattering involving dense distributions of discrete scatterers is often a full-fledged 3-D scattering problem. The additional degree of freedom makes direct simulations of scattering coefficients rather difficult. Radiative transfer theory is commonly used for such problems, but the conventional approach fails to take into account of coherent multiple interactions between the scatterers. A better approach is to perform the scattering simulations on a test volume that contains a large number of scatterers but forms only a small part of the whole system. Coherent interactions are captured through the simulated extinction coefficients and phase functions, which can then be used in the dense medium radiative transfer equation (rigorously derived in Volume III) to solve the large-scale problem. These concepts are discussed in Chapter 7, where idealized randomly distributed point scatterers are used to illustrate the methods. The multiple scattering problem is formulated using the Foldy-Lax self-consistent equations.

In a dense medium, the correlation of scatterer positions could significantly affect the scattering results. The pair-distribution function quantifies the two-particle correlation property of the scatterers. In Chapter 8, we introduce the Percus–Yevick equation for the pair-distribution function and give closed-form solutions for hard and sticky spheres. For Monte Carlo simulations, statistical realizations of scatterer configurations are needed. Two
methods are commonly employed to generate the particle positions: sequential addition and Metropolis shuffling, the latter method being more efficient when the particles are very closely packed. We show simulation results of the pair distribution functions for hard spheres and spheroids as well as sticky spheres. The simulated pair distribution functions are found to compare well with the Percus–Yevick pair distribution functions. Before dealing with 3-D dense media scattering, it is instructional to first study, in Chapter 9, the simpler problem of 2-D dense media scattering, where the volume scatterers are chosen to be infinitely long cylinders. We describe analytical pair distribution function and Monte Carlo simulations of particle positions in the 2-D case. The Foldy-Lax multiple scattering equations are then used to simulate extinction coefficients for densely packed hard and sticky cylinders. Finally, the SMCG method used in rough surface scattering is generalized to the volume scattering simulations. In Chapter 10, we perform 3-D dense media scattering calculations with dielectric spheres and spheroids. The volume integral equation approach as well as the T-matrix approach based on the Foldy-Lax equations are described in details. Simulation results for the extinction coefficients and phase matrices are shown and compared with analytical approximations.

In Chapter 11, we describe the novel correlation phenomenon in random media scattering known as the memory effect, which manifests itself in wave scattering through the angular correlation function (ACF). ACF has been discussed in Chapter 6 of Volume I in the context of single scattering by point scatterers. Here, we provide a general derivation of the memory effect based on the statistical translational invariance of the random medium. The special property of ACF for random medium makes it a good candidate for the detection of a target embedded in random clutter. We explore such ideas by studying targets buried under rough surface and volume scatterers.

The subject of multiple scattering by finite cylinders has important applications in the remote sensing of vegetation as well as signal coupling among multiple vias in high frequency circuits. In Chapter 12, we consider scattering by vertical cylinders in the presence of reflective boundaries, which introduce additional complications. We discuss Monte Carlo simulations of these systems as well as simple analytical results that take into account of first and second order scattering. In Chapter 13, more realistic modeling of vegetation structures through stochastic Lindenmayer systems are presented. We compare scattering results from such systems obtained using the methods of DDA, the coherent addition approximation, and independent scattering.
This book should provide a good mix of basic principles and current research topics. An introductory course in Monte Carlo simulations can cover most of Chapters 1, 2, 4, 5, 7, and 9.

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SCATTERING OF ELECTROMAGNETIC WAVES
Chapter 1

MONTE CARLO SIMULATIONS OF LAYERED MEDIA

1 One-Dimensional Layered Media with Permittivity Fluctuations 2
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1 One-Dimensional Layered Media with Permittivity Fluctuations

We study Monte Carlo simulations of solutions of the Maxwell equations in Volume II. The simplest case of random medium is one where the permittivity is a random function of positions in a one-dimensional problem. In Fig. 1.1.1, we show a stratified medium of many layers. The permittivity fluctuates from layer to layer. The basic theory of waves in layered medium was covered in Chapter 5 of Volume I. Nevertheless, even in this simple case, there can be two distinct kinds of layering. The first kind is a continuous random medium in which the random medium permittivity $\epsilon(z)$ is a random process that is a continuous function of $z$. The second kind is discrete layering in which there are abrupt changes of permittivity from layer to layer. To further illustrate the difference, we apply both models to thermal emission of a layered medium and make a comparison with observed brightness temperatures of Antarctica. We found that in order to match the observed brightness temperatures, the two models have to use drastically different physical parameters. The results illustrate the difference between a continuous random medium and a discrete random medium.

Figure 1.1.1 Stratified medium with permittivity fluctuations from layer to layer.

1.1 Continuous Random Medium

A common approach is to assume a Gaussian random process of the permittivity fluctuations. Figure 1.1.2 illustrates a realization of Gaussian random process as a function of position. The density of snow is used for illustration.
§1.1 Continuous Random Medium

Figure 1.1.2 A single realization of a continuous Gaussian random profile with a mean density of 0.4 g/cm$^3$, a correlation length of 2 mm, and a standard deviation in density of 0.0156 g/cm$^3$.

For layered random media, one can assume $\epsilon(z)$ as a one-dimensional Gaussian random process with mean $\epsilon_m$ and variance $\sigma^2 = \delta \epsilon_m^2$. The probability density function is

$$p(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\epsilon - \epsilon_m)^2}{2\sigma^2}\right) \quad (1.1.1)$$

Let $z_1$ and $z_2$ be two positions and let $\epsilon_1 = \epsilon(z_1)$ and $\epsilon_2 = \epsilon(z_2)$. Then the joint probability density function is

$$p(\epsilon_1, \epsilon_2) = \frac{1}{2\pi\sigma^2\sqrt{1-r^2}} \exp\left[- \frac{1}{2\sigma^2(1-r^2)} \left((\epsilon_1 - \epsilon_m)^2 \right. \right. \right.$$

$$\left. \left. - 2r(\epsilon_1 - \epsilon_m)(\epsilon_2 - \epsilon_m) + (\epsilon_2 - \epsilon_m)^2\right)\right] \quad (1.1.2)$$

where $r$ is the correlation coefficient that depends on $|z_1 - z_2|$. If the correlation coefficient is of exponential form, then

$$r(z_1 - z_2) = \exp\left(-\frac{|z_1 - z_2|}{l_z}\right) \quad (1.1.3)$$
where \( l_z \) is the correlation length. Let \( \epsilon_f(z) = \epsilon(z) - \epsilon_m \) be the fluctuating part of the permittivity. Then the covariance function of the permittivity is

\[
\langle \epsilon_f(z)\epsilon_f(z') \rangle = \delta \epsilon_m^2 \exp \left( -\frac{|z - z'|}{l_z} \right)
\]  

(1.1.4)

where angular bracket denotes average. Given a realization of permittivity profile, we can discretize the medium into fine layers (say up to 30,000 layers). We note that in Fig. 1.1.2 of the Gaussian random process, the permittivity is a continuous function of depth.

### 1.2 Generation of One-Dimensional Continuous Gaussian Random Medium

If we assume that \( f(z) \) is a real Gaussian process with normalized correlation function \( C(z) \). Then

\[
\langle f(z)f(z') \rangle = \sigma^2 C(z - z')
\]  

(1.1.5)

Let \( W(K) \) be the spectral density

\[
\sigma^2 C(z) = \int_{-\infty}^{\infty} dK e^{iKz} W(K)
\]  

(1.1.6)

\[
W(K) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz \sigma^2 C(z) e^{-iKz}
\]  

(1.1.7)

For the case that the correlation is exponential

\[
C(z) = \exp \left( -\frac{|z|}{l_z} \right)
\]  

(1.1.8)

the spectral density is

\[
W(K) = \frac{\sigma^2 l_z}{\pi} \frac{l_z}{1 + K^2 l_z^2}
\]  

(1.1.9)

Let the sample be generated for \( 0 \leq z \leq L \). Outside \( L \), we can assume that \( \epsilon_f(z) \) is periodic. Then using a Fourier series,

\[
f(z) = \frac{1}{L} \sum_{n=-\infty}^{\infty} b_n e^{i2\pi nz/L}
\]  

(1.1.10)

The discretization is

\[
\Delta K = \frac{2\pi}{L}
\]  

(1.1.11)

\[
K_n = \frac{2\pi n}{L} = n\Delta K
\]  

(1.1.12)
The $b_n$'s are complex and

$$\langle f(z_1) f(z_2) \rangle = \int_{-\infty}^{\infty} dK e^{iK(z_1-z_2)} W(K)$$

$$= \frac{1}{L^2} \sum_n \sum_m \langle b_n b_m^* \rangle e^{i \frac{2\pi n}{L} z_1 - i \frac{2\pi n}{L} z_2}$$

$$= \sum_n \frac{2\pi}{L} e^{iK_n(z_1-z_2)} W(K_n)$$

(1.1.13)

Thus

$$\langle b_n b_m^* \rangle = \delta_{nm} 2\pi LW(K_n)$$

(1.1.15)

Since $f$ is real,

$$b_n = b_{-n}^*$$

(1.1.16)

$$\langle |b_n'|^2 \rangle = \langle |b_n''|^2 \rangle = \pi LW(K_n)$$

(1.1.17)

where $b_n = b_n' + ib_n''$. The real and imaginary parts are independent Gaussian random variables. Thus $\langle b_n b_{-n}^* \rangle = \langle b_n b_n \rangle = 0$. Let $L$ be divided with $N$ intervals,

$$\Delta z = \frac{L}{N}$$

(1.1.18)

and $N$ be a power of 2.

$$f(z_l) = \frac{1}{L} \sum_{n=-N/2+1}^{N/2} b_n \exp \left( i \frac{2\pi nl}{N} \right)$$

(1.1.19)

Then $b_0$ and $b_{N/2}$ are real. We first obtain $N$ independent Gaussian random numbers with zero mean and unit variance. We next multiply the numbers by a normalization factor to $b_0$, $b_{N/2}$, $b_n'$ and $b_n''$ with $n = 1, 2, \ldots, N/2 - 1$, such that (1.1.17) holds. We then use

$$b_{-n} = b_n^*$$

(1.1.20)

to get $b_n$ with $n = -1, -2, \ldots, -N/2 + 1$. The permittivity is then calculated by (1.1.19).

### 1.3 Numerical Results and Applications to Antarctica

In this section we illustrate the numerical results and application to the Antarctic firn. The Antarctic firn has a layering structure. The permittivity of snow is around $1.5\epsilon_o$. Thus if a half-space medium is assumed, the reflectivity at $\theta_o = 0$ is 0.01 so that with $T = 240$ K, the brightness temperature is 237.6 K. However, the measured brightness temperature is significantly
less than that. The difference can be attributed to the reflections by the layering structure. Snow is a mixture of ice and air, so that the density of snow \( \rho \) indicates the fractional volume of ice in snow. Ice has a density of 0.91 g/cm\(^3\). The density of snow is

\[ \rho = 0.91 f \]  

(1.1.21)

where \( f \) is the fractional volume of ice in snow. We model \( \rho(z) \) as a random process. First we assume that \( \rho(z) \) is a Gaussian random process with

\[ \langle \rho \rangle = \rho_m \]  

(1.1.22)

\[ \rho(z) = \rho_m + \rho_f(z) \]  

(1.1.23)

\[ \langle \rho_f(z_1) \rho_f(z_2) \rangle = \sigma^2 \rho \exp \left( -\frac{|z_1 - z_2|}{l_z} \right) \]  

(1.1.24)

In Fig. 1.1.2 we show a simulated density profile of a single realization using \( l_z = 2 \) mm, \( \sigma_p = 0.0156 \) g/cm\(^3\), and \( \rho_m = 0.4 \) g/cm\(^3\). The continuous profile of each realization is generated down to a depth of 21 m and is discretized with \( 2^{14} = 32,768 \) layers. This gives a \( \Delta z \) discretization thickness of 0.6 mm. The permittivity of each layer is calculated using the following empirical mixing formula for dry snow

\[ \frac{\epsilon'}{\epsilon_o} = 1 + \frac{1.60 \rho}{1 - 0.35 \rho} \]  

(1.1.25)

\[ \frac{\epsilon''}{\epsilon_o} = \frac{\epsilon_{ice}''}{\epsilon_o} \left( 0.52 \rho + 0.62 \rho^2 \right) \]  

(1.1.26)

where \( \epsilon_{ice}'' \) is the imaginary part of the permittivity of pure ice and is temperature-dependent. If \( \sigma_p \ll \rho_m \), we can linearize (1.1.25) and (1.1.26), so that \( \epsilon_m' \) and \( \rho_m \) are related by the same relation as in (1.1.25) and \( \epsilon_m'' \) and \( \rho_m \) are related by the same relation as in (1.1.26).

\[ \frac{\epsilon_m'}{\epsilon_o} = 1 + \frac{1.60 \rho_m}{1 - 0.35 \rho_m} \]  

(1.1.27a)

\[ \frac{\epsilon_m''}{\epsilon_o} = \frac{\epsilon_{ice}''}{\epsilon_o} (0.52 \rho_m + 0.62 \rho_m^2) \]  

(1.1.27b)

Let \( \epsilon = \epsilon_m + \epsilon_f \). Then \( \epsilon_f \), the fluctuating part is

\[ \frac{\epsilon_f'}{\epsilon_o} = \frac{1.60}{(1 - 0.35 \rho_m)^2} \rho_f \]  

(1.1.28)

\[ \frac{\epsilon_f''}{\epsilon_o} = \frac{\epsilon_{ice}''}{\epsilon_o} (0.52 + 1.24 \rho_m) \rho_f \]  

(1.1.29)

The permittivity fluctuation is also a Gaussian random process.
Figure 1.1.3 Computed brightness temperatures using fluctuation dissipation theory and a discretized continuous Gaussian random density profile with a mean density of 0.4 g/cm$^3$, a correlation length of 2 mm, and a standard deviation in density of 0.0156 g/cm$^3$. The temperature profile is: $T(z) = 222 + 34 \exp(0.81 z)$ (z is 0 at the top and negative in the medium). Both profiles are carried down to a depth of 21 m, and are discretized into 32,768 layers, giving a layer thickness of 0.6 mm. Both vertically and horizontally polarized brightness temperatures are shown, with $T_v > T_h$.

The brightness temperature of such a profile is then calculated using the layered medium model of Chapter 5 of Volume I. The layered medium model also accounts for a temperature profile. The temperature profile is assumed to have the form of $T_0 + T_h \exp(\gamma z)$. This form of temperature profile is characteristic of Antarctic firn in the summer. We use Eqs. (5.2.36a) and (5.2.36b) of Volume I to compute the brightness temperature. Figure 1.1.3 shows the brightness temperatures of two different realizations which have the same correlation length and variance as the realization shown in Fig. 1.1.2. A single realization of permittivity profile means that a single sample of random permittivity fluctuation is produced. The brightness temperatures are then computed. Since the layered medium model is based on a coherent approach, the results have to be averaged over many realizations. In a real-life situation, there can be built-in incoherence. For example, the interfaces of the layered structure can be rough with rms height larger than 1/16 of a wavelength so that the reflection is rendered incoherent. In Fig. 1.1.3, we also show the brightness temperature averaged over 200 realizations. The
averaging shows that all the coherent oscillations have been smoothed out in the average. However, in order to produce a significant amount of decrease in brightness temperature due to reflection, a small correlation length of 2 mm is required as shown in Fig. 1.1.2. The reasons are that the permittivity in a Gaussian random process is a continuous function of \( z \). As we see in some of the examples in Chapter 5 of Volume I, a continuous profile usually does not produce much reflection. In order to produce reflection, the continuous profile must have a substantial change of permittivity over a short distance, say 2 mm. Over a long distance of 2.5 m, this means more than 1200 reflections. Thus to match brightness temperature experimental data, a small standard deviation of 0.0156 g/cm\(^3\) is used for the density fluctuations. This will reduce the amount of power reflections for each reflection. Hence, the choice of parameters of \( l_z = 2 \) mm and \( \sqrt{\langle \rho_f^2 \rangle} = 0.0156 \) g/cm\(^3\) is dictated by the underlying assumption of Gaussian random process.

By choosing the parameters of the Gaussian random process, we can get reasonable brightness temperatures. However, the question is whether these physical parameters are reasonable. In the next section we discuss the discrete layering model.

2 Random Discrete Layering and Applications

The ground truth measurements of snow density profile have been taken by Rott et al. [1993]. Figure 1.2.1 illustrates the results for the station at Vestestraumen. The profiles indicate discrete layering with layer thickness of the order of 5 cm. Abrupt changes of densities are associated with discrete layering. The ground truth layering geometry does not correspond to the continuous Gaussian random process that is discussed in Section 1. Thus a satisfactory theory needs to (1) give an accurate and correct solution of Maxwell’s equations; (2) match experimental measurements, and (3) use a correct medium characterization with parameters that are verified by ground truth measurements.

To incorporate ground truth data on the density profile, we apply a centimeter discrete layering model instead of a millimeter correlation length continuous random medium model. The measured profile in Fig. 1.2.1 shows a background trend of the form \( 1 - \exp(\delta z) \) \( (z < 0) \) which saturates below about 1 m of depth. A theoretical profile similar to the measured profile can be generated using two random variables and a background exponential trend. The two random variables are the layer thickness and the density. The layer thickness is assumed to be exponentially distributed. The layer-to-
Random Discrete Layering and Applications

Figure 1.2.1 The snow density profile measured by H. Rott at Vestestraumen. The profile was obtained by measuring the average density in consecutive 5-cm layers.

Layer density variations are assumed to be normally distributed and are then superimposed on top of the background exponential profile. The profile is carried down to 10-m depth. Below this depth, layered scattering is expected to drop off. The temperature profile is again assumed to have the form of $T_0 + T_h \exp(\gamma z)$. Since the measurements were made in the Antarctic summer, the temperature distribution decays from a high temperature at the surface down to the mean annual temperature at depths greater than 10 m. Figure 1.2.2 shows two sample theoretical profiles generated. The layer thickness is exponentially distributed with a mean layer thickness of 4.1 cm. The density is

$$\rho(z) = 0.25 + 0.16 [1 - \exp(0.05z)] + \rho_f(z)$$

(1.2.1)

with $z$ in centimeters. The fluctuating part $\rho_f(z)$ is normally distributed with standard deviation of 0.04 g/cm$^3$. Both parameters of layer thickness and density fluctuation are very different from that of the continuous random medium model. The continuous random medium model used $l_z = 2$ m and density fluctuation of 0.0156 g/cm$^3$. Figure 1.2.3 shows the corresponding histogram of the densities in a theoretical profile along with the histogram of the actual densities. The background exponential profile was set to provide the correct density level in the theoretical profile. Using the layered medium model, the theoretical brightness temperatures for a range of ob-
Figure 1.2.2 Two sample realizations of a discrete random profile. The profiles are generated with an exponential distribution of layer thickness and a mean thickness of 4.1 cm. The density in each layer is the sum of a deterministic part given by $0.25 \text{ (g/cm}^3) + 0.16(1 - \exp(z/(20 \text{ cm})))\text{ (g/cm}^3)$ and a normally distributed random variable with zero mean and a standard deviation of $0.04 \text{ g/cm}^3$ ($z$ is 0 at the top and negative in the medium). For display purposes, the resulting profile is then averaged over 5-cm intervals just as Rott’s measured profile was (see Fig. 1.1.2). Calculation of brightness temperatures uses the original profile without the 5-cm averaging.

Observation angles are computed and averaged over many realizations. Figure 1.2.4 shows the results when 600 such realizations are averaged. The measured brightness temperatures are also shown in Fig. 1.2.4, along with the results which would be expected from a uniform density profile and the same temperature profile. The layered scattering model gives good agreement of brightness temperature with the measured results out to an observation angle of $50^\circ$. Note that the discrete layering used by the theory (Fig. 1.2.2) is statistically similar to the observed profile (Fig. 1.2.1). No ad-hoc correction factors are required. The half-space model of uniform density does not give adequate results. The half-space model results show much less polarization contrast. The half-space model of homogeneous density gives much higher brightness temperatures that does not agree with experimental observations. These simulations show that layer scattering with centimeter layer thickness is an important phenomenon at C-band passive remote sensing of Antarctica.

Extensions have been made to a Poisson process with a modified spectral density. Good agreement with data have also been found for Vestestraumen, Amundsen Ice and Base Camp stations [West, 1994].
Figure 1.2.3 A histogram of the measured density profile superimposed on a histogram of one realization of a density profile using the discrete random profile described in Fig. 1.2.2.

Figure 1.2.4 A comparison of the measured brightness temperatures with theoretical results using the discrete random profile described in Fig. 1.2.2. Average layer thickness is 4.1 cm, standard deviation of density variation is 0.04 g/cm$^3$, and a background trend is given by $0.25 \text{ (g/cm}^3) + 0.16(1-\exp(z/(20 \text{ cm}))))(\text{g/cm}^3)$. The temperature profile is: $T(z) = 234 x + 24 \exp(0.81 z)$ ($z$ is 0 at the top and negative in the medium). Both profiles are carried down to a depth of 10 m. Vertically and horizontally polarized brightness temperatures are shown, with $T_v > T_h$ at all viewing angles.
REFERENCES AND ADDITIONAL READINGS


West, R., D. P. Winebrenner, L. Tsang, and H. Rott (1996), Microwave emission from density stratified Antarctic firn at 6 cm wavelength, *J. of Glaciology*, 42(140), 63-76.
Chapter 2

INTEGRAL EQUATION FORMULATIONS
AND BASIC NUMERICAL METHODS

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In this chapter, we discuss integral equation formulation of boundary value problems. We will give a brief overview with more detailed analysis to be given in subsequent chapters where the numerical methods are applied to specific problems. We will also describe the basic numerical methods that include the method of moments, discrete dipole approximation, product of Toeplitz matrix and column vector using FFT, and conjugate gradient method. These numerical methods will be used extensively in subsequent chapters.

1 Integral Equation Formulation for Scattering Problems

1.1 Surface Integral Equations

Integral equations can be derived by using Green’s functions. The advantage of surface integral equation is that they reduce the dimension of the problem by one. In the following we first consider a two-dimensional scattering problem so that the surface integral equation becomes one-dimensional.

Consider an incident wave impinging upon an object. Let the problem be uniform in the \( \hat{y} \)-direction so that there is no variation in the \( \hat{y} \)-direction i.e., \( \frac{\partial}{\partial \hat{y}} = 0 \) (Fig. 2.1.1).

We first consider the TE case with electric field in the \( \hat{y} \)-direction

\[
\overline{E}_{\text{inc}} = \hat{y}\psi_{\text{inc}}(x, z) \tag{2.1.1}
\]

\[
\overline{E} = \hat{y}\psi(x, z) \tag{2.1.2}
\]

The \( \overline{H} \) field is

\[
i\omega\mu\overline{H} = \hat{x}\left(-\frac{\partial\psi}{\partial z}\right) + \hat{z}\frac{\partial\psi}{\partial x} \tag{2.1.3}
\]

For the TM case, the \( \overline{H} \) field will be in the \( \hat{y} \)-direction so that

\[
\overline{H}_{\text{inc}} = \hat{y}\psi_{\text{inc}}(x, z) \tag{2.1.4}
\]

\[
\overline{H} = \hat{y}\psi(x, z) \tag{2.1.5}
\]

Then the electric field is

\[
-i\omega\epsilon\overline{E} = \hat{x}\left(-\frac{\partial\psi}{\partial z}\right) + \hat{z}\frac{\partial\psi}{\partial x} \tag{2.1.6}
\]

If the scattering object is a perfect electric conductor, then the boundary condition is

\[
\hat{n} \times \overline{E} = 0 \tag{2.1.7}
\]
Let $\hat{n} = n_x \hat{x} + n_z \hat{z}$. We note from (2.1.6) that
\[
\hat{n} \times \left( -\hat{x} \frac{\partial \psi}{\partial z} + \hat{z} \frac{\partial \psi}{\partial x} \right) = -\hat{y} \left( n_x \frac{\partial \psi}{\partial x} + n_z \frac{\partial \psi}{\partial z} \right) = -\hat{y} \frac{\partial \psi}{\partial n}
\]
(2.1.8)
where $\frac{\partial \psi}{\partial n} = \hat{n} \cdot \nabla \psi$.

Thus for two-dimensional problem, we can simply use $\psi$. Then
\[
\nabla^2 \psi + k^2 \psi = 0
\]
(2.1.9)

(i) For TE problem of perfect electric conductor, the boundary condition is
\[
\psi = 0 \quad \text{at } S
\]
(2.1.10)

(ii) For TM problem of perfect electric conductor, the boundary condition is
\[
\frac{\partial \psi}{\partial n} = 0 \quad \text{at } S
\]
(2.1.11)

For two-dimensional problems, the Green’s function is
\[
g(\rho, \rho') = \frac{i}{4} H_0^{(1)} (k|\rho - \rho'|)
\]
(2.1.12)
where $\rho = x\hat{x} + z\hat{z}$ and $H_0^{(1)}$ is the zeroth order Hankel function of the first kind.

The Green’s function obeys the equation
\[
(\nabla^2 + k^2) g(\rho, \rho') = -\delta (\rho - \rho')
\]
(2.1.13)

Applying the scalar Green’s theorem
\[
\int d\rho \left( \psi_1 \nabla^2 \psi_2 - \psi_2 \nabla^2 \psi_1 \right) = \oint d\bar{s} \cdot (\psi_1 \nabla \psi_2 - \psi_2 \nabla \psi_1)
\]
(2.1.14)
Let $\psi_2 = \psi$ and $\psi_1 = g$ in (2.1.14). Then
\[
\int d\bar{\rho} \left( g \nabla^2 \psi - \psi \nabla^2 g \right)
= \int d\bar{\rho} \left[ g \left( -k^2 \psi \right) - \psi \left( -k^2 g - \delta \left( \bar{\rho} - \bar{\rho}' \right) \right) \right]
= \begin{cases} 
\psi(\bar{\rho}') & \text{if } \bar{\rho}' \text{ in } V \\
0 & \text{if } \bar{\rho}' \text{ in } V_p
\end{cases}
= - \int dS \left( g \frac{\partial \psi}{\partial n} - \psi \frac{\partial g}{\partial n} \right) + \psi_{inc}(\bar{\rho}') \tag{2.1.15}
\]
where $\hat{n}$ is the outward normal to surface $S$. In (2.1.14), the surface integral at infinity gives the incident wave $\psi_{inc}(\bar{\rho})$. For TE case of PEC, we apply (2.1.10) to get
\[
\begin{cases} 
\psi(\bar{\rho}') & \text{if } \bar{\rho}' \text{ in } V \\
0 & \text{if } \bar{\rho}' \text{ in } V_p
\end{cases}
= - \int dS g(\bar{\rho}, \bar{\rho}') \frac{\partial \psi}{\partial n}(\bar{\rho}) + \psi_{inc}(\bar{\rho}') \tag{2.1.16}
\]
To obtain a surface integral equation, we let $\bar{\rho}'$ approach surface $S$, then we have
\[
0 = \psi_{inc}(\bar{\rho}') - \int dS g(\bar{\rho}, \bar{\rho}') \frac{\partial \psi}{\partial n}(\bar{\rho}) \tag{2.1.17}
\]
for $\bar{\rho}' \in S$.

Equation (2.1.17) is a surface integral equation because $\bar{\rho}$ and $\bar{\rho}'$ both belong to the same domain $S$. Equation (2.1.17) is Fredholm equation of the first kind. The source domain $\bar{\rho}$ and the field domain $\bar{\rho}'$ belong to the same domain. As $\bar{\rho} \to \bar{\rho}'$, $g(\bar{\rho}, \bar{\rho}')$ is large which means the matrix equation will have strong diagonal elements which makes (2.1.17) well conditioned usually. This is unlike Fredholm equation of the first kind in inverse scattering problems. In such inverse scattering problems, the source domain and the field domain are different. The matrix equation does not have large diagonal elements and the equation is often ill-conditioned.

For TM problem of PEC, we apply boundary conditions (2.1.11). Then
\[
\begin{cases} 
\psi(\bar{\rho}') & \text{if } \bar{\rho}' \text{ in } V \\
0 & \text{if } \bar{\rho}' \text{ in } V_p
\end{cases}
= \psi_{inc}(\bar{\rho}') + \int dS \psi(\bar{\rho}) \frac{\partial g}{\partial n}(\bar{\rho}, \bar{\rho}') \tag{2.1.18}
\]
To get a surface integral equation, we let $\bar{\rho}'$ approach surface $S$. However, since $\psi(\bar{\rho}')$ experiences a discontinuity of $S$ from $V$ to $V_p$ which is also manifested in the fact that $\frac{\partial g}{\partial n}(\bar{\rho}, \bar{\rho}')$ has a non-integrable singularity at $\bar{\rho} = \bar{\rho}'$, care has to be exercised. We will address these problems later when we implement these equations numerically in later chapters. At this point
we let $\rho' \to \rho'_+$ when $+$ stands for the fact that we approach $S$ from $V$. Then

$$\psi (\rho'_+) = \psi_{inc} (\rho') + \lim_{\rho' \to \rho'_+} \int dS \psi (\rho) \frac{\partial g}{\partial n} (\rho, \rho')$$

for $\rho'$ on $S$.

1.2 Volume Integral Equations

Consider an incident wave $\mathbf{E}^{inc}(\mathbf{r})$ impinging upon the scatterer with permittivity $\epsilon_p(\mathbf{r})$ (Fig. 2.1.2). Maxwell’s equations are

$$\nabla \times \mathbf{E} = +i\omega \mu \mathbf{H}$$
$$\nabla \times \mathbf{H} = -i\omega \epsilon_p(\mathbf{r}) \mathbf{E}$$

where

$$\epsilon_p(\mathbf{r}) = \begin{cases} \epsilon_p(\mathbf{r}) & \text{if } \mathbf{r} \in V_p \\ \epsilon & \text{if } \mathbf{r} \in V \end{cases}$$

It follows that

$$\nabla \times \nabla \times \mathbf{E} - k^2 \mathbf{E} = k^2 (\epsilon_r(\mathbf{r}) - 1) \mathbf{E}$$

where $\epsilon_r(\mathbf{r}) = \epsilon_p(\mathbf{r})/\epsilon$ is the relative permittivity. Thus the scattered field is

$$\mathbf{E}_s(\mathbf{r}) = \int d\mathbf{r}' \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot k^2 (\epsilon_r(\mathbf{r}') - 1) \mathbf{E}(\mathbf{r}')$$

Adding $\mathbf{E}_s(\mathbf{r})$ to $\mathbf{E}^{inc}(\mathbf{r})$ gives the total field $\mathbf{E}(\mathbf{r})$. Then

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{inc}(\mathbf{r}) + k^2 \int d\mathbf{r}' \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot (\epsilon_r(\mathbf{r}') - 1) \mathbf{E}(\mathbf{r}')$$

We can also regard

$$\mathbf{P}(\mathbf{r}) = \epsilon (\epsilon_r(\mathbf{r}) - 1) \mathbf{E}(\mathbf{r})$$
as the induced polarization density. When solving (2.1.25) numerically, we have to take into account the singularity of the dyadic Green’s function.

A volume integral equation can also be obtained by using vector and scalar potentials.

\[
\begin{align*}
\nabla \times \bar{E} &= +i\omega \mu \bar{H} \\
\nabla \times \bar{H} &= -i\omega \varepsilon_p(\bar{r}) \bar{E} \\
&= -i\omega \varepsilon \bar{E} - i\omega \varepsilon(\varepsilon_r(\bar{r}) - 1) \bar{E} \\
\nabla \cdot \bar{H} &= 0 \\
\n\nabla \cdot (\varepsilon_p(\bar{r}) \bar{E}) &= 0 = \nabla \cdot [(\varepsilon + (\varepsilon_r(\bar{r}) - 1)\varepsilon) \bar{E}]
\end{align*}
\]

Using equivalent current of

\[
\bar{J}(\bar{r}) = -i\omega \varepsilon (\varepsilon_r(\bar{r}) - 1) \bar{E}(\bar{r})
\]

From (2.1.30), \(\nabla \cdot (\varepsilon \bar{E}) = \nabla \cdot [\varepsilon \bar{E} - \varepsilon_r(\bar{r}) \varepsilon \bar{E}]\). Thus

\[
\rho_f(\bar{r}) = \frac{1}{i\omega} \nabla \cdot \bar{J}(\bar{r}) = -\varepsilon \nabla \cdot [(\varepsilon_r(\bar{r}) - 1) \bar{E}(\bar{r})]
\]

We can make use of the scalar Green’s function

\[
g(\bar{r}, \bar{r}') = \frac{e^{ik|\bar{r} - \bar{r}'|}}{4\pi |\bar{r} - \bar{r}'|}
\]

The solutions of scalar and vector potentials are

\[
\begin{align*}
\bar{A}(\bar{r}) &= \int d\bar{r}' g(\bar{r}, \bar{r}') \mu \bar{J}(\bar{r}') \\
\Phi(\bar{r}) &= \int d\bar{r}' g(\bar{r}, \bar{r}') \frac{\rho_f(\bar{r}')}{\varepsilon}
\end{align*}
\]

Since \(\bar{E}_s = i\omega \bar{A} - \nabla \Phi\), we have

\[
\bar{E}_s(\bar{r}) = i\omega \int d\bar{r}' g(\bar{r}, \bar{r}') \mu \bar{J}(\bar{r}') - \nabla \int d\bar{r}' g(\bar{r}, \bar{r}') \frac{\rho_f(\bar{r}')}{\varepsilon}
\]

Using (2.1.31) and (2.1.32) in (2.1.36), we get

\[
\bar{E}(\bar{r}) = \bar{E}^{inc}(\bar{r}) + k^2 \int d\bar{r}' g(\bar{r}, \bar{r}') (\varepsilon_r(\bar{r}') - 1) \bar{E}(\bar{r}') \\
+ \nabla \int d\bar{r}' g(\bar{r}, \bar{r}') \nabla' \cdot [(\varepsilon_r(\bar{r}') - 1) \bar{E}(\bar{r}')]
\]

The volume integral over \(d\bar{r}'\) is carried over infinite space. Thus if \(\varepsilon(\bar{r}')\) is discontinuous, the divergence term inside the integrand of (2.1.37) can give rise to surface charge density. This happens when there is a boundary separating two media of different permittivities.
1.3 Dyadic Green’s Function Singularity and Electrostatics

From (2.1.25), the volume integral equation is in terms of the dyadic Green’s function. Using

$$\overline{G}(\bar{r}, \bar{r}') = \left( \bar{I} + \frac{\nabla \nabla}{k^2} \right) g(\bar{r}, \bar{r}')$$  \hspace{1cm} (2.1.38)

we have

$$\bar{E}(\bar{r}) = \bar{E}^{inc}(\bar{r}) + k^2 \int d\bar{r}' (\epsilon_r(\bar{r}') - 1) \bar{E}(\bar{r}')$$

$$+ \int d\bar{r}' (\nabla \nabla g(\bar{r}, \bar{r}')) \cdot (\epsilon_r(\bar{r}') - 1) \bar{E}(\bar{r}')$$  \hspace{1cm} (2.1.39)

To take into account of the singularity of the dyadic Green’s function, let

$$\overline{G}(\bar{r}, \bar{r}') = \text{PV}\overline{G}(\bar{r}, \bar{r}') - \frac{\bar{L}\delta(\bar{r} - \bar{r}')}{k^2}$$  \hspace{1cm} (2.1.40)

where $\text{PV}$ stands for principal value integral and $\delta(\bar{r} - \bar{r}')$ is the three-dimensional Dirac delta function. The volume integration in $\text{PV}$ is over the volume with a volume $V_\delta$ excluded from the observation point $\bar{r}$ (Fig. 2.1.3). The volume $V_\delta$ is infinitesimal. Nevertheless the shape of the exclusion volume has to be specified. The dyad $\bar{L}$ depends on the shape of the exclusion volume.

The volume integral equation becomes

$$\bar{E}(\bar{r}) = \bar{E}^{inc}(\bar{r}) + \int_{V - V_\delta} d\bar{r}' \overline{G}(\bar{r}, \bar{r}') (\epsilon_r(\bar{r}') - 1) k^2 \bar{E}(\bar{r}') + \bar{E}_{\text{self}}(\bar{r})$$  \hspace{1cm} (2.1.41)

where

$$\bar{E}_{\text{self}}(\bar{r}) = - (\epsilon_r(\bar{r}) - 1) \bar{L} \cdot \bar{E}(\bar{r})$$  \hspace{1cm} (2.1.42)

is the self field. The source is an infinitesimal volume $V_\delta$ of relative permittivity $\epsilon_r = \epsilon_p / \epsilon$ (i.e. relative to the background $\epsilon$), and with internal field $\bar{E}(\bar{r})$ inside $V_\delta$. On the other hand, the first two terms on the right-hand side of (2.1.41) is the contribution to $\bar{E}(\bar{r})$ from the incident field and its surrounding medium. Since $V_\delta \to 0$, the self field $\bar{E}_{\text{self}}(\bar{r})$ can be interpreted in terms of electrostatic field created by free charge and polarization charge densities and surface charge densities.

On the other hand, if the vector potential and scalar potential are used, we have the volume integral equation of (2.1.37). The subject of singularity of the dyadic Green’s function are discussed in [van Bladel, 1961; Livesay and Chen, 1974; Yaghjian, 1980; Tsang et. al. 1985; Chew, 1990]. We note that by comparing (2.1.37) and (2.1.39) that the term due to electric current...
\( J \) is benign. The singularity comes from the electrostatic part of electric field due to charges that are in the third term of (2.1.37) and (2.1.39). Thus we shall use electrostatics and examine how electric charges and polarization charges produce electric field in the source region.

In the electrostatic limit

\[
g(\vec{r}, \vec{r}') = \frac{1}{4\pi|\vec{r} - \vec{r}'|} \tag{2.1.43}
\]

The electrostatic equations are

\[
\nabla \cdot \vec{D} = \rho_f \tag{2.1.44}
\]

\[
\nabla \times \vec{E} = 0 \tag{2.1.45}
\]

The electrostatic potential is \( \Phi \) such that

\[
\vec{E} = -\nabla \Phi \tag{2.1.46}
\]

The boundary condition is

\[
\hat{n} \cdot (\vec{D}_{\text{out}} - \vec{D}_{\text{in}}) = \rho_s \tag{2.1.47}
\]

where “out” and “in” represent the outside and inside of the particle respectively. If we use polarization density, with \( \epsilon \) being the background permittivity,

\[
\vec{D} = \epsilon \vec{E} + \vec{P} \tag{2.1.48}
\]

\[
\vec{P} = (\epsilon_p(\vec{r}) - \epsilon)\vec{E} \tag{2.1.49}
\]

Then

\[
\nabla \cdot \epsilon \vec{E} = \rho_f + \rho_p \tag{2.1.50}
\]

where

\[
\rho_p = -\nabla \cdot \vec{P} = -\nabla \cdot \left[ (\epsilon_p(\vec{r}) - \epsilon)\vec{E} \right] \tag{2.1.51}
\]

is the polarization charge density. The surface polarization charge is

\[
-\hat{n} \cdot (\vec{P}_{\text{out}} - \vec{P}_{\text{in}}) = \sigma_p \tag{2.1.52}
\]

The electrostatic potential can be calculated from the superposition integral of these charges

\[
\Phi(\vec{r}) = \frac{1}{\epsilon} \int d\vec{r}' g(\vec{r}, \vec{r}') \left[ \rho_f(\vec{r}') + \rho_p(\vec{r}') \right] \\
+ \frac{1}{\epsilon} \int dS' g(\vec{r}, \vec{r}') \left[ \sigma_s(\vec{r}') + \sigma_p(\vec{r}') \right] \tag{2.1.53}
\]

For the case of an infinitesimal volume \( V_\delta \), we can assume that it is of homogeneous permittivity \( \epsilon_p \) inside \( V_\delta \) (Fig. 2.1.4). The field inside is \( \vec{E} \).

\[
\vec{P}_{\text{in}} = (\epsilon_p - \epsilon)\vec{E} \tag{2.1.54}
\]

\[
\vec{P}_{\text{out}} = 0 \tag{2.1.55}
\]
Note that $\overline{P}_{\text{in}} = \text{constant inside } V_{\delta}$ so that $\rho_p = -\nabla \cdot \overline{P}_{\text{in}} = 0$. For dielectric problem, $\rho_f = \sigma_s = 0$. Thus we only have

$$\sigma_p = -\hat{n} \cdot (\overline{P}_{\text{out}} - \overline{P}_{\text{in}}) = \hat{n} \cdot (\epsilon_r - 1) \epsilon \overline{E} \tag{2.1.56}$$

Thus for $\overline{r}$ inside $V_{\delta}$, from (2.1.53) and (2.1.56),

$$\Phi_{\text{self}}(\overline{r}) = \frac{1}{\epsilon} \int dS' g(\overline{r}, \overline{r}') \sigma_p(\overline{r}') = \int dS' \frac{1}{4\pi |\overline{r} - \overline{r}'|} \hat{n}' \cdot (\epsilon_r - 1) \overline{E}(\overline{r}') \tag{2.1.57}$$

The electric field is $\overline{E}_{\text{self}} = -\nabla \Phi_{\text{self}}(\overline{r})$. Let $\hat{R} = (\overline{r} - \overline{r}') / R$ with $R = |\overline{r} - \overline{r}'|$ and $\hat{R}' = -\hat{R}$. Then $-\nabla (1/R) = \hat{R}/R^2$. Also $V_{\delta}$ is small so that $\overline{E}$ is constant inside $V_{\delta}$.

$$\overline{E}_{\text{self}}(\overline{r}) = \int_{S_{\delta}} dS' \frac{\hat{R} \hat{n}'}{4\pi |\overline{r} - \overline{r}'|^2} \cdot (\epsilon_r - 1) \overline{E}(\overline{r}') = -(\epsilon_r - 1) \overline{L} \cdot \overline{E} \tag{2.1.58}$$

where

$$\overline{L} = \int_{S_{\delta}} dS' \frac{\hat{R}' \hat{n}'}{4\pi |\overline{r} - \overline{r}'|^2} \tag{2.1.59}$$

Note that $\overline{r}$ is at the center of $V_{\delta}$ and $\hat{R}'$ is a unit vector pointing from $\overline{r}$ to $\overline{r}'$.

**Example 1:** Without loss of generality, let $\overline{r} = 0$. If $V_{\delta}$ is a sphere of radius $\delta$ and $\delta \to 0$, then $\hat{R}' = \hat{n}' = \hat{r} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}$. We have

$$\overline{L} = \frac{1}{4\pi} \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\phi \ \hat{r} \hat{r} \tag{2.1.60a}$$
and

\[
\int d\Omega \, \hat{r} \hat{r} = \int d\Omega (\sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}) \\
\cdot (\sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}) \\
= \frac{4\pi \bar{I}}{3} \tag{2.1.60b}
\]

We have used the result that on integration, the cross terms in (2.1.60) vanish. Hence

\[
\bar{L} = \frac{\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}}{3} = \frac{\bar{I}}{3} \tag{2.1.61}
\]

**Example 2:** Let \( V_b \) be a rectangular parallelepiped with sides equal to \( \delta_x, \delta_y \) and \( \delta_z \), respectively. Also let \( \delta_x = a\delta, \delta_y = b\delta \) and \( \delta_z = c\delta \) and \( \delta \to 0 \). Thus \( a, b \) and \( c \) are finite numbers and the ratios among them are important to determine \( \bar{L} \). In this case there are six faces for the surface integral of (2.1.60). The sum of the contributions from the top and bottom faces to \( \bar{L} \) is

\[
\frac{1}{4\pi} \lim_{\delta \to 0} \int_{-\delta_z/2}^{\delta_z/2} dx \int_{-\delta_y/2}^{\delta_y/2} dy \frac{\dot{z}(x\dot{x} + y\dot{y} + (\delta_z/2)\dot{z}) - \dot{z}(x\dot{x} + y\dot{y} - (\delta_z/2)\dot{z})}{(x^2 + y^2 + (\delta_z/2)^2)^{3/2}} \\
= \frac{\dot{z}\dot{z}}{2\pi} \int_{0}^{\delta_z/2} dx \frac{1}{(x^2 + (\delta_z/2)^2)(x^2 + (\delta_y/2)^2 + (\delta_z/2)^2)^{3/2}} \\
= \frac{\dot{z}\dot{z}}{2\pi} \tan^{-1} \frac{\delta_x\delta_y}{\delta_z(\delta_x^2 + \delta_y^2 + \delta_z^2)^{1/2}} \tag{2.1.62}
\]

The integration over \( dy \) and \( dx \) can be found in Gradshteyn and Ryzhik [1965]. Note that in (2.1.62), the result only depends on the ratios of the lengths of the three sides of the rectangular parallelepiped. Similar expressions can be derived for the other four faces.

\[
\bar{L} = \frac{2}{\pi} \left\{ \hat{x}\hat{x} \tan^{-1} \frac{bc}{a(a^2 + b^2 + c^2)^{1/2}} + \hat{y}\hat{y} \tan^{-1} \frac{ca}{b(a^2 + b^2 + c^2)^{1/2}} \\
+ \hat{z}\hat{z} \tan^{-1} \frac{ab}{c(a^2 + b^2 + c^2)^{1/2}} \right\} \tag{2.1.63}
\]

For the special case of a cube, we set \( a = b = c \) in (2.1.63). That gives

\[
\bar{L} = \frac{\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}}{3} = \frac{\bar{I}}{3} \tag{2.1.64}
\]

Examples of other shapes can be found in Yaghjian [1980].
2 Method of Moments

The method of moments (MoM) is a numerical technique that has been used extensively in the solution of electromagnetic boundary value problems. Many excellent texts have been written on this subject [Harrington, 1968]. The technique is used extensively in this book in Monte Carlo simulations. A characteristic of this technique is that it leads to a full matrix equation which can be solved by matrix inversion. In later chapters, we will describe techniques that can speed up the numerical solution of these matrix equations.

With the use of Green’s function, integral equations can be derived. Consider a one dimensional integral equation of the form

\[ \int_a^b dx' G(x, x') f(x') = c(x) \]  

(2.2.1)

where \( G(x, x') \) is the Green’s function, \( f(x) \) is the unknown for the domain \( a \leq x \leq b \), and \( c(x) \) is known for \( a \leq x \leq b \). To solve (2.2.1), two sets of functions are used in the MoM: basis functions and weighting functions.

(1) Basis functions. A set of \( N \) basis functions in the domain of \( a \leq x \leq b \) is chosen. Let the basis functions be \( f_1, f_2, \ldots, f_N \). The unknown function \( f(x) \) is expanded in terms of a linear combination of these basis functions.

\[ f(x) = \sum_{n=1}^{N} b_n f_n(x) \]  

(2.2.2)

The linear combination of \( f_n(x) \) should well represent the unknown \( f(x) \) in the domain. Substitute (2.2.2) into (2.2.1), we have

\[ \sum_{n=1}^{N} b_n \int_a^b dx' G(x, x') f_n(x') = c(x) \]  

(2.2.3)

The unknown coefficients \( b_1, b_2, \ldots, b_N \) are to be determined.

(2) Next a set of \( N \) weighting functions (testing functions) \( w_1(x), w_2(x), \ldots, w_N(x) \) is chosen. Multiply (2.2.3) by \( w_m(x) \) and integrate over the domain

\[ \sum_{n=1}^{N} b_n \int_a^b dx w_m(x) \int_a^b dx' G(x, x') f_n(x') = \int_a^b dx w_m(x) c(x) \]  

(2.2.4)
This gives the matrix equation

$$\sum_{n=1}^{N} G_{mn} b_n = c_m$$

(2.2.5)

where

$$m = 1, 2, \ldots, N,$$ where

$$c_m = \int_a^b dx w_m(x)c(x) = \langle w_m, c \rangle$$

(2.2.6)

$$G_{mn} = \int_a^b dx w_m(x) \int_a^b dx' G(x, x') f_n(x') = \langle w_m, Gf_n \rangle$$

(2.2.7)

where the inner product notation is used.

$$\langle f, g \rangle = \int_a^b dx f(x) g(x)$$

(2.2.8)

**Computational Considerations**

Generally (2.2.5) is a full matrix equation. We note the following

(1) Matrix solution: To solve a full matrix equation of order \(N\) by full matrix inversion (e.g., Gaussian elimination) requires \(O(N^3)\) number of operations. This increases rapidly with \(N\).

(2) Matrix filling: To calculate \(G_{mn}\), \(m, n = 1, 2, \ldots, N\) can be computationally intensive because there are \(N^2\) values of \(G_{mn}\). Also \(G_{mn}\) can require the evaluation of a double integral as given in (2.2.7). The matrix filling can be more computationally intensive than matrix solution because \(G(x, x')\) can be of a complicated form. Also since there are \(N^2\) elements of \(G_{mn}\), this can impose a large memory requirement.

(3) The study of \(f_n\), \(n = 1, 2, \ldots, N\) is also an important subject as the choice of \(f_n\) must well represent the correct solution. Often they have to satisfy differentiation and continuity properties.

**Basis Functions**

Basis functions can use full domain functions such as sines, cosines, special functions, polynomials, modal solutions, etc. A set that is useful for practical problem is the subsectional basis function. This means that each \(f_n\) is only nonzero over a subsection of the domain of \(f\).

A common choice is the pulse function (Fig. 2.2.1a)

$$f_n(x) = \begin{cases} 1 & \text{if } a_n \leq x \leq b_n \\ 0 & \text{otherwise} \end{cases}$$

(2.2.9)
where the interval $a \leq x \leq b$ have been divided into $N$ intervals with end-
points $a_n$ and $b_n$, $n = 1, 2, \ldots, N$.

Another choice is the triangle basis functions (Fig. 2.2.1b). In Fig. 2.2.1b we show $f_n(x)$ and $f_{n+1}(x)$. Note that $f_n(x)$ and $f_{n+1}(x)$ overlap.

**Weighting Functions**

Two common choices are

1. Galerkin's method. In this case the weighting functions, $n = 1, 2, \ldots, N$, are the same as the basis functions, i.e., $\omega_n(x) = f_n(x)$.

2. Point matching. One can pick a set of points $x = x_1, x_2, \ldots, x_N$ to enforce (2.2.3). Then

$$\sum_{n=1}^{N} b_n \int_{a}^{b} dx' G(x_m, x') f_n(x') = c(x_m)$$

where

$$c_m = c(x_m)$$

$$G_{mn} = \int_{a}^{b} dx' G(x_m, x') f_n(x')$$

This particular choice of testing procedure is called point matching. In terms of weighting functions, this means that the weighting functions are

$$\omega_m(x) = \delta(x - x_m)$$

where $m = 1, 2, \ldots, N$ and $\delta$ is the Dirac delta function.

In Chapter 1 of Volume I, we have used an infinite cylinder approximation to calculate the scattering by a cylinder of finite length. The surface
fields are then used to calculate the scattering by integrating the surface fields only over the finite length of the cylinder. Numerically, one can use the method of moment body of revolution code [Glisson and Wilton, 1979] to calculate scattering from a finite length cylinder by solving the surface integral equations. The variations of the unknown electric and magnetic surface fields are approximated by staggered pulse functions in the $t$-direction and are expanded in Fourier series in the $\phi$-direction.

In Fig. 2.2.2 we make a comparison of total surface fields for $m = 0$ harmonic, computed based on infinite cylinder (IC) approximation and MoM solution. The incident wave is of unit amplitude in a direction perpendicular to the axis of the cylinder with polarization parallel to the axis of the cylinder. Equivalent electric surface currents $\eta J_t$ and equivalent magnetic surface current $M_\phi$ are shown. The $t$ coordinate and the $t$ direction is as indicated in Fig. 2.2.2. The $t$ coordinate starts from center of bottom face, radially outward to the edge, along the curved side and then ends at the center of the top face with range $2.5 \text{ cm} + 15 \text{ cm} + 2.5 \text{ cm} = 20 \text{ cm}$. Thus the infinite cylinder approximation has uniform current densities on the curved surface of the cylinder while the MoM code predicts a maximum at the midpoint.
3 Discrete Dipole Approximation

In this section we discuss how the volume integral equation of Sections 1.2 and 1.3 can be discretized and solved numerically based on the discrete dipole approximation (DDA) [Purcell and Pennypacker, 1973; Goodman et al. 1991].

The volume integral equation is

\[
\mathcal{E}(\vec{r}) = \mathcal{E}^{\text{inc}}(\vec{r}) + k^2 \int_{V-V_s} d\vec{r}' \bar{G}(\vec{r}, \vec{r}') \cdot (\varepsilon_r(\vec{r}') - 1) \mathcal{E}(\vec{r}') - (\varepsilon_r(\vec{r}) - 1) \bar{L} \cdot \mathcal{E}(\vec{r})
\]

(2.3.1)

If we define polarization \( \mathcal{P} \) by

\[
(\varepsilon_p(\vec{r}) - \varepsilon) \mathcal{E}(\vec{r}) = \mathcal{P}(\vec{r})
\]

(2.3.2)

Then

\[
\mathcal{E}(\vec{r}) = \mathcal{E}^{\text{inc}}(\vec{r}) + \frac{k^2}{\varepsilon} \int_{V-V_s} d\vec{r}' \bar{G}(\vec{r}, \vec{r}') \cdot \mathcal{P}(\vec{r}') - (\varepsilon_r(\vec{r}) - 1) \bar{L} \cdot \mathcal{E}(\vec{r})
\]

(2.3.3)

We discretize (2.3.3) into volumes \( \Delta V_j \) with centers at \( \vec{r}_j \), \( j = 1, 2, \ldots, N \). Inside \( \Delta V_j \), there is uniform field \( \bar{E}_j \) and polarization \( \mathcal{P}_j \). Then

\[
\mathcal{E}(\vec{r}) = \mathcal{E}^{\text{inc}}(\vec{r}) + \frac{k^2}{\varepsilon} \sum_{j=1}^{N} \bar{G}(\vec{r}_i, \vec{r}_j) \cdot \mathcal{P}_j \Delta V_j - (\varepsilon_r(\vec{r}) - 1) \bar{L} \cdot \bar{E}_i
\]

(2.3.4)

Let \( \hat{R} = \) unit vector from \( \vec{r}' \) to \( \vec{r} \), \( R = |\vec{r} - \vec{r}'| \) and \( \bar{R} = \vec{r} - \vec{r}' \). For \( \vec{r} \neq \vec{r}' \), by straightforward differentiation,

\[
\bar{G}(\vec{r}, \vec{r}') = G_1(R) \bar{I} + G_2(R) \hat{R} \bar{R}
\]

(2.3.5)

where

\[
G_1(R) = (-1 + ikR + k^2 R^2) \frac{e^{ikR}}{4\pi k^2 R^3}
\]

(2.3.6)

\[
G_2(R) = (3 - 3ikR - k^2 R^2) \frac{e^{ikR}}{4\pi k^2 R^3}
\]

(2.3.7)

We let

\[
\bar{A}(\vec{r}, \vec{r}') = -\frac{k^2}{\varepsilon} \bar{G}(\vec{r}, \vec{r}')
\]

\[
= \frac{e^{ikR}}{4\pi \varepsilon R^3} \left\{ k^2(-R^2 \bar{I} + \bar{R} \bar{R}) + \frac{(1 - ikR)}{R^2} (R^2 \bar{I} - 3R \bar{R}) \right\}
\]

(2.3.8)
3.1 Small Cubes

If the volumes $\Delta V_j$ are cubes, then

$$\bar{p}_j = (\Delta V) P_j$$

(2.3.9)

where $\Delta V = V/N = d^3$ and $d$ is the length of each volume cube. Then the discretized version of the volume integral equation is, with $\overline{L} = \overline{I}/3$,

$$\overline{E}_i = \overline{E}_i^{inc} - \sum_{j=1, j \neq i}^{N} \overline{A}(\overline{r}_i, \overline{r}_j) \cdot \overline{p}_j - \left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right) \frac{\overline{E}_i}{3}$$

(2.3.10)

where $\overline{E}_i$, $\overline{E}_i^{inc}$, $\overline{p}_i$, $\epsilon_{pi}$ are the values in the $i$th elemental cube. Note that the second term excludes $j = i$ in accordance with principal value and the last term is a result of the $\overline{L}$ factor associated with cubic volume. The dipole moment for each cube is

$$\bar{p}_i = d^3 (\epsilon_{pi} - \epsilon) \overline{E}_i$$

(2.3.11)

Putting the last term in (2.3.10) on the left-hand-side and using (2.3.11) gives the matrix equation for the dipole moment of each cube

$$\bar{p}_i = \alpha_i \overline{E}_i^{inc} - \alpha_i \sum_{j=1, j \neq i}^{N} \overline{A}_{ij} \cdot \bar{p}_j$$

(2.3.12)

where $\overline{A}_{ij} = \overline{A}(\overline{r}_i, \overline{r}_j)$,

$$\alpha_i = \alpha_i^C = 3\epsilon d^3 \left( \frac{n_i^2 - 1}{n_i^2 + 2} \right) = 3\epsilon \Delta V \left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right)$$

(2.3.13)

and $n = \sqrt{\epsilon_p/\epsilon}$ is the complex relative refractive index. In (2.3.13) $\alpha_i^C$ is the familiar Clausius-Mossoti polarizability. However $\alpha_i$ in (2.3.13) does not obey optical theorem and will subsequently be changed to include more correction terms.

We note that the matrix elements $\overline{A}$ is that of the dyadic Green’s function which is translational invariant. Thus the product of $\overline{A}$ and a column vector can be computed by FFT. That is

$$\sum_{j=1, j \neq i}^{N} \overline{A}_{ij} \cdot \bar{p}_j$$
where the summation over all cubes except the $i$th one can be computed by FFT. Thus solution of (2.3.12) using conjugate gradient method combined with FFT makes the solution much faster than that of the Gaussian elimination [Goodman et al. 1991].

However, if $\epsilon_{pi}$ is the same as $\epsilon$ in most of the the region, it may be more efficient to use the electric field equation from (2.3.11) and (2.3.12)

$$\frac{d^3(\epsilon_{pi} - \epsilon)}{\alpha_i} \bar{E}_i = \bar{E}_i^{inc} - \sum_{j=1, j \neq i}^{N} \bar{A}_{ij} \cdot d^3(\epsilon_{pj} - \epsilon) \bar{E}_j$$  \hspace{1cm} (2.3.14)

where $N$ now only need to include those cubes that have $\epsilon_{pj} \neq \epsilon$. Note also that $(\epsilon_{pi} - \epsilon)/\alpha_i$ is finite as can be seen from (2.3.13) even when $\epsilon_{pi} = \epsilon$.

For the case of a single small cube, the scattering solution is calculated by dropping the $\sum \bar{A}_{ij} \cdot \bar{p}_j$ term from (2.3.10). The equation can be solved readily to give $\bar{E}_i = \bar{E}_i^{inc} [1 + \frac{1}{3} \left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right)]^{-1}$. We note the similarity between a small cube and a small sphere. The polarizability of a small sphere is $\alpha_s = 3v_0\epsilon(n^2 - 1)/(n^2 + 2)$ where $n = \epsilon_p/\epsilon$ and $v_0 = (4\pi/3)a^3$ is the same as (2.3.13) with $d^3$ replaced by $(4\pi/3)a^3$. The internal field of a small sphere is $(3\epsilon/(\epsilon_p + 2\epsilon))\bar{E}^{inc}$ which becomes the same as that of a small cube.

As we examine the optical theorem for a small sphere in Chapter 2, Section 8.2 of Volume I, we have noted that the Clausius-Mossoti internal field is not accurate enough because when one applies the optical theorem using the result forward scattering amplitudes, it does not give the contribution due to the scattering part. For the case of small cube, the same reasoning applies. Thus to ensure that the final scattering obeys energy conservation, one has to take into account radiative correction. In doing so, the expression of $\alpha_i$ in (2.3.14) is modified with the new expression given below.

### 3.2 Radiative Corrections

In numerical implementations, the cubes are not infinitesimal. One major correction is to improve the self-term impedance matrix element. This will give correction to the Clausius-Mossoti polarizability.

From (2.3.1), the self field $\bar{E}_{self}$ should be, for volume cube of finite size,

$$\bar{E}_{self} = k^2 \int_{V_c \setminus V_\delta} d\bar{r}' \bar{G}(\bar{r}, \bar{r}') \cdot (\epsilon_r - 1)\bar{E} - (\epsilon_r - 1)\bar{L} \cdot \bar{E}$$  \hspace{1cm} (2.3.15)

where $V_c$ is the self cube, $V_\delta$ is the exclusion volume, and $\bar{r}$ is at the center of the cube. Thus

$$\bar{E}_{self} = k^2 \bar{S} \cdot (\epsilon_r - 1)\bar{E}$$  \hspace{1cm} (2.3.16)
where
\[ \overline{S} = \int_{V_c - V_n} d\tau' \overline{G}(\tau', \tau') - \frac{L}{k^2} = -\frac{\epsilon}{k^2} \int_{V_c - V_n} d\tau' \overline{A}(\tau, \tau') - \frac{L}{k^2} \quad (2.3.17) \]
and
\[ \overline{A} = -\frac{k^2}{\epsilon} \overline{G} \quad (2.3.18) \]

Then the DDA equation becomes
\[ \overline{E}_i = \overline{E}_i^{inc} + \frac{k^2}{\epsilon} \sum_{j=1 \atop j \neq i}^N \overline{G}(\tau_i, \tau_j) \cdot \overline{P}_j \Delta V_j + k^2 \overline{S} \cdot (\epsilon_r(\tau_i) - 1) \overline{E}_i \quad (2.3.19) \]

Because of the similarity between a small cube and a small sphere, a small equivalent spherical volume of radius \(a\) where \((4\pi/3)a^3 = d^3 = v_0\) will be assumed. Then, using \(G_1\) and \(G_2\) as given by (2.3.6) and (2.3.7)
\[ \overline{S} = -\frac{I}{3k^2} + \lim_{\delta \to 0} \int_\delta^a d\tau' r'^2 \int_{4\pi} d\Omega' [G_1(r')I + G_2(r')\hat{r}' \hat{r}'] \]
\[ = -\frac{I}{3k^2} + \lim_{\delta \to 0} 4\pi \int_\delta^a d\tau' r'^2 \left[ G_1(r') + \frac{G_2(r')}{3} \right] \overline{I} \quad (2.3.20) \]
The second equality in (2.3.20) is a result of (2.1.60b). Since
\[ G_1(r') + \frac{G_2(r')}{3} = \frac{e^{ikr'}}{6\pi r'} \quad (2.3.21) \]
we have
\[ \overline{S} = \overline{I} S \quad (2.3.22) \]
where
\[ S = -\frac{1}{3k^2} + \frac{2}{3} \lim_{\delta \to 0} \int_{\delta}^a d\tau' r' e^{ikr'} = -\frac{1}{3k^2} + \frac{2}{3k^2} \left[ -1 + e^{ika}(1 - ika) \right] \]
\[ \approx -\frac{1}{3k^2} + \frac{2}{3k^2} \left[ \frac{k^2 a^2}{2} - \frac{ik^3 a^3}{3} \right] \quad (2.3.23) \]
in the limit of small \(a\). Putting (2.3.22) in (2.3.19)
\[ \overline{E}_i = \overline{E}_i^{inc} + \left( \frac{\epsilon_p}{\epsilon} - 1 \right) sk^2 \overline{E}_i - \sum_{j=1 \atop j \neq i}^N \overline{A}_{ij} \cdot \overline{P}_j \quad (2.3.24) \]
Thus
\[ \overline{E}_i = \frac{\overline{E}_i^{inc}}{1 - \left( \frac{\epsilon_p}{\epsilon} - 1 \right) sk^2} - \frac{1}{1 - \left( \frac{\epsilon_p}{\epsilon} - 1 \right) sk^2} \sum_{j=1 \atop j \neq i}^N \overline{A}_{ij} \cdot \overline{P}_j \quad (2.3.25) \]
Multiply by $\Delta V (\epsilon_{pi} - \epsilon_i)$, and noting that
\[
\overline{p}_i = \Delta V (\epsilon_{pi} - \epsilon_i) \overline{E}_i
\]  
(2.3.26)

we have
\[
\overline{p}_i = \alpha_i \overline{E}_i^{inc} - \alpha_i \sum_{j=1}^{N} A_{ij} \cdot \overline{p}_j
\]  
(2.3.27)

with
\[
\alpha_i = \frac{\Delta V (\epsilon_{pi} - \epsilon)}{1 - \left(\frac{\epsilon_{pi}}{\epsilon} - 1\right) s k^2}
\]  
(2.3.28)

Putting (2.3.23) in (2.3.28) gives
\[
\alpha_i = \frac{3 \epsilon \Delta V \left(\frac{\epsilon_{pi}}{\epsilon} - 1\right)}{\frac{\epsilon_{pi}}{\epsilon} + 2 - 2 \left(\frac{\epsilon_{pi}}{\epsilon} - 1\right) \left(\frac{k^2 a^2}{2} + i \frac{k^3 a^3}{3}\right)}
\]
(2.3.29)

\[
= \frac{\alpha_i^C}{1 - \frac{2}{3 \epsilon \Delta V} \left[\frac{k^2 a^2}{2} + i \frac{k^3 a^3}{3}\right]}
\]

Using $a = (3/4\pi)^{1/3} d$ and $\Delta V = d^3$ in (2.3.29) gives
\[
\alpha_i = \frac{\alpha_i^C}{1 - \frac{\alpha_i^C}{4\pi \epsilon d^3} \left[\left(\frac{4\pi}{3}\right)^{1/3} \frac{k^2 d^2}{3} + \frac{2k^3 d^3}{3}\right]}
\]
(2.3.30)

The term with imaginary part in the denominator of (2.3.30) is known as radiative correction, which arises for the same reasoning as when scattering by Rayleigh spheres was discussed in Chapter 2, Section 8.2 of Volume I.

### 3.3 Other Shapes

Let the medium be discretized into rectangular parallelepipeds $V_s$ of sizes $d_x \times d_y \times d_z$. We let $d_x = ad$, $d_y = bd$, $d_z = cd$ where $a$, $b$ and $c$ are dimensionless quantities and their ratios denote the relative sizes of the three sides of the rectangular parallelepiped. The exclusion volume $V_\delta$ for the dyadic Green’s function in this function will be an infinitesimal parallelepiped with dimensions $\delta_x = a\delta$, $\delta_y = b\delta$ and $\delta_z = c\delta$ and the $\overline{L}$ is as given in (2.1.63). Note that the ratios of the sides of the finite small rectangular parallelepiped $V_s$ is the same as that of the infinitesimal rectangular parallelepiped $V_\delta$. Then
it is useful to write a low frequency approximation of $G_0(\mathbf{R})$. We note that for $\mathbf{R} \neq 0$

$$
\overline{G}(\mathbf{R}) = -\frac{\epsilon}{k^2} \overline{A}(\mathbf{R}) = -\frac{e^{ik\mathbf{R}}}{4\pi k^2 R^3} \left\{ k^2(-R^2 \mathbf{\hat{I}} + \mathbf{R} \mathbf{R}) + \frac{(1 - i k R)}{R^2} (R^2 \mathbf{\hat{I}} - 3\mathbf{R} \mathbf{R}) \right\}
$$

(2.3.31)

When expanding $\overline{G}(\mathbf{R})$ of (2.3.31), it is important to see that there is a singular part of $O(1/(k^2 R^3))$ that is non-integrable over the origin. We also have to expand to the leading term in the imaginary part because that accounts for radiative correction. The Green’s function $\overline{G}(\mathbf{R})$, on expansion will give $O(1/(k^2 R^3)) + O(1/R) + iO(k)$. Thus in (2.3.31), we write $\exp(i k R) \simeq 1 + i k R - k^2 R^2/2 - i k^3 R^3/6$. We have to include $-i k^3 R^3/6$ because this gives a term of order $iO(k)$ when multiplied with the second term inside the curly bracket of (2.3.31). Thus for $\mathbf{R} \neq 0$ and $kR \ll 1$

$$
\overline{G}(\mathbf{R}) \simeq -\frac{1}{4\pi k^2 R^3} \left\{ k^2(-R^2 \mathbf{\hat{I}} + \mathbf{R} \mathbf{R})(1 + i k R) + \frac{(1 - i k R)}{R^2} (R^2 \mathbf{\hat{I}} - 3\mathbf{R} \mathbf{R}) \left( 1 + i k R - \frac{k^2 R^2}{2} - \frac{i k^3 R^3}{6} \right) \right\}
$$

$$
= -\frac{1}{4\pi k^2 R^5} (R^2 \mathbf{\hat{I}} - 3\mathbf{R} \mathbf{R}) + \frac{1}{8\pi} \left\{ \frac{1}{R^3} (R^2 \mathbf{\hat{I}} + \mathbf{R} \mathbf{R}) + \frac{4i k R}{3} \right\}
$$

(2.3.32)

Note that the imaginary part term of (2.3.32) is just the product of a constant and a unit dyad. Following (2.3.17), let

$$
\overline{S} = -\frac{\epsilon}{k^2} \int_{V_s - V_s} d\mathbf{r}' \overline{A}(\mathbf{r}, \mathbf{r}') - \frac{\overline{L}}{k^2}
$$

(2.3.33)

We use (2.3.32) to write $\overline{A}$ as a sum of a regular part $\overline{A}_o$ that is integrable over the origin and a singular part $\overline{A}_s$ that is non-integrable over the origin. Thus

$$
\overline{A}(\mathbf{R}) \simeq \overline{A}_o(\mathbf{R}) + \overline{A}_s(\mathbf{R})
$$

(2.3.34)

where

$$
\overline{A}_o(\mathbf{R}) = -\frac{k^2}{8\pi \epsilon R^3} (R^2 \mathbf{\hat{I}} + \mathbf{R} \mathbf{R}) - \frac{i k^3}{6\pi \epsilon} \mathbf{\hat{I}}
$$

(2.3.35a)

$$
\overline{A}_s(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi \epsilon R^5} (R^2 \mathbf{\hat{I}} - 3\mathbf{R} \mathbf{R})
$$

(2.3.35b)

Thus

$$
\overline{S} = -\frac{\epsilon}{k^2} \int_{V_s} d\mathbf{r}' \overline{A}_o(\mathbf{r}, \mathbf{r}') - \frac{\epsilon}{k^2} \int_{V_s - V_s} d\mathbf{r}' \overline{A}_s(\mathbf{r}, \mathbf{r}') - \frac{\overline{L}}{k^2}
$$

(2.3.36)
Note that $\bar{A}_s$ is non-integrable over the origin. However, the origin is excluded in the integration over $V_s - V_\delta$.

The second integral in (2.3.36) can be shown generally to be zero. Here we perform it for the case of rectangular parallelepipeds of $V_s$ and $V_\delta$. The volume $V_s - V_\delta$ can be formed from 8 octants. In integration, the cross terms vanish. The volume integration can also be combined into that of one octant. Thus

$$\frac{\epsilon}{k^2} \int_{V_s - V_\delta} d\bar{r}' \bar{A}_s(\bar{r}, \bar{r}')$$

$$= -\frac{2}{\pi k^2} \left\{ \int_0^{\delta_x} dx \int_0^{\delta_y} dy \int_0^{\delta_z} \frac{dz}{2} \right\} + \int_0^{\delta_x} dx \int_0^{\delta_y} dy \int_0^{\delta_z} \frac{dz}{2} \times \frac{1}{(x^2 + y^2 + z^2)^{5/2}} \left[ \hat{x} \hat{x}(-2x^2 + y^2 + z^2) + \hat{y} \hat{y}(-2y^2 + x^2 + z^2) + \hat{z} \hat{z}(x^2 + y^2 - 2z^2) \right] = 0 \quad (2.3.37)$$

The integral over $\bar{A}_{o}$ can be performed as follows. The dyad $\bar{S}$ is diagonal so that

$$\bar{S} = S_x \hat{x} \hat{x} + S_y \hat{y} \hat{y} + S_z \hat{z} \hat{z} \quad (2.3.38)$$

$$\bar{L} = L_x \hat{x} \hat{x} + L_y \hat{y} \hat{y} + L_z \hat{z} \hat{z} \quad (2.3.39)$$

and

$$\bar{S} = \bar{D} - \frac{\bar{L}}{k^2} \quad (2.3.40)$$

$$\bar{D} = D_x \hat{x} + D_y \hat{y} + D_z \hat{z} \quad (2.3.41)$$

where

$$L_x = \frac{2}{\pi} \tan^{-1} \frac{bc}{a(a^2 + b^2 + c^2)^{1/2}} \quad (2.3.42)$$

$$L_y = \frac{2}{\pi} \tan^{-1} \frac{ca}{b(a^2 + b^2 + c^2)^{1/2}} \quad (2.3.43)$$

$$L_z = \frac{2}{\pi} \tan^{-1} \frac{ab}{c(a^2 + b^2 + c^2)^{1/2}} \quad (2.3.44)$$
\[ D_x = \frac{1}{\pi} \left\{ \frac{d_x}{2} \int_0^{\frac{d_x}{2}} dy \ln \frac{\frac{d_y}{2} + \sqrt{y^2 + \left(\frac{d_x}{2}\right)^2}}{\frac{d_y}{2} + \sqrt{y^2 + \left(\frac{d_x}{2}\right)^2}} + \sqrt{\left(\frac{d_x}{2}\right)^2 + x^2 + \left(\frac{d_x}{2}\right)^2} \right\} + \frac{ik}{6} \Delta V \] (2.3.45)

\[ D_y = \frac{1}{\pi} \left\{ \frac{d_y}{2} \int_0^{\frac{d_y}{2}} dx \ln \frac{\frac{d_z}{2} + \sqrt{z^2 + \left(\frac{d_y}{2}\right)^2}}{\frac{d_z}{2} + \sqrt{z^2 + \left(\frac{d_y}{2}\right)^2}} + \sqrt{\left(\frac{d_y}{2}\right)^2 + y^2 + \left(\frac{d_y}{2}\right)^2} \right\} + \frac{ik}{6} \Delta V \] (2.3.46)

\[ D_z = \frac{1}{\pi} \left\{ \frac{d_z}{2} \int_0^{\frac{d_z}{2}} dx \ln \frac{\frac{d_x}{2} + \sqrt{x^2 + \left(\frac{d_z}{2}\right)^2}}{\frac{d_x}{2} + \sqrt{x^2 + \left(\frac{d_z}{2}\right)^2}} + \sqrt{\left(\frac{d_x}{2}\right)^2 + z^2 + \left(\frac{d_x}{2}\right)^2} \right\} + \frac{ik}{6} \Delta V \] (2.3.47)

Substituting (2.3.40) into (2.3.19), we get

\[ \frac{\bar{P}_i}{\epsilon \Delta V} = \frac{\bar{\alpha}_i}{\epsilon \Delta V} \cdot \vec{E}_i^{inc} - \frac{\bar{\alpha}_i}{\epsilon \Delta V} \cdot \sum_{j=1\atop j \neq i}^{N} (\epsilon \Delta V) \bar{A}_{ij} \cdot \frac{\bar{p}_j}{\epsilon \Delta V} \] (2.3.48)

where

\[ \bar{\alpha}_i = \alpha_{ix} \hat{x} \hat{x} + \alpha_{iy} \hat{y} \hat{y} + \alpha_{iz} \hat{z} \hat{z} = \left(\frac{\epsilon_{pi}}{\epsilon} - 1\right) \bar{\beta}_i \] (2.3.49)

\[ \frac{\beta_{ix}}{\epsilon \Delta V} = \frac{1}{1 + \left(\frac{\epsilon_{pi}}{\epsilon} - 1\right) (L_x - D_x k^2)} \] (2.3.50)


\[ \frac{\beta_{xy}}{\epsilon \Delta V} = \frac{1}{1 + \left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right) (L_y - D_y k^2)} \]  
\[ \frac{\beta_{xz}}{\epsilon \Delta V} = \frac{1}{1 + \left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right) (L_z - D_z k^2)} \]

and \( \Delta V = d_x d_y d_z \).

In the case of cells of circular cylindrical shape of radius \( a \) and length \( l \), the corresponding results of \( L_x, L_y, L_z \) and \( D_x, D_y \) and \( D_z \) are

\[ L_x = L_y = \frac{l}{2(4a^2 + l^2)^{1/2}} \]  
\[ L_z = 1 - \frac{l}{(4a^2 + l^2)^{1/2}} \]

\[ D_x = D_y = \frac{ika^2 l}{6} + \frac{l}{8} \left\{ \sqrt{l^2 + 4a^2} - l \right\} + \frac{a^2}{4} \ln \left( \frac{l + \sqrt{l^2 + 4a^2}}{2a} \right) \]  
\[ D_z = \frac{ika^2 l}{6} + \frac{a^2}{2} \ln \left( \frac{l + \sqrt{l^2 + 4a^2}}{2a} \right) \]

Equation (2.3.48) is the DDA matrix equation and is to be solved numerically. After the solution is obtained, we have the solution of the induced dipole moment \( \vec{p}_i \) for every cell. The electric field at cell \( i \) is given by

\[ \vec{E}_i = \frac{1}{\left( \frac{\epsilon_{pi}}{\epsilon} - 1 \right) \epsilon \Delta V} \frac{\vec{p}_i}{\epsilon \Delta V} \]  

for \( \epsilon_{pi} \neq \epsilon \) for cell \( i \). For the case of \( \epsilon_{pi} = \epsilon \),

\[ \vec{E}_i = \frac{\vec{\beta}_i}{\epsilon \Delta V} \cdot \vec{E}^{inc}_i - \frac{\vec{\beta}_i}{\epsilon \Delta V} \cdot \sum_{j=1}^{N} (\epsilon \Delta V) \vec{A}_{ij} \cdot \frac{\vec{p}_j}{\epsilon \Delta V} \]

For the case of rectangular parallelepipeds the matrix equation of (2.3.48) is of dimension \( 3N \times 3N \) where \( N \) is the number of rectangular parallelepipeds and the factor 3 arises from the \( x \), \( y \) and \( z \) components of the polarization vector. In the standard form, the matrix equation is

\[ \vec{Z} \vec{x} = \vec{b} \]

where \( \vec{Z} \) is the impedance matrix and \( \vec{x} \) is the unknown column vector and \( \vec{b} \) is the right-hand side. Let the rectangular parallelepipeds be equally spaced in \( \hat{x} \), \( \hat{y} \) and \( \hat{z} \) directions. Then (2.3.48) can be solved by using conjugate
gradient method (CGM) combined with fast Fourier transform (FFT) that will be discussed in Section 4. In applying CGM, we need to take the product $\overline{Z} \overline{d}$ and the product $\overline{Z}^\dagger \overline{r}$ where $\dagger$ denotes adjoint, $\overline{d}$ is the direction vector and $\overline{r}$ is the residual vector. For example, if there are two rectangular parallelepipeds, $N = 2$, then the impedance matrix $\overline{Z}$ is of dimension $6 \times 6$ and is

$$\overline{Z} = \begin{bmatrix} \overline{I} & \frac{\overline{\alpha}_1}{\epsilon \Delta V} (\epsilon \Delta V) \overline{A}_{i2} \\ \frac{\overline{\alpha}_2}{\epsilon \Delta V} (\epsilon \Delta V) \overline{A}_{i2} & \overline{I} \end{bmatrix}$$

(2.3.56)

Note that

$$\overline{A}_{ij} = \overline{A}_{ji}$$

(2.3.57)

and

$$\overline{A}_{ij} = \overline{A}_{ji}$$

(2.3.58)

where $t$ denotes transpose of the dyad. Then the adjoint of the impedance matrix is

$$\overline{Z}^\dagger = \begin{bmatrix} \overline{I} & (\epsilon \Delta V) \overline{A}_{i2}^* \cdot \frac{\overline{\alpha}_2^*}{\epsilon \Delta V} \\ (\epsilon \Delta V) \overline{A}_{i2}^* \cdot \frac{\overline{\alpha}_1^*}{\epsilon \Delta V} & \overline{I} \end{bmatrix}$$

(2.3.59)

where $*$ denotes complex conjugate.

After the matrix equation (2.3.48) is solved, the far field scattered field in direction $\hat{k}_s$ is

$$\overline{E}^s(\overline{r}) = \frac{e^{ikr}}{4\pi r} k^2 \Delta V (\hat{v}_s \hat{v}_s + \hat{h}_s \hat{h}_s) \cdot \sum_i e^{-ik_s \overline{r}_i} \frac{\overline{p}_i}{\epsilon \Delta V}$$

(2.3.60)

The time-averaged power absorbed is equal to

$$\langle P_a \rangle = \frac{1}{2} \omega \sum_i \epsilon''_{pi} |\overline{E}_i|^2 \Delta V$$

(2.3.61)

where $\epsilon''_{pi}$ is the imaginary part of $\epsilon_{pi}$ for the $i$th cell. In terms of dipole moment of each cell, we have

$$\langle P_a \rangle = \frac{1}{2} \omega \sum_i \begin{cases} 0 & \text{if } \epsilon''_{pi} = 0 \\ \epsilon''_{pi} \Delta V \frac{1}{\epsilon_{pi} - 1} \left| \frac{\overline{p}_i}{\epsilon \Delta V} \right|^2 & \text{if } \epsilon''_{pi} \neq 0 \end{cases}$$

(2.3.62)
Calculation of Matrix Elements by Numerical Integration

In the matrix equation of (2.3.48), the $A_{ij}$ elements are calculated by taking the value of $A(\vec{r}, \vec{r}')$ at the point $\vec{r}_i$ and $\vec{r}_j$, for $\vec{r}_i \neq \vec{r}_j$

$$\overline{A}_{ij} = \overline{A}(\vec{r}_i, \vec{r}_j) \quad (2.3.63)$$

These may not be accurate enough particularly for $\vec{r}_i$ and $\vec{r}_j$ in the neighborhood of each other. Accuracy can be improved by numerical integration over the cell $V_j$ centered at $\vec{r}_j$. Thus we can define a neighborhood distance $r_d$ so that

$$\overline{A}_{ij} = \begin{cases} \frac{1}{\Delta V} \int_{V_j} d\vec{r}' \overline{A}(\vec{r}_i, \vec{r}') & \text{for } |\vec{r}_i - \vec{r}_j| < r_d \\ \overline{A}(\vec{r}_i, \vec{r}_j) & \text{for } |\vec{r}_i - \vec{r}_j| \geq r_d \end{cases} \quad (2.3.64)$$

The expression of $\overline{A}_{ij}$ of (2.3.64) will still preserve the translational invariant property so that the FFT can still be taken when the matrix equation is solved by iterative method.

4 Product of Toeplitz Matrix and Column Vector

In matrix equation, the product of a matrix and a column vector is

$$\overline{y} = \overline{g} \overline{x} \quad (2.4.1)$$

where $\overline{x}$ and $\overline{y}$ are column vectors of dimension $N$ and $\overline{g}$ is a matrix of dimension $N \times N$. In matrix notation

$$y(n) = \sum_{m=1}^{N} g(n, m)x(m) \quad (2.4.2)$$

$n = 1, 2, \ldots, N$. The domain has $N$ points. If the kernel $g(n, m)$ is translational invariant, then

$$y(n) = \sum_{m=1}^{N} g(n - m)x(m) \quad (2.4.3)$$

If $g_{nm} = g_{n-m}$, the matrix $\overline{g}$ is known as a Toeplitz matrix.

Equation (2.4.3) looks like a discrete convolution. A fast way to do such a computation is to use FFT. However, since $1 \leq n \leq N$ and $1 \leq m \leq N$, the range of $n - m$ is such that $-(N - 1) \leq n - m \leq N - 1$ so that the argument of $g$ has $2N - 1$ points. Thus Fourier transform of (2.4.3) should be taken over at least $2N - 1$ points. In the following, we briefly review discrete Fourier transform.
4.1 Discrete Fourier Transform and Convolutions

Consider a sequence \( x(n) \) that has length \( N \) such that \( x(n) = 0 \) except in the range \( 1 \leq n \leq N \). A periodic sequence \( \tilde{x}(n) \) can be formed from \( x(n) \) by repeating \( x(n) \) periodically outside the range \( 1 \leq n \leq N \). Suppose \( N = 4 \) and we have a sequence \( x(n) \) as shown in Fig. 2.4.1. We can form a periodic sequence with period \( N \) as shown in Fig. 2.4.2.

\[
\tilde{x}(n) = \sum_{r=-\infty}^{\infty} x(n + rN)
\]  

Let \( U_N(n) \) be a rectangular sequence of length \( N \).

\[
U_N(n) = \begin{cases} 1 & \text{for } 1 \leq n \leq N \\ 0 & \text{otherwise} \end{cases}
\]

Then

\[
x(n) = \tilde{x}(n)U_N(n)
\]

To take discrete Fourier transform, we define the complex number

\[
W_N = \exp\left(\frac{2\pi i}{N}\right)
\]  

so that

\[
W_N^N = 1
\]

\[
\sum_{k=1}^{N} W_N^k(n-n') = \sum_{k=0}^{N-1} W_N^k(n-n') = \begin{cases} N & \text{if } n - n' = \text{integer multiples of } N \\ 0 & \text{otherwise} \end{cases}
\]
Then the discrete Fourier transform is, for all $k$

$$\tilde{X}(k) = \sum_{n=1}^{N} \tilde{x}(n)W_N^{(k-1)(n-1)} = \sum_{n=1}^{N} x(n)W_N^{(k-1)(n-1)} \quad (2.4.7)$$

From (2.4.7), $\tilde{X}(k)$ is periodic with period $N$. It follows that for all $n$

$$\tilde{x}(n) = \frac{1}{N} \sum_{k=1}^{N} \tilde{X}(k)W_N^{-(k-1)(n-1)} \quad (2.4.8)$$

The discrete Fourier transform pairs are defined as in (2.4.7) and (2.4.8). Next define $X(k)$ as one period of $\tilde{X}(k)$.

$$X(k) = \tilde{X}(k)U_N(k) = \begin{cases} \tilde{X}(k) & k = 1, \ldots, N \\ 0 & \text{otherwise} \end{cases} \quad (2.4.9)$$

Thus from (2.4.7) and (2.4.9), for $k = 1, \ldots, N$

$$X(k) = \sum_{n=1}^{N} x(n)W_N^{(k-1)(n-1)} \quad (2.4.10)$$

From (2.4.8) and (2.4.10), for $n = 0, 1, \ldots, N - 1$

$$x(n) = \frac{1}{N} \sum_{k=1}^{N} X(k)W_N^{-(k-1)(n-1)} \quad (2.4.11)$$

Note that the right-hand sides of (2.4.10) and (2.4.11) are periodic while left-hand sides are only nonzero over one period. The advantage of using fast
Fourier transform (FFT) is that both (2.4.7) and (2.4.8) can be computed in \( N \log_2 N \) steps rather than \( N^2 \) steps.

The periodic convolution is as follows. Let \( \tilde{x}_1(n) \) and \( \tilde{x}_2(n) \) be periodic sequences of period \( N \) and \( \tilde{X}_1(k) \) and \( \tilde{X}_2(k) \) be their respective DFT. Let

\[
\tilde{X}_3(k) = \tilde{X}_1(k)\tilde{X}_2(k)
\]

(2.4.12)

and \( \hat{x}_3(n) \) be the inverse discrete Fourier transform

\[
\hat{x}_3(n) = \frac{1}{N} \sum_{k=1}^{N} \tilde{X}_3(k) W_N^{-(k-1)(n-1)}
\]

\[
= \frac{1}{N} \sum_{k=1}^{N} \sum_{m=1}^{N} \sum_{r=1}^{N} \hat{x}_1(m)\hat{x}_2(r) W_N^{(k-1)(m+r-n-1)}
\]

\[
= \begin{cases} 
\sum_{m=1}^{N} \hat{x}_1(m)\hat{x}_2(r) & m + r - n - 1 = \text{integer multiples of } N \\
0 & \text{otherwise}
\end{cases}
\]

\[
= \sum_{m=1}^{N} \hat{x}_1(m)\hat{x}_2(n + 1 - m)
\]

(2.4.13)

Equation (2.4.13) is known as periodic convolution. Note that \( \hat{x}_3(n) \) is also a periodic sequence. However, (2.4.13) is not the usual (linear) convolution. This is because the periodic sequence \( \hat{x}_2(n + 1 - m) \), when it is "shifted" outside the period \( N \), re-enters on the other side because of the periodic property. Thus

\[
x_3^{(c)}(n) = \left[ \sum_{m=1}^{N} \hat{x}_1(m)\hat{x}_2(n - m + 1) \right] U_N(n)
\]

(2.4.14)

is known as circular convolution.

Circular convolution is not equal to linear convolution of

\[
\sum_{n=1}^{N} x_1(n)x_2(m - n + 1)
\]

(2.4.15)

Steps of linear convolution is as shown in Fig. 2.4.3. To use circular convolution to get the result of linear convolution, we need zero padding (Fig. 2.4.4). We also note from Fig. 2.4.3 that to obtain linear convolution from circular convolution, zero padding such that the period becomes \( 2N \) is sufficient.

Let \( x_1(n) \) and \( x_2(n) \) be of length \( N \) and zero outside \( 1 \leq n \leq N \). The
linear convolution is

\[ x_3(n) = \sum_{m=1}^{N} x_1(m)x_2(n - m + 1) \]  

(2.4.16)

and \( x_3(n) \) can be nonzero for \( 1 \leq n \leq 2N - 1 \). Thus there are \( 2N - 1 \) points in \( x_3(n) \).

To use DFT to reform the convolution, we need to “pad” \( x_1(n) \) and \( x_2(n) \) with zeroes to have sequences of length \( M \geq 2N - 1 \)

\[
    x_{1p}(n) = \begin{cases} 
    x_1(n) & 1 \leq n \leq N \\
    0 & N + 1 \leq n \leq M 
    \end{cases}  
    \]

(2.4.17)

\[
    x_{2p}(n) = \begin{cases} 
    x_2(n) & 1 \leq n \leq N \\
    0 & N + 1 \leq n \leq M 
    \end{cases}  
    \]

(2.4.18)

Usually \( M \) is chosen as \( 2N \). Then define \( \tilde{x}_{1p}(n) \) and \( \tilde{x}_{2p}(n) \) as periodic sequences with period \( M \). That is, they are periodic replicas of \( x_{1p}(n) \) and \( x_{2p}(n) \) respectively. Then from (2.4.16)–(2.4.18)

\[
    x_3(n) = \sum_{m=1}^{M} \tilde{x}_{1p}(n)\tilde{x}_{2p}(n - m)  
    \]

(2.4.19)
for $n = 1, 2, \ldots, 2N$. Thus the DFT pairs that give (2.4.16) are

\[
\tilde{X}_1^p(k) = \sum_{n=1}^{M} \tilde{x}_1^p(n)W_M^{(n-1)(k-1)} \tag{2.4.20}
\]

\[
\tilde{X}_2^p(k) = \sum_{n=1}^{M} \tilde{x}_2^p(n)W_M^{(n-1)(k-1)} \tag{2.4.21}
\]

\[
\tilde{X}_3^p(k) = \tilde{X}_1^p(k)\tilde{X}_2^p(k) \tag{2.4.22}
\]

\[
\tilde{x}_3^p(n) = \frac{1}{M} \sum_{k=1}^{M} \tilde{X}_3^p(k)W_M^{-((n-1)(k-1)} \tag{2.4.23}
\]

The equation (2.4.23) gives the relation in which $x_3(n)$ as defined by (2.4.16) is computed. Note that the relations (2.4.16)-(2.4.23) are exact. $\tilde{x}_3^p(n)$ is a periodic sequence of period $M$ and $x_3(n) = \tilde{x}_3^p(n)$ for $n = 1, 2, \ldots, 2N$.

### 4.2 FFT for Product of Toeplitz Matrix and Column Vector

Next we address the equation (2.4.3) that describes the product of a matrix and a column vector.

\[
y(n) = \sum_{m=1}^{N} g(n - m)x(m) \tag{2.4.24}
\]

The equation of (2.4.24) has the following features:

(i) only $N$ values of $y(n)$ are needed. That is, we need to compute $y(n)$, $n = 1, 2, \ldots, N$. 

![Figure 2.4.4 Zero padding of $x(n)$. ($N = 4$)](image)
§4.2 FFT for Product of Toeplitz Matrix and Column Vector

Figure 2.4.5 Zero padding with period of $2N$.

(ii) $g(n)$ is needed for $n = -N + 1, -N + 2, \ldots, 0, \ldots, N - 2, N - 1$, a total of $2N - 1$ distinct values.

(iii) $x(n)$ is defined for $n = 1, \ldots, N$.

For simplicity, we take $M = 2N$.

To illustrate for the case $N = 4$, we need

(i) $x(n)$, $n = 1, 2, 3, 4$

(ii) $y(n)$, $m = 1, 2, 3, 4$

(iii) $g(n - m)$, $n - m = -3, -2, -1, 0, 1, 2, 3$

First we do zero padding of $x(n)$ (Fig. 2.4.5) to get $x_1(n)$. Let $\tilde{x}_1(n)$ be the periodic version of $x_1(n)$ with period $2N$.

$$x_1(n) = \begin{cases} 
  x(n) & \text{for } n = 1, 2, 3, \ldots, N \\
  0 & \text{for } n = N + 1, N + 2, \ldots, 2N 
\end{cases} \quad (2.4.25)$$

Then

$$y(n) = \sum_{m=1}^{2N} g(n - m) \tilde{x}_1(m) \quad (2.4.26)$$

Note that the summation has been changed to $2N$.

Define

$$g'(n) = g(n - 1) \quad (2.4.27)$$

See Fig. 2.4.6 for $g'(n)$. Then

$$y(n) = \sum_{m=1}^{2N} g'(n - m + 1) \tilde{x}_1(m) \quad (2.4.28)$$
Define $x_2(n)$ by

\[
x_2(n) = \begin{cases} 
g'(n) & \text{for } 1 \leq n \leq N \\
0 & \text{for } n = N + 1 \\
g'(n - 2N) & \text{for } N + 2 \leq n \leq 2N \end{cases}
\]  

(2.4.29)

for $n = 1, 2, \ldots, 2N$. Let $\tilde{x}_2(n)$ be the periodic version of $x_2(n)$ with period $2N$. Then

\[
\tilde{x}_2(n) = g'(n) \quad \text{for } -N + 2 \leq n \leq N
\]  

(2.4.30)

Note that

\[
\tilde{x}_2(n) = \begin{cases} 
g(n - 1) & 1 \leq n \leq N \\
0 & n = N + 1 \\
g(n - 2N - 1) & N + 2 \leq n \leq 2N \end{cases}
\]  

(2.4.31)

Hence

\[
y(n) = \sum_{m=1}^{2N} \tilde{x}_2(n - m + 1)\tilde{x}(m)
\]  

(2.4.32)
Define
\[ \tilde{y}(n) = \sum_{m=1}^{2N} \tilde{x}_2(n - m + 1) \tilde{x}(n) \] (2.4.33) for all \( n \). The result of \( \tilde{y}(n) \) is periodic with period \( 2N \). Also
\[ y(n) = \tilde{y}(n) \quad \text{for} \quad 1 \leq n \leq N \] (2.4.34)
Now (2.4.33) satisfies the properties of periodic convolution.
We apply periodic convolution.
\[ \tilde{X}(k) = \sum_{n=1}^{2N} \tilde{x}(n) W_{2N}^{(k-1)(n-1)} \] (2.4.35)
\[ \tilde{X}_2(k) = \sum_{n=1}^{2N} \tilde{x}_2(n) W_{2N}^{(k-1)(n-1)} \]
Then
\[ \tilde{Y}(k) = \tilde{X}_2(k) \tilde{X}(k) \] (2.4.36)
\[ \tilde{y}(n) = \frac{1}{2N} \sum_{k=1}^{2N} \tilde{Y}(k) W_{2N}^{-(k-1)(n-1)} \] (2.4.37)
We can extend to the case of three-dimensional convolution with three indices as needed for the discrete dipole approximation. Let \( N_x, N_y \) and \( N_z \) points, respectively, in \( \hat{x}, \hat{y} \) and \( \hat{z} \) directions with \( N_x, N_y \) and \( N_z \) all equal to powers of 2. Let
\[ y(n, m, l) = \sum_{n'=1}^{N_x} \sum_{m'=1}^{N_y} \sum_{l'=1}^{N_z} g(n - n', m - m', l - l') x(n', m', l') \] (2.4.38)
is to be computed. For the sake of simplicity, we illustrate the scalar case. The vector case follows by a simple extension. Then we have 3-D periodic sequences \( \hat{x} \) and \( \hat{x}_2 \) with period \( M_x = 2N_x, M_y = 2N_y \) and \( M_z = 2N_z \), respectively in \( \hat{x}, \hat{y} \) and \( \hat{z} \) directions. For one period of \( \hat{x}(n, m, l) \) it is
\[ \hat{x}(n, m, l) = \begin{cases} x(n, m, l) & 1 \leq n \leq N_x \text{ and } 1 \leq m \leq N_y \text{ and } 1 \leq l \leq N_z \\ 0 & \text{when } N_x + 1 \leq n \leq 2N_x \\
 & \text{or } N_y + 1 \leq m \leq 2N_y \text{ or } N_z + 1 \leq l \leq 2N_z \end{cases} \] (2.4.39)
The \( \hat{x}_2 \) for nonzero values can be computed as in Table 2.4.1. Then the 3-D DFT and inverse DFT can be performed accordingly.
### Table 2.4.1 Computations for the nonzero values of $\bar{x}_2(n,m,l)$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$m$</th>
<th>$l$</th>
<th>$\bar{x}_2(n,m,l)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[1,N_x]$</td>
<td>$[1,N_y]$</td>
<td>$[1,N_z]$</td>
<td>$g(n-1,m-1,l-1)$</td>
</tr>
<tr>
<td>$[N_x+2,2N_x]$</td>
<td>$[1,N_y]$</td>
<td>$[1,N_z]$</td>
<td>$g(n-2N_x-1,m-1,l-1)$</td>
</tr>
<tr>
<td>$[1,N_x]$</td>
<td>$[N_y+2,2N_y]$</td>
<td>$[1,N_z]$</td>
<td>$g(n-1,m-2N_y-1,l-1)$</td>
</tr>
<tr>
<td>$[N_x+2,2N_x]$</td>
<td>$[N_y+2,2N_y]$</td>
<td>$[1,N_z]$</td>
<td>$g(n-2N_x-1,m-2N_y-1,l-1)$</td>
</tr>
<tr>
<td>$[1,N_x]$</td>
<td>$[1,N_y]$</td>
<td>$[N_z+2,2N_z]$</td>
<td>$g(n-1,m-1,l-2N_z-1)$</td>
</tr>
<tr>
<td>$[N_x+2,2N_x]$</td>
<td>$[1,N_y]$</td>
<td>$[N_z+2,2N_z]$</td>
<td>$g(n-2N_x-1,m-1,l-2N_z-1)$</td>
</tr>
<tr>
<td>$[1,N_x]$</td>
<td>$[N_y+2,2N_y]$</td>
<td>$[N_z+2,2N_z]$</td>
<td>$g(n-1,m-2N_y-1,l-2N_z-1)$</td>
</tr>
<tr>
<td>$[N_x+2,2N_x]$</td>
<td>$[N_y+2,2N_y]$</td>
<td>$[N_z+2,2N_z]$</td>
<td>$g(n-2N_x-1,m-2N_y-1,l-2N_z-1)$</td>
</tr>
</tbody>
</table>

5 Conjugate Gradient Method

Consider a matrix equation of the form

$$\bar{A}\bar{x} = \bar{b}$$  \hspace{1cm} (2.5.1)

where $\bar{A}$ is a $N \times N$ nonsingular matrix, $\bar{x}$ is the unknown column vector and $\bar{b}$ is the right hand side. Both $\bar{x}$ and $\bar{b}$ are $N \times 1$ column vectors.

In the following we briefly describe the conjugate gradient method. Details can be found in textbooks on matrix computation [Hestenes and Stiefel, 1952; Golub and Van Loan, 1996].

5.1 Steepest Descent Method

Let $\bar{A}$ be a real symmetric matrix and positive definite and $\phi(\bar{x})$ be the functional

$$\phi(\bar{x}) = \frac{1}{2} \bar{x}^t \bar{A} \bar{x} - \bar{x}^t \bar{b}$$ \hspace{1cm} (2.5.2)

where $t$ denotes transpose so that $\bar{x}^t$ is a row vector of dimension $1 \times N$. In index notation

$$\phi(\bar{x}) = \frac{1}{2} \sum_{ij} x_i A_{ij} x_j - \sum_i x_i b_i$$  \hspace{1cm} (2.5.3)

Taking the derivatives

$$-\frac{\partial \phi}{\partial x_i} = -\frac{1}{2} \sum_j A_{ij} x_j - \frac{1}{2} \sum_j x_j A_{ji} + b_i$$
\(\frac{5.1}{2}\) Steepest Descent Method

The second equality is due to the fact that
\[
A_{ij} = A_{ji}
\]  
(2.5.5)

Thus the gradient is
\[
-\nabla \phi = \bar{b} - \bar{A} \bar{x}
\]  
(2.5.6)

Optimizing \(\phi\) with respect to \(\bar{x}\) gives
\[
0 = -\nabla \phi = \bar{b} - \bar{A} \bar{x}
\]  
(2.5.7)

This means that optimizing \(\phi\) is equivalent to solving the matrix equation \(\bar{A} \bar{x} = \bar{b}\).

The residual is the “left over” or the “remainder”. Let \(\bar{x}_{i-1}\) be the \((i-1)\)th iterative solution. The residual is
\[
\bar{r}_{i-1} = \bar{b} - \bar{A} \bar{x}_{i-1}
\]  
(2.5.8)

The direction vector \(\bar{d}_i\) gives the next solution
\[
\bar{x}_i = \bar{x}_{i-1} + \alpha_i \bar{d}_i
\]  
(2.5.9)

In the method of steepest descent, the direction vector is chosen to be the same as the residual vector.
\[
\bar{d}_i = \bar{r}_{i-1}
\]  
(2.5.10)

Then the \(i\)th solution is
\[
\bar{x}_i = \bar{x}_{i-1} + \alpha_i \bar{r}_{i-1}
\]  
(2.5.11)

Substituting in (2.5.2), we have
\[
\phi(\bar{x}_i) = \phi(\bar{x}_{i-1} + \alpha_i \bar{d}_i)
\]  
(2.5.12)

\[
= \frac{1}{2} (\bar{x}_{i-1} + \alpha_i \bar{d}_i)^t \bar{A} (\bar{x}_{i-1} + \alpha_i \bar{d}_i) - (\bar{x}_{i-1} + \alpha_i \bar{d}_i)^t \bar{b}
\]

\[
= \phi(\bar{x}_{i-1}) + \alpha_i \bar{d}_i^t \bar{A} \bar{x}_{i-1} + \frac{\alpha_i^2}{2} \bar{d}_i^t \bar{A} \bar{d}_i - \alpha_i \bar{d}_i^t \bar{b}
\]

\[
= \phi(\bar{x}_{i-1}) + \alpha_i \bar{r}_{i-1}^t \bar{A} \bar{x}_{i-1} + \frac{\alpha_i^2}{2} \bar{r}_{i-1}^t \bar{A} \bar{r}_{i-1} - \alpha_i \bar{r}_{i-1}^t \bar{b}
\]

\[
= \phi(\bar{x}_{i-1}) - \alpha_i \bar{r}_{i-1}^t \bar{r}_{i-1} + \frac{\alpha_i^2}{2} \bar{r}_{i-1}^t \bar{A} \bar{r}_{i-1}
\]  
(2.5.13)

Optimizing \(\phi(\bar{x}_i)\) by taking its derivative with respect to \(\alpha_i\) and setting it to zero gives
\[
\alpha_i = \frac{\bar{r}_{i-1}^t \bar{r}_{i-1}}{\bar{r}_{i-1}^t \bar{A} \bar{r}_{i-1}}
\]  
(2.5.13)