NUMERICAL METHODS FOR SOLVING WAVE SCATTERING PROBLEMS

by

NHAN THANH TRAN

B.S., University of Science, Vietnam, 2003

M.S., McNeese State University, 2010

AN ABSTRACT OF A DISSERTATION

submitted in partial fulfillment of the requirements for the degree

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Department of Mathematics College of Arts and Sciences

KANSAS STATE UNIVERSITY Manhattan, Kansas

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Abstract

In this thesis, the author presents several numerical methods for solving scalar and electromagnetic wave scattering problems. These methods are taken from the papers of Professor Alexander Ramm and the author, see [1] and [2].

In Chapter 1, scalar wave scattering by many small particles of arbitrary shapes with impedance boundary condition is studied. The problem is solved asymptotically and numerically under the assumptions $a \ll d \ll \lambda$, where $k = 2\pi/\lambda$ is the wave number, λ is the wave length, a is the characteristic size of the particles, and d is the smallest distance between neighboring particles. A fast algorithm for solving this wave scattering problem by billions of particles is presented. The algorithm comprises the derivation of the (ORI) linear system and makes use of Conjugate Orthogonal Conjugate Gradient method and Fast Fourier Transform. Numerical solutions of the scalar wave scattering problem with 1, 4, 7, and 10 billions of small impedance particles are achieved for the first time. In these numerical examples, the problem of creating a material with negative refraction coefficient is also described and a recipe for creating materials with a desired refraction coefficient is tested.

In Chapter 2, electromagnetic (EM) wave scattering problem by one and many small perfectly conducting bodies is studied. A numerical method for solving this problem is presented. For the case of one body, the problem is solved for a body of arbitrary shape, using the corresponding boundary integral equation. For the case of many bodies, the problem is solved asymptotically under the physical assumptions $a \ll d \ll \lambda$, where a is the characteristic size of the bodies, d is the minimal distance between neighboring bodies, $\lambda = 2\pi/k$ is the wave length and k is the wave number. Numerical results for the cases of one and many small bodies are presented. Error analysis for the numerical method are also provided.

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In Chapter 2, electromagnetic (EM) wave scattering problem by one and many small perfectly conducting bodies is studied. A numerical method for solving this problem is presented. For the case of one body, the problem is solved for a body of arbitrary shape, using the corresponding boundary integral equation. For the case of many bodies, the problem is solved asymptotically under the physical assumptions $a \ll d \ll \lambda$, where a is the characteristic size of the bodies, d is the minimal distance between neighboring bodies, $\lambda = 2\pi/k$ is the wave length and k is the wave number. Numerical results for the cases of one and many small bodies are presented. Error analysis for the numerical method are also provided.

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Chapter 1

Fast Algorithm for Solving Scalar Wave Scattering Problem by Billions of Particles

1.1 Introduction

Wave scattering is a natural phenomenon that happens in everyday life, for example, light scattering in the atmosphere, light scattering by cosmic dust and by the dust in atmosphere, sound wave scattering by packs of fish in the ocean, etc. Studying wave scattering is a subject that has attracted much attention from scientists and engineers since it has many practical applications, for example, in medical image processing, geophysical prospecting, quantum theory, materials science, etc. The wave scattering theory gives insights into the structure of the materials, see [3] and [4]. Wave scattering by small particles was studied by Lord Rayleigh, see [5], who understood that the main term in the scattered field is the dipole radiation. For particles of an arbitrary shape he did not give formulas for calculating the induced dipole moment with a desired accuracy for bodies of arbitrary shapes. This was done in [6] and [7]. Scalar wave scattering by small impedance particles, developed in [8], and used in this paper, has practically important physical features: the field scattered by such particles is $O(a^{2-\kappa})$, as $a \to 0$, which is much larger than the field in Rayleigh scattering which is $O(a^3)$. Here *a* is the characteristic size of small particles and it is assumed that the boundary impedance of a particle is $\zeta = ha^{-\kappa}$, where *h* is a continuous function and $\kappa \in [0, 1)$ is a constant. The theory of wave scattering by many small impedance particles of an arbitrary shape has been developed in [9] and [8], and is a basis for the computational results in this paper. Our basic physical assumptions are $a \ll d \ll \lambda$, where λ is the wavelength and *d* is the minimal distance between neighboring particles. The theory corresponding to the assumption that the effective field in the medium is equal to the incident field. In quantum mechanics it is called the Born approximation, and elsewhere the term weak scattering is used, see [3] and [4].

We do not assume that the particles are distributed in the vertices of a fixed grid with the step size d. They can be distributed randomly or not randomly. The small particles can be described by the inequality $ka \ll 1$, where k is the wave number, $k = 2\pi/\lambda$. In [8] one can find a detailed presentation of this theory. In [9] and [8] the developed theory has been applied to materials science: it was proved that by distributing small particles with prescribed boundary impedances in a given bounded domain, one can create materials with any desired refraction coefficient, in particular, with negative refraction coefficient, which is of interest for the theory of meta-materials, see [10].

Earlier numerical results on wave scattering by not more than one million particles, based on the above theory, were reported in [11] and [12]. In this paper, for dealing with 10¹⁰ small impedance particles, an essentially novel computational procedure which requires parallel computations at a large scale is developed. The numerical solution of the wave scattering problem with so many small particles, ten billions, is obtained, apparently, for the first time. There are many papers on waves and static fields in the many-body systems. We mention just a few papers [13],[14], [15], and [16]. In these and many other papers in this area the theoretical basis for the computational results is quite different from ours, and there were no computational results on scattering by billions of particles, to our knowledge. In Section 1.3 the computational difficulties that we have faced and the methods to overcome these are briefly described.

In Section 1.2 the theory, on which the computational results are based, is outlined. In Section 1.3 a fast algorithm for solving wave scattering problem with many small impedance particles of arbitrary shapes is described. The algorithm is based on 3D convolution, Fast Fourier Transforms (FFT), and Conjugate Orthogonal Conjugate Gradient method (COCG), see [17, 18] and [19]. It exploits the structure of the Green's function of the Helmholtz equation in the wave scattering problem and drastically reduces the total number of operations required for solving this problem. The fast computational methods, such as (FFT), have been widely used in various computational problems, see [20, 21] and [22], but the scale of the problem we deal with requires new computational techniques briefly described in 1.3. Numerical examples are presented in Section 1.4 to illustrate the practical usage of the algorithm. In these numerical examples the algorithm is implemented in parallel and the scalar wave scattering problem is solved with one, four, seven, and ten billions of particles using Gordon super computer at the Extreme Science and Engineering Discovery Environment (XSEDE).

1.2 Scalar wave scattering by many small impedance particles

Consider a bounded domain $\Omega \subset \mathbb{R}^3$ filled with a material whose refraction coefficient is $n_0(x)$. The assumptions on this coefficient are formulated below (1.2.5). Suppose there are M small particles D_m distributed in Ω so that the minimal distance between neighboring particles, d, is much greater than the maximal radius of the particles, $a = \frac{1}{2} \max_{1 \leq m \leq M} \operatorname{diam} D_m$, and much less than the wave length, λ , $a \ll d \ll \lambda$. Let D be the union of D_m , $D := \bigcup_{m=1}^M D_m$, $D \subset \Omega$, and $D' := \mathbb{R}^3 \setminus D$ be the exterior domain. Suppose that the boundary impedance of the mth particle is ζ_m , $\zeta_m = \frac{h(x_m)}{a^{\kappa}}$, where h(x) is a given continuous function in D such that Im $h \leq 0$ in D, and x_m is a point inside D_m . This point gives the position of the mth particle in \mathbb{R}^3 . Let κ be a given constant, $\kappa \in [0, 1)$.

formulated as follows:

$$(\nabla^2 + k^2 n_0^2(x))u = 0$$
 in D' , $k = \text{const} > 0$, $ka \ll 1$ (1.2.1)

$$u_N = \zeta_m u$$
 on $S_m := \partial D_m$, Im $\zeta_m \le 0$, $1 \le m \le M$, (1.2.2)

$$u(x) = u_0(x) + v(x), (1.2.3)$$

$$u_0(x) = e^{ik\alpha \cdot x}, \quad |\alpha| = 1,$$
 (1.2.4)

$$v_r - ikv = o(1/r), \quad r := |x| \to \infty.$$
 (1.2.5)

Here k is the wave number, $k = 2\pi/\lambda$, u_0 is the incident plane wave, v is the scattered wave, α is the direction of the incident wave, \vec{N} is the outer unit normal to S_m , the refraction coefficient $n_0(x) = 1$ in $\Omega' := \mathbb{R}^3 \setminus \Omega$. It is assumed that $n_0(x)$ is a Riemann-integrable function and that Im $n_0^2(x) \ge 0$ in Ω . Equation (1.2.5) is called the radiation condition. It was proved in [8] that if Im $n_0^2(x) \ge 0$ and Im $h(x) \le 0$, then the scattering problem (1.2.1)-(1.2.5) has a unique solution and it can be found in the form

$$u(x) = u_0(x) + \sum_{m=1}^{M} \int_{S_m} G(x,t)\sigma_m(t)dt.$$
 (1.2.6)

Note that u in (1.2.6) satisfies (1.2.1) and (1.2.5) for any σ_m . Thus, one just needs to find σ_m so that u satisfies (1.2.2).

In (1.2.6), G(x, y) is the Green's function of the Helmholtz equation (1.2.1), G satisfies the equation

$$[\nabla^2 + k^2 n_0^2(x)]G = -\delta(x - y) \quad \text{in } \mathbb{R}^3$$
(1.2.7)

and the radiation condition (1.2.5). The functions $\sigma_m(t)$ are unknown continuous functions. These functions are uniquely defined by the boundary condition (1.2.2), see [9]. If $n_0^2 = 1$ in \mathbb{R}^3 , then

$$G(x,y) = \frac{e^{ik|x-y|}}{4\pi|x-y|}.$$
(1.2.8)

The assumption $n_0^2 = 1$ in \mathbb{R}^3 is not a restriction in the problem of creating materials with

a desired refraction coefficient. In the general case, when n_0^2 is a function of x, the Green's function G has to be computed.

From (1.2.6), one gets

$$u(x) = u_0(x) + \sum_{m=1}^M G(x, x_m)Q_m + \sum_{m=1}^M \int_{S_m} [G(x, t) - G(x, x_m)]\sigma_m(t)dt,$$
(1.2.9)

where

$$Q_m := \int_{S_m} \sigma_m(t) dt. \tag{1.2.10}$$

It is proved in [8] that in (1.2.9)

$$|G(x, x_m)Q_m| \gg \left| \int_{S_m} [G(x, t) - G(x, x_m)]\sigma_m(t)dt \right|,$$
 (1.2.11)

as $a \to 0$ and $|x - x_m| \ge a$. Therefore, the solution to the scattering problem can be well approximated by the sum

$$u(x) \sim u_0(x) + \sum_{m=1}^M G(x, x_m) Q_m.$$
 (1.2.12)

Thus, instead of finding the unknown functions $\sigma_m(t)$ from a system of boundary integral equations, as is usually done when one solves a wave scattering problem, we just need to find the unknown numbers Q_m to get the accurate approximation of the solution. This makes it possible to solve problems with so large number of particles that it was not possible to do earlier.

To find the numbers Q_m , let us define the effective field $u_e(x)$. The effective field acting on the jth particle is defined as follows

$$u_e(x_j) := u(x_j) - \int_{S_j} G(x_j, t) \sigma_j(t) dt, \qquad (1.2.13)$$

or equivalently

$$u_e(x_j) = u_0(x_j) + \sum_{m=1, m \neq j}^M \int_{S_m} G(x_j, t) \sigma_m(t) dt, \qquad (1.2.14)$$

where x_j is a point in D_j . The asymptotic formula for Q_m is derived in [8]:

$$Q_m = -c_S a^{2-\kappa} h(x_m) u_e(x_m) [1+o(1)], \quad a \to 0,$$
(1.2.15)

where $c_S > 0$ is a constant depending on the shape of the particle,

$$|S_m| = c_S a^2, (1.2.16)$$

where $|S_m|$ is the surface area of S_m . If S_m is a sphere of radius a, then $c_S = 4\pi$. We assume for simplicity that c_S does not depend on m, that is, all the particles are of the same shape.

Let us derive a formula for the effective field. From (1.2.14)-(1.2.15) one gets

$$u_e(x_j) \simeq u_0(x_j) - c_S \sum_{m=1, m \neq j}^M G(x_j, x_m) h(x_m) u_e(x_m) a^{2-\kappa}, \qquad (1.2.17)$$

as $a \to 0$ and $1 \le j \le M$.

Denote $u_j := u_e(x_j), u_{0j} := u_0(x_j), G_{jm} := G(x_j, x_m)$, and $h_m := h(x_m)$. Then (1.2.17) can be rewritten as a linear algebraic system for the unknown numbers u_m :

$$u_j = u_{0j} - c_S \sum_{m=1, m \neq j}^M G_{jm} h_m a^{2-\kappa} u_m, \quad \text{as } a \to 0, \quad 1 \le j \le M.$$
 (1.2.18)

In (1.2.18), the numbers u_j , $1 \le j \le M$, are unknowns. We call (1.2.18) the original linear algebraic system (ORI). It was proved in [8] that under the assumptions

$$d = O\left(a^{\frac{2-\kappa}{3}}\right), \quad \text{and } M = O\left(\frac{1}{a^{2-\kappa}}\right), \quad \text{for } \kappa \in [0,1), \tag{1.2.19}$$

the numbers u_j , $1 \leq j \leq M$, can be uniquely found by solving (ORI) for all sufficiently small a. If the numbers u_m are known, then the numbers Q_m can be calculated by formula (1.2.15) and the approximate solution to the wave scattering problem (1.2.1)-(1.2.5) can be computed by (1.2.12). This solution is asymptotically exact as $a \to 0$.

The method for solving many-body wave scattering problem, described above, differs in principle from the Fast Multipole Method (FMM), used in many papers, of which we mention just two: [13] and [14]. The FMM is one of the ten most important algorithms in scientific computing discovered in the 20th century by Vladimir Rokhlin and Leslie Greengard. The FMM is an efficient method to do matrix-vector multiplication. A problem involving N degrees of freedom might be solved by using FMM in $CN^{iter}N \log N$ operations, see [23]. Here C is a constant depending on the implementation of the method. The difference between the FMM and our method briefly can be explained as follows: the theoretical basis is different, our method is developed for scattering by small impedance particles of arbitrary shapes and is based on the asymptotically exact formula for the field, scattered by one small particle, and on the asymptotic of many small particles as $a \to 0$. We do not use multipole expansions. One of the advantages of our method is in the asymptotic exactness of the method as $a \to 0$.

Next, let us derive the reduced order linear system for solving the wave scattering problem. Let Δ be an arbitrary subdomain of Ω . Assume that the distribution of particles in Δ satisfies this law

$$\mathcal{N}(\Delta) = \frac{1}{a^{2-\kappa}} \int_{\Delta} N(x) dx [1+o(1)], \quad \text{as } a \to 0.$$
(1.2.20)

Here $N(x) \ge 0$ is a given continuous function in Ω . The function N(x) and the number $\kappa \in [0, 1)$ can be chosen by the experimenter as he(she) desired. The number $\mathcal{N}(\Delta)$ is the total number of the embedded particles in Δ .

Let Ω be partitioned into P non-intersecting sub-cubes Δ_p of side b such that $b \gg d \gg a$, where b = b(a), d = d(a), and $\lim_{a\to 0} \frac{d(a)}{b(a)} = 0$. Here $P \ll M$, and each sub-cube contains many particles. If the function N(x) in (1.2.20) is continuous and $b \ll 1$, then

$$\mathcal{N}(\Delta_p)a^{2-\kappa} = N(x_p)|\Delta_p|[1+o(1)] = a^{2-\kappa}\sum_{x_m\in\Delta_p} 1, \text{ as } a \to 0,$$
 (1.2.21)

where $|\Delta_p|$ is the volume of Δ_p and $x_p \in \Delta_p$ is an arbitrary point, for example, the center of Δ_p . Thus, (1.2.18) can be rewritten as

$$u_q = u_{0q} - c_S \sum_{p=1, p \neq q}^{P} G_{qp} h_p N_p u_p |\Delta_p|, \quad \text{for } 1 \le q \le P,$$
(1.2.22)

where $N_p := N(x_p)$ and x_p is a point in Δ_p , for example, the center of Δ_p . We call (1.2.22) the reduced linear algebraic system (RED). This system is much easier to solve since $P \ll M$.

Let $|\Delta_p| \to 0$. Then it follows from (1.2.22) that the limiting integral equation for u = u(x) holds

$$u(x) = u_0(x) - c_S \int_{\Omega} G(x, y) h(y) N(y) u(y) dy, \text{ for } x \in \mathbb{R}^3,$$
 (1.2.23)

if the assumption (1.2.20) is satisfied. The sum in (1.2.22) is the Riemannian sum for the integral in (1.2.23) which converges to this integral when $\max_p |\Delta_p| \to 0$ (see [8] for the proof of convergence).

Let

$$p(x) := c_S N(x) h(x).$$
(1.2.24)

Then (1.2.23) can be written as

$$u(x) = u_0(x) - \int_{\Omega} G(x, y) p(y) u(y) dy, \text{ for } x \in \mathbb{R}^3.$$
 (1.2.25)

Here u = u(x) is the limiting field in the medium created by embedding many small impedance particles distributed according to equation (1.2.20). We call (1.2.25) the *limiting integral equation* (IE).

Now, applying the operator $(\nabla^2 + k^2 n_0^2)$ to (1.2.25) and using the equation $(\nabla^2 + k^2 n_0^2)G(x, y) = -\delta(x - y)$, one gets

$$(\nabla^2 + k^2 n_0^2) u(x) = p(x) u(x).$$
(1.2.26)

This implies

$$(\nabla^2 + k^2 n^2)u = 0, \qquad (1.2.27)$$

where

$$n^{2}(x) := n_{0}^{2}(x) - k^{-2}p(x), \qquad (1.2.28)$$

and n(x) is the new refraction coefficient of the limiting medium. Since Im $h(x) \leq 0$ and Im $n_0^2(x) \geq 0$, one concludes that Im $n^2(x) \geq 0$. From (1.2.28), one gets

$$p(x) = k^{2} [n_{0}^{2}(x) - n^{2}(x)].$$
(1.2.29)

By equation (1.2.24), h(x) can be computed as

$$h(x) = \frac{p(x)}{c_S N(x)}.$$
 (1.2.30)

This gives a method for creating new materials with a desired refraction coefficient n(x) by embedding many small impedance particles into a given material with the original refraction coefficient n_0 using the distribution law (1.2.20). These engineered materials are called metamaterials which have not been found in nature and have many interesting applications such as creating super-lens, cloaking devices, etc, see [24] and [25].

1.3 A fast algorithm for solving wave scattering problem by billions of particles

For solving the (RED) linear system, one can use any iterative method, namely GMRES, see [26]. Since the order of (RED) can be made much smaller than that of (ORI), the computation is very fast. Therefore, our remaining goal is to develop a fast algorithm for solving (ORI) in order to get the solution of the scattering problem (1.2.1)-(1.2.5). Our algorithm is a combination of the Conjugate Orthogonal Conjugate Gradient (COCG) method, 3D convolution, and FFT. When one solves a linear algebraic system using iterations, matrix-vector

multiplications are carried out in the iterative process. These multiplications take most of the computation time. If the linear system is very large, it takes a huge amount of time to finish only one matrix-vector multiplication in a standard way, since this multiplication is of the order $O(n^2)$. In some cases it is practically impossible to perform such computations, for example, when the system is dense and has more than one billion equations and unknowns. In this section we present an algorithm that greatly reduces the total number of operations (from $O(n^2)$ to $O(n \log n)$) and decreases the overall computation time of the iterative process by handling the matrix-vector multiplication by using 3D convolution and FFT.

There are numerous methods which also employ FFT to solve different problems, for example, Precorrected-FFT method for electrostatic analysis of complicated 3D structures [16], or Particle mesh Ewald method for Ewald sums in large systems [15], etc. Nevertheless, none of these papers deals with the scale that we face solving the scalar wave scattering problem with ten billion particles, i.e., solving a $10^{10} \times 10^{10}$ linear system. This is done for the first time in our work. We have to develop a new algorithm that can solve two major problems in our computing: memory and time. First, it is impossible to store a $10^{10} \times 10^{10}$ dense matrix in any currently available super computer. Suppose we use only single precision. Then it would take 800 million terabytes of memory to store only one matrix to do the computation, since each complex number is 8 bytes. Furthermore, we will suffer network latency and traffic jams which cause a halt in our computation if we use such an amount of memory in any parallel cluster. Second, it is impossible to do the computation at order $O(n^2)$ for a $10^{10} \times 10^{10}$ linear system in a reasonable and permitted time. We deal with the first computing problem, memory, by finding a way to store the $n \times n$ matrix in a 3D cube which is equivalent to only one $n \times 1$ vector in size and avoid moving terabytes of data around. The second computing problem, time, is resolved by reducing the number of operations from $O(n^2)$ to $O(n \log n)$. The details on how to deal with these two major computing problems at our scale and how to set up the wave scattering problem in order to solve it in parallel clusters are described in this section.

Consider the following summation in the original linear system (1.2.18) of the wave

scattering problem

$$\sum_{m=1,m\neq j}^{M} G(\mathbf{x_j}, \mathbf{x_m}) u(\mathbf{x_m}), \qquad (1.3.1)$$

where by bold letters vectors are denoted. G in equation (1.3.1) is the Green's function of the form

$$G(\mathbf{x}_{\mathbf{j}}, \mathbf{x}_{\mathbf{m}}) = \frac{e^{ik|\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{m}}|}}{4\pi|\mathbf{x}_{\mathbf{j}}-\mathbf{x}_{\mathbf{m}}|},$$
(1.3.2)

where $\mathbf{x}_{\mathbf{j}}, \mathbf{x}_{\mathbf{m}}$ are the positions of the jth and mth particles in \mathbb{R}^3 , respectively. If we write $G(\mathbf{x} - \mathbf{y}) := G(\mathbf{x}, \mathbf{y})$, the summation in (1.3.1) will be

$$\sum_{m=1,m\neq j}^{M} G(\mathbf{x_j} - \mathbf{x_m}) u(\mathbf{x_m}), \qquad (1.3.3)$$

which is a discrete convolution of G and u, G * u, if $m \neq j$ is dropped.

In the linear system (1.2.18), G is an $M \times M$ matrix, where M is the total number of particles, and u is an $M \times 1$ vector. When solving the linear system (1.2.18) using COCG iterative algorithm, the matrix-vector multiplication in (1.3.3) needs to be executed. If we do this matrix-vector multiplication in the standard way, it would take $O(M^2)$ operations. This is very expensive in terms of computation time if M is very large, for example, $M \ge 10^6$. Therefore, we have to find a new way to do the matrix-vector multiplication.

The convolution in (1.3.3) can be carried out by using Convolution theorem as follows:

$$G * u = \mathcal{F}^{-1}(\mathcal{F}(G * u)) = \mathcal{F}^{-1}(\mathcal{F}(G) \cdot \mathcal{F}(u)), \qquad (1.3.4)$$

where the \cdot stands for the component-wise multiplication of two vectors and its result is a vector.

If particles are distributed uniformly, one can just use FFT to quickly compute this convolution. Otherwise, one can use Nonequispaced Fast Fourier Transform (NFFT), see [27], [28], and [29]. Our method is valid for variable N(x), see formulas (1.2.22) and (1.2.23). Alternatively, one can just use the (RED) linear system or (IE) with much lower order to solve the wave scattering problem without using FFT nor NFFT. The theory in Section 1.2

shows that the solution to (RED) or (IE) yields a solution to (ORI) with high accuracy, the error tends to zero as $a \to 0$.

To illustrate the idea, let us assume for simplicity that particles are distributed uniformly, that is, N(x) = const in (1.2.20). Let $\mathbf{m} = (x_m, y_m, z_m)$ be the position of the mth particle in \mathbb{R}^3 , where x_m , y_m , and z_m are real numbers. We will assume our domain is a unit cube (different domains can be treated similarly), this cube is placed in the first octant and the origin is one of its vertices, then \mathbf{m} can be rewritten as a product of the scalar factor d > 0and a vector (m_1, m_2, m_3) :

$$\mathbf{m} = d(m_1, m_2, m_3), \tag{1.3.5}$$

where d is the distance between neighboring particles, a scalar, (m_1, m_2, m_3) is a vector whose components m_1, m_2 , and m_3 are integers in [0, b), and $b = M^{1/3}$ is the number of particles on a side of the cube.

In the convolution (1.3.3) suppose that $\mathbf{x}_j = d(j_1, j_2, j_3)$ and $\mathbf{x}_m = d(m_1, m_2, m_3)$, one can write (1.3.3) as

$$G * u = \sum_{m=1, m \neq j}^{M} G(\mathbf{x}_{j} - \mathbf{x}_{m})u(\mathbf{x}_{m})$$
(1.3.6)

$$= \sum_{\substack{m_1, m_2, m_3 = 0 \\ (m_1, m_2, m_3) \neq (j_1, j_2, j_3)}}^{b-1} G(j_1 - m_1, j_2 - m_2, j_3 - m_3)u(m_1, m_2, m_3).$$
(1.3.7)

This is a 3D convolution of G and u.

In order to do this convolution, we need to store matrix G as a vector. This reduces drastically the amount of memory for storing the original $M \times M$ matrix to a much smaller amount for storing an $M \times 1$ vector, which is also denoted by G. Since this vector depends on the three components, $G = G(j_1 - m_1, j_2 - m_2, j_3 - m_3)$ where $j_1, m_1, j_2, m_2, j_3, m_3$ are integers in [0, b) and $(j_1, j_2, j_3) \neq (m_1, m_2, m_3)$, we can alternatively store it as a cube of size $b \times b \times b$. Similarly, vector $u(m_1, m_2, m_3)$ is also stored as a cube of size $b \times b \times b$. Each cube is a stack of planes which will be distributed across all machines in a cluster for



Figure 1.1: Dividing a cube into a stack of planes for storing across machines.

parallelizing the computations and reducing moving data around to prevent traffic jam and network latency, see Figure 1.1. Each machine will work on its local data. Information can be shared among machines but as minimal as possible. Matrix-vector multiplication is done via a function handle without storing any matrix.

When implementing the 3D convolution we need to pad the cubes G and u as follows:

- Pad in x-direction
- Pad in y-direction
- Pad in z-direction



For each direction, the padding is illustrated by this example

For G:

1	2	3	4		1	2	3	4	3	2
5	6	7	8	Pad	5	6	7	8	7	6
9	10	11	12		9	10	11	12	11	10
13	14	15	16		13	14	15	16	15	14

For u:

1	2	3	4		1	2	3	4	0	0
5	6	7	8	Pad	5	6	7	8	0	0
9	10	11	12		9	10	11	12	0	0
13	14	15	16		13	14	15	16	0	0

This means that we pad G using its entries and pad u with zeros. As described in the example above, for padding G we copy all columns except the first and the last ones and put them symmetrically through the last column. This will create a periodic signal G. In fact, if one places padded G continuously, one can see a periodic signal. Since we only need to perform linear convolution on M-length vectors, the result we need is an M-length vector. All the entries after the M-th entry in the convolution will be discarded. So, we pad u with zeros just to have the same length with the padded G to do the cyclic convolution in computer. Cyclic convolutions allow us to compute linear convolutions by means of Discrete Fourier Transforms (DFT). After padding G and u will have size $(2b - 2)^3$.

The Fourier transform and inverse Fourier transform are of order $O(n \log n)$, and vector pointwise multiplication is of order O(n) if the vectors are $n \times 1$. In our case the total number of operations for computing $G * u = \mathcal{F}^{-1}(\mathcal{F}(G) \cdot \mathcal{F}(u))$ is

$$n\log n + n\log n + n + n\log n = O(n\log n), \quad n = (2b-2)^3,$$
 (1.3.8)

since the Fourier transforms $\mathcal{F}(G)$ and $\mathcal{F}(u)$ are of order $O(n \log n)$, the vector point-wise multiplication $\mathcal{F}(G) \cdot \mathcal{F}(u)$ is of order O(n), and the inverse Fourier transform $\mathcal{F}^{-1}(\mathcal{F}(G) \cdot \mathcal{F}(u))$ is of order $O(n \log n)$. If we compare this with the standard matrix-vector multiplication which takes M^2 operations $(M = b^3)$, this is a huge reduction of the number of operations and computation time, when M is very large, say $M \ge 10^9$.

This algorithm is applicable not only to solving scalar wave scattering problems but also to other PDE problems, for example, aeroacoustics, signal processing, etc.

1.4 Experiments

The algorithm described in Section 1.3 is implemented in parallel using the Portable, Extensible Toolkit for Scientific Computation (PETSc) library developed at Argonne National Laboratory (ANL), see [30]. For implementing FFT, Fastest Fourier Transform in the West (FFTW) library is used, see [31]. The wave scattering problem is solved using Gordon super computer at XSEDE. "Gordon is a dedicated XSEDE cluster designed by Appro and SDSC consisting of 1024 compute nodes and 64 I/O nodes. Each compute node contains two 8-core 2.6 GHz Intel EM64T Xeon E5 (Sandy Bridge) processors and 64 GB of DDR3-1333 memory", see [32]. Table 1.1 shows the technical information of one compute node in Gordon. "The network topology of Gordon is a 4x4x4 3D torus with adjacent switches connected by

Table 1.1: Compute node In	tel EM041 Aeon E5.
System Component	Configuration
Sockets	2
Cores	16
Clock speed	$2.6~\mathrm{GHz}$
Flop speed	333 Gflop/s
Memory capacity	64 GB DDR3-1333
Memory bandwidth	85 GB/s
STREAM Triad bandwidth	60 GB/s

 Table 1.1: Compute node Intel EM64T Xeon E5.

three 4x QDR InfiniBand links (120 Gbit/s). Compute nodes (16 per switch) and I/O nodes (1 per switch) are connected to the switches by 4x QDR (40 Gbit/s). The theoretical peak performance of Gordon is 341 TFlop/s", see [32]. Table 1.2 shows information about the network of Gordon.

Table 1.2:Network summary.					
QDR InfiniBand Interconnect					
Topology	3D Torus				
Link bandwidth	8 GB/s (bidirectional)				
MPI latency	$1.3 \ \mu s$				

The program code is written in C & C++, compiled with Intel compiler, and linked with

MPI library MVAPICH2. The code uses 64-bit integers and single precision. The relative error tolerance used for the convergence of COCG iterations is 2×10^{-5} .

We assume that the domain Ω , which contains all the particles, is a unit cube, placed in the first octant such that the origin is one of its vertices, and particles are distributed uniformly in Ω . Suppose we want to create a new meta-material with the refraction coefficient n(x) = -1 in Ω given a material with the refraction coefficient $n_0(x) = 1$ by embedding many small particles into the given material. We assume the particles are spheres, so $c_S = 4\pi$. The new refraction coefficient is computed by the following formula

$$n(x) = [n_0^2(x) - k^{-2}c_S h(x)N(x)]^{1/2}, \qquad (1.4.1)$$

where N(x) and h(x) are at our choices. For simplicity we choose N(x) = 1. The choice of h(x) is subject to the physical condition Im $h \leq 0$. If Im $h(x) \leq 0$ and Im $n_0^2 \geq 0$, then Im $n^2(x) \geq 0$. The square root in formula (1.4.1) is of the form

$$z^{1/2} = |z|^{1/2} e^{i\frac{\phi}{2}}, \quad \phi := \arg z, \quad \phi \in [0, 2\pi].$$
 (1.4.2)

Formula (1.4.2) defines a one-valued branch of analytic function $z^{1/2}$ in the complex plane with the cut $[0, +\infty)$. If one wants to get $n = Be^{i(\pi-\epsilon)}$, where B > 0 and $\epsilon > 0$, then $n^2 = B^2 e^{i(2\pi-2\epsilon)}$. When $\epsilon > 0$ is very small, one gets practically negative refraction coefficient n. In this experiment, we choose Im n = 0.001. This violates the assumption Im $h(x) \leq 0$. To justify this violation for very small values of Im h(x) we argue as follows. The integral equation (1.2.23) is an equation with compact integral operator T

$$Tu := c_S \int_D G(x, y)h(y)N(y)u(y)dy.$$
(1.4.3)

It is of Fredholm type with index zero. It is proved in [8] that equation (1.2.23) has at most one solution for Im $h \leq 0$. Therefore, the inverse operator $(I+T)^{-1}$ is bounded for Im $h \leq 0$. The set of boundedly invertible operators is open. Therefore the inverse operator $(I+T)^{-1}$ exists and is bounded also for sufficiently small Im $h \ge 0$.

The radius a of the particles and the distance d between neighboring particles are chosen so that

$$d = \frac{1}{M^{1/3}} = a^{\frac{2-\kappa}{3}}, \text{ and } M = \frac{1}{a^{2-\kappa}},$$
 (1.4.4)

where M is the total number of particles embedded in the domain Ω . To solve (IE), we use a collocation method, dividing the domain into many sub-cubes, taking the collocation points as the centers of these cubes, and then approximating the integral equation by the corresponding Riemannian sum.

The following physical parameters are used to conduct the experiment:

- Speed of wave, v = 34400 cm/sec,
- Frequency, f = 1000 Hz,
- Wave number, $k = 0.182651 \text{ cm}^{-1}$,
- Direction of plane wave, $\alpha = (1, 0, 0)$,
- The constant $\kappa = 0.5$,
- Volume of the domain that contains all particles, $|\Omega| = 1 \text{ cm}^3$,
- Distribution of particles, $N = Ma^{2-\kappa}/|\Omega| = 1$, i.e. particles are distributed uniformly in the unit cube,
- Function h(x) = 2.65481E-09 + i5.30961E-06,
- Original refraction coefficient, $n_0 = 1 + i0$,
- Desired refraction coefficient, n = -1 + i0.001 $(n = [n_0^2(x) - k^{-2}c_Sh(x)N(x)]^{1/2} = [1^2 - 0.182651^{-2}4\pi (2.65481\text{E-}09 + i5.30961\text{E-}06)1]^{1/2} = -1 + i0.001),$
- Number of small subcubes after partitioning the domain Ω for solving (RED), P = 8000.

• Number of collocation points for solving (IE), C = 64000.

Table 1.3 and Figure 1.2 show the time usage in Gordon for solving the wave scattering problem with 1, 4, 7, and 10 billion particles using the algorithm described in Section 1.3. The computation time is measured by Service Unit (SU), 1 SU corresponds to 1 hour/core. Table 1.4 and Figure 1.3 show the differences (errors) between the solutions of (ORI) vs.

Table 1.3: Time usage for solving the wave scattering problem.						
Number of particles	1 billion	4 billions	7 billions	10 billions		
Time usage (second)	103	1076	2082	1674		
Node usage	8	28	49	74		
Number of SUs	3.66	133.90	453.41	550.56		

600 500 400 300 200 100 0 1 billion 4 billions 7 billions 10 billions Number of particles

Figure 1.2: Time usage for solving the wave scattering problem.

(RED), (RED) vs. (IE), and (ORI) vs. (IE). Since the numbers of unknowns in (ORI), (RED), and (IE) are different, $M \gg P$ and P < C, we use interpolation procedure to compare their solutions. For example, let x and y be the solutions of (ORI) and (RED), respectively. We find all the particles x_i that lie in the subcube Δ_q corresponding to y_q and then find the difference $|x_i - y_q|$. Then, we compute

$$\sup_{y_q} \frac{1}{\mathcal{N}(\Delta_q)} \sum_{x_i \in \Delta_q} |x_i - y_q|, \qquad (1.4.5)$$

where $\mathcal{N}(\Delta_q)$ is the number of particles in the subcube Δ_q . This gives the difference between the solutions of (ORI) and (RED). The solution differences between (RED) vs. (IE) and (ORI) vs. (IE) are computed similarly. The numbers in Table 1.4 are rounded to the nearest ten-thousandths.

Table 1.4: Solution differences (errors).							
Number of particles	1 billion	4 billions	7 billions	10 billions			
(ORI) vs. (RED) (RED) vs. (IE) (ORI) vs. (IE)	$0.0045 \\ 0.0022 \\ 0.0022$	$0.0045 \\ 0.0022 \\ 0.0022$	$0.0045 \\ 0.0022 \\ 0.0022$	$0.0045 \\ 0.0022 \\ 0.0022$			



Figure 1.3: Solution differences (errors).

For example, Figures 1.4, 1.5 and 1.6 display vertical slice planes of the solutions, scattering fields, of (ORI), (RED), and (IE), respectively, at the center of the domain Ω , when $M = 10^9$ particles, P = 8000 subcubes, and C = 64000 collocation points. The relative errors of the convergence of the solutions to (ORI), (RED), and (IE) are 1.72448E-05, 1.94613E-05, and 1.93914E-05, respectively. The relative errors are residual-based and computed using this ratio $\frac{||r||}{||RHS||}$, where r is the residual vector and RHS is the right-hand-side vector. The solution differences between (ORI) vs. (RED), (RED) vs. (IE), and (ORI) vs. (IE) are 0.0045, 0.0022, and 0.0022, respectively. The color bars indicate the values of the corresponding colors. The values used here are the real part and imaginary part of the scattering fields at the grid points on the slices.

For reference, Tables 1.5, 1.6, and 1.7 show the solutions of (ORI), (RED), and (IE), respectively, at the grid points $5 \times 5 \times 5$ in the unit cube Ω .

1.5 Conclusions

The numerical results in this paper allow one to solve (ORI) for $1 \leq M \leq 10^{10}$. These results show that the solution by (RED) for $M = 10^{10}$ agrees with the solution by (ORI) with high accuracy (99.55 %), and agrees with the solution of (IE) also with high accuracy (99.78%). Therefore, practically for solving problems with $M \geq 10^6$ one may use (RED) or (IE). For solving the scattering problem for $M < 10^6$ numerically one can use (ORI). The accuracy of our numerical method is high if the quantity $ka + ad^{-1}$ is small. Furthermore, it is important to note that this method is of the same order of number of operations as that of Fast Multipole Method (FMM), $O(n \log n)$. However, we do not use multipole expansions and our method is easier to implement compared to FMM. In addition, our method can give an asymptotically exact solution to the wave scattering problem.



Figure 1.4: Solution of (ORI) when $M = 10^9$.

Table 1.5: Solution of (ORI) at the grid points $5 \times 5 \times 5$ in the cube.

	0 (/ 1		
0.999990+0.004392i	0.999990+0.004392i	0.999990 + 0.004392i	0.999990 + 0.004392i	0.999990 + 0.004392i
0.999990 + 0.004392i				
0.999990 + 0.004392i				
0.999990 + 0.004392i				
0.999990 + 0.004392i				
0.999163 + 0.040911i				
0.999163 + 0.040911i				
0.999163 + 0.040911i				
0.999163 + 0.040911i				
0.999163 + 0.040911i				
0.997002 + 0.077375i				
0.997002 + 0.077375i				
0.997002 + 0.077375i				
0.997002 + 0.077375i				
0.997002 + 0.077375i				
$0.993511 {+} 0.113736i$				
$0.993511 {+} 0.113736i$				
$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	0.993511 + 0.113736i
$0.993511 {+} 0.113736i$				
$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	$0.993511 {+} 0.113736i$	0.993511 + 0.113736i
0.988694 + 0.149945i				
0.988694 + 0.149945i				
0.988694 + 0.149945i				
0.988694 + 0.149945i				
0.988694 + 0.149945i				



Figure 1.5: Solution of (RED) when $M = 10^9$ and P = 8000.

Table 1.6: Solution of (RED) at the grid points $5 \times 5 \times 5$ in the cube.

	J (/ .	L	
0.9999999+0.000010i	0.999999+0.000010i	0.999999+0.000010i	0.999999 + 0.000010i	0.9999999+0.000010i
0.999999 + 0.000010i	0.9999999 + 0.000010i	0.999999 + 0.000010i	0.9999999 + 0.000010i	0.999999 + 0.000010i
0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.999999 + 0.000010i
0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.999999 + 0.000010i
0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.9999999 + 0.000010i	0.999999 + 0.000010i
0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i
0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i
0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i
0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i
0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i	0.999332 + 0.036532i
$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	0.997331 + 0.073005i
$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	0.997331 + 0.073005i
$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	0.997331 + 0.073005i
$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	0.997331 + 0.073005i
$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	$0.997331 {+} 0.073005i$	0.997331 + 0.073005i
0.993999 + 0.109381i	0.993999 + 0.109381i	$0.993999 {+} 0.109381 i$	0.993999 + 0.109381i	0.993999 + 0.109381i
0.993999 + 0.109381i	0.993999 + 0.109381i	$0.993999 {+} 0.109381 i$	0.993999 + 0.109381i	0.993999 + 0.109381i
0.993999 + 0.109381i	0.993999 + 0.109381i	$0.993999 {+} 0.109381 i$	0.993999 + 0.109381i	0.993999 + 0.109381i
0.993999 + 0.109381i	$0.993999 {+} 0.109381 i$	$0.993999 {+} 0.109381 i$	0.993999 + 0.109381i	0.993999 + 0.109381i
0.993999 + 0.109381i	$0.993999 {+} 0.109381 i$	$0.993999 {+} 0.109381 i$	0.993999 + 0.109381i	0.993999 + 0.109381i
0.989341 + 0.145611i	$0.989341 {+} 0.145611i$	0.989341 + 0.145611i	0.989341 + 0.145611i	0.989341 + 0.145611i
0.989341 + 0.145611i	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	0.989341 + 0.145611i
0.989341 + 0.145611i	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	0.989341 + 0.145611i
0.989341 + 0.145611i	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	$0.989341 {+} 0.145611i$	0.989341 + 0.145611i
0.989341 + 0.145611i	0.989341 + 0.145611i	$0.989341 {+} 0.145611i$	0.989341 + 0.145611i	0.989341 + 0.145611i



Figure 1.6: Solution of (IE) when $M = 10^9$, P = 8000, and C = 64000.

Table 1.7: Solution of (IE) at the grid points $5 \times 5 \times 5$ in the cube.

	J			
1.000000 + 0.000010i				
1.000000 + 0.000010i				
1.000000 + 0.000010i				
1.000000 + 0.000010i				
1.000000 + 0.000010i				
0.999332 + 0.036532i				
0.999332 + 0.036532i				
0.999332 + 0.036532i				
0.999332 + 0.036532i				
0.999332 + 0.036532i				
0.997332 + 0.073005i				
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Chapter 2

Numerical Method for Solving Electromagnetic Wave Scattering by One and Many Small Perfectly Conducting Bodies

2.1 Introduction

Many real-world electromagnetic (EM) problems like EM wave scattering, EM radiation, etc [33], cannot be solved analytically and exactly to get a solution in a closed form. Thus, numerical methods have been developed to tackle these problems approximately. Computational Electromagnetics (CEM) has evolved enormously in the past decades to a point that its methods can solve EM problems with extreme accuracy. These methods can be classified into two categories: Integral Equation (IE) method and Differential Equation (DE) method. Typical IE methods include: Method of Moment (MoM) developed by Roger F. Harrington (1968) [34], Fast Multipole Method (FMM) first introduced by Greengard and Rokhlin (1987) [13] and then applied to EM by Engheta et al (1992) [35], Partial Element Equivalent Circuit (PEEC) method [36], and Discrete Dipole Approximation [37]. Typical DE methods are: Finite Difference Time Domain (FDTD) developed by Kane Yee (1966) [38], Finite Element Method (FEM) [39], Finite Integration Technique (FIT) proposed by Thomas Weiland (1977) [40], Pseudospectral Time Domain (PSTD) [41], Pseudospectral Spatial Domain (PSSD) [42], and Transmission Line Matrix (TLM) [43]. Among these methods, FDTD has emerged as one of the most popular techniques for solving EM problems due to its simplicity and ability to provide animated display of the EM field. However, FDTD requires the entire computational domain be gridded [44], that results in very long solution times. Furthermore, as a DE method, it does not take into account the radiation condition in exact sense [45, 46], which leads to certain error in the solution. On the other hand, spurious solutions might exist in DE methods [47–49]. Most importantly, most of DE methods are not suitable if the number of bodies is very large.

In [8, 50–54], A. G. Ramm has developed a theory of EM wave scattering by many small perfectly conducting and impedance bodies. In this theory, the EM wave scattering problem is solved asymptotically under the physical assumptions: $a \ll d \ll \lambda$, where a is the characteristic size of the bodies, d is the minimal distance between neighboring bodies, $\lambda = 2\pi/k$ is the wave length and k is the wave number. In this paper, the problem of EM wave scattering by one and many small perfectly conducting bodies is considered. A numerical method for solving this problem asymptotically based on the above theory is presented. For the case of one body, the problem is solved for a body of arbitrary shape, using the corresponding boundary integral equation. For the case of many small bodies, the problem is solved under the basic assumptions $a \ll d \ll \lambda$ and the assumption about the distribution of the small bodies

$$\mathcal{N}(\Delta) = \frac{1}{a^3} \int_{\Delta} N(x) dx [1 + o(1)], \quad a \to 0,$$
 (2.1.1)

in which Δ is an arbitrary open subset of the domain Ω that contains all the small bodies, $\mathcal{N}(\Delta)$ is the number of the small bodies in Δ , and N(x) is the distribution function of the bodies

$$N(x) \ge 0, \quad N(x) \in C(\Omega). \tag{2.1.2}$$

In Sections 2.2 and 2.3, the theory of EM wave scattering by one and many small perfectly conducting bodies is presented. The numerical methods for solving these problems are also described in details. Furthermore, error analysis for the numerical methods of solving the EM scattering problem are also provided. In Section 2.4 these methods are tested and numerical results are discussed.

2.2 EM wave scattering by one perfectly conducting body

Let D be a bounded perfectly conducting body, $a = \frac{1}{2} \operatorname{diam} D$, S be its C^2 -smooth boundary, and $D' := \mathbb{R}^3 \setminus D$. Let ϵ and μ be the dielectric permittivity and magnetic permeability constants of the medium in D'. Let E and H denote the electric and magnetic fields, respectively, E_0 be the incident field and v_E be the scattered field. The problem of electromagnetic wave scattering by one perfectly conducting body can be stated as follows

$$\nabla \times E = i\omega\mu H, \quad \text{in } D' := \mathbb{R}^3 \setminus D, \tag{2.2.1}$$

$$\nabla \times H = -i\omega\epsilon E, \quad \text{in } D', \tag{2.2.2}$$

$$[N, [E, N]] = 0, \text{ on } S := \partial D,$$
 (2.2.3)

$$E = E_0 + v_E, (2.2.4)$$

$$E_0 = \mathcal{E}e^{ik\alpha \cdot x}, \quad \mathcal{E} \cdot \alpha = 0, \quad \alpha \in S^2,$$
 (2.2.5)

$$\frac{\partial v_E}{\partial r} - ikv_E = o\left(\frac{1}{r}\right), \quad r := |x| \to \infty, \tag{2.2.6}$$

where $\omega > 0$ is the frequency, $k = 2\pi/\lambda = \omega\sqrt{\epsilon\mu}$ is the wave number, $ka \ll 1$, λ is the wave length, \mathcal{E} is a constant vector, and α is a unit vector that indicates the direction of the incident wave E_0 . This incident wave satisfies the relation $\nabla \cdot E_0 = 0$. The scattered field v_E satisfies the radiation condition (2.2.6). Here, N is the unit normal vector to the surface S, pointing out of D. By $[\cdot, \cdot]$ the vector product is denoted and $\alpha \cdot x$ is the scalar product

of two vectors.

The solution to problem (2.2.1)-(2.2.6) can be found in the form

$$E(x) = E_0(x) + \nabla \times \int_S g(x,t)J(t)dt, \quad g(x,t) := \frac{e^{ik|x-t|}}{4\pi|x-t|}, \quad (2.2.7)$$

see [50]. Here, E is a vector in \mathbb{R}^3 and $\nabla \times E$ is a pseudo-vector, that is a vector-like object which changes sign under reflection of its coordinate axes. E_0 is the incident plane wave defined in (2.2.5) and J is an unknown pseudo-vector that is to be found. J is assumed to be tangential to S and continuous. J can be found by applying the boundary condition (2.2.3), or equivalently [N, E] = 0, to (2.2.7) and solving the resulting boundary integral equation

$$\frac{J}{2} + AJ := \frac{J(s)}{2} + \int_{S} [N_s, [\nabla_s g(s, t), J(t)]] dt = -[N_s, E_0], \qquad (2.2.8)$$

or, equivalently

$$(I+2A)J = F,$$
 (2.2.9)

where $F := -2[N_s, E_0]$. Equation (2.2.9) is of Fredholm type since A is compact, see [51].

Once we have J, E can be computed by formula (2.2.7) and H can be found by the formula

$$H = \frac{\nabla \times E}{i\omega\mu}.$$
 (2.2.10)

If D is sufficiently small, then equation (2.2.9) is uniquely solvable in C(S) and its solution J is tangential to S, see [50]. The asymptotic formula for E when the radius a of the body D tends to zero can be derived as follows, see [50]. Rewrite equation (2.2.7) as

$$E(x) = E_0(x) + [\nabla g(x, x_1), Q] + \nabla \times \int_S [g(x, t) - g(x, x_1)] J(t) dt, \qquad (2.2.11)$$

where $x_1 \in D$, an arbitrary point inside the small body D, and

$$Q := \int_{S} J(t)dt. \tag{2.2.12}$$

Since

$$|\nabla g(x, x_1)]| = O\left(\frac{k}{d} + \frac{1}{d^2}\right), \quad d = |x - x_1|,$$
(2.2.13)

$$|g(x,t) - g(x,x_1)| = O\left(\left(\frac{k}{d} + \frac{1}{d^2}\right)a\right), \quad a = |t - x_1|, \text{ and } (2.2.14)$$

$$|\nabla[g(x,t) - g(x,x_1)]| = O\left(\frac{ak^2}{d} + \frac{ak}{d^2} + \frac{a}{d^3}\right),$$
(2.2.15)

the second term in (2.2.11) is much greater than the last term

$$\left|\left[\nabla g(x,x_1),Q\right]\right| \gg \left|\nabla \times \int_S [g(x,t) - g(x,x_1)]J(t)dt\right|, \quad a \to 0.$$
(2.2.16)

Then, the asymptotic formula for E when a tends to zero is

$$E(x) = E_0(x) + [\nabla_x g(x, x_1), Q], \quad a \to 0,$$
(2.2.17)

where $|x - x_1| \gg a$, $x_1 \in D$. Thus, when D is sufficiently small, instead of finding J, we can just find one pseudovector Q.

The analytical formula for Q is derived as follows, see [51]. By integrating both sides of (2.2.8) over S, one gets

$$\int_{S} \frac{J(s)}{2} ds + \int_{S} ds \int_{S} dt [N_s, [\nabla_s g(s, t), J(t)]] = -\int_{S} [N_s, E_0] ds.$$
(2.2.18)

This is equivalent to

$$\frac{Q}{2} + \int_{S} dt \int_{S} ds \nabla_{s} g(s,t) N_{s} \cdot J(t) - \int_{S} dt J(t) \int_{S} ds \frac{\partial g(s,t)}{\partial N_{s}} = -\int_{D} \nabla \times E_{0} dx. \quad (2.2.19)$$

When $a \to 0$, this equation becomes

$$\frac{Q}{2} + e_p \int_S dt \int_S ds \frac{\partial g(s,t)}{\partial s_p} N_q(s) J_q(t) + \frac{1}{2} \int_S dt J(t) = -|D| \nabla \times E_0, \quad 1 \le p, q \le 3, \quad (2.2.20)$$

where in the second term, summations over the repeated indices are understood, e_p , $1 \le p \le 3$, are the orthogonal unit vectors in \mathbb{R}^3 , |D| is the volume of D, $|D| = c_D a^3$, and in the third term we use this estimate

$$\int_{S} ds \frac{\partial g(s,t)}{\partial N_s} \simeq \int_{S} ds \frac{\partial g_0(s,t)}{\partial N_s} = -\frac{1}{2}, \quad g_0(s,t) := \frac{1}{4\pi |s-t|}.$$
 (2.2.21)

Let

$$\Gamma_{pq}(t) := \int_{S} ds \frac{\partial g(s,t)}{\partial s_p} N_q(s), \qquad (2.2.22)$$

then equation (2.2.20) can be rewritten as follows

$$\frac{Q}{2} + e_p \int_S dt \Gamma_{pq}(t) J_q(t) + \frac{Q}{2} = -|D| \nabla \times E_0, \qquad (2.2.23)$$

or

$$Q + \Gamma Q = -|D|\nabla \times E_0, \qquad (2.2.24)$$

where Γ is a 3 \times 3 constant matrix and it is defined by

$$\Gamma Q = e_p \int_S dt \Gamma_{pq}(t) J_q(t), \qquad (2.2.25)$$

in which summations are understood over the repeated indices. Thus, Q can be written as

$$Q = -|D|(I+\Gamma)^{-1}\nabla \times E_0, \quad a \to 0,$$
(2.2.26)

where $I := I_3$, the 3 × 3 identity matrix. This formula is asymptotically exact as $a \to 0$.

2.2.1 Numerical method for solving EM wave scattering by one perfectly conducting spherical body

In this section, we consider the EM wave scattering problem by a small perfectly conducting spherical body. Instead of solving the problem (2.2.1)-(2.2.6) directly, we will solve its

corresponding boundary integral equation (2.2.8) for the unknown vector J

$$\frac{J(s)}{2} + \int_{S} [N_s, [\nabla_s g(s, t), J(t)]] dt = -[N_s, E_0].$$
(2.2.27)

Then the solution E to the EM wave scattering problem by one perfectly conducting body can be computed by either the exact formula (2.2.7) or the asymptotic formula (2.2.17).

Scattering by a sphere has been discussed in many papers, for example [55] in which Mie solves the EM wave scattering problem by separation of variables. The EM field, scattered by a small body, is proportional to $O(a^3)$.

Suppose S is a smooth surface of a spherical body. Let S be partitioned into P nonintersecting subdomains $S_{ij}, 1 \le i \le m_{\theta}, 1 \le j \le m_{\phi}$, using spherical coordinates, where m_{θ} is the number of intervals of θ between 0 and 2π and m_{ϕ} defines the number of intervals of ϕ between 0 and π . Then $P = m_{\theta}m_{\phi} + 2$, which includes the two poles of the sphere. m_{θ} is defined in this way: $m_{\theta} = m_{\phi} + |\phi - \frac{\pi}{2}| 6m_{\phi}$. This means the closer it is to the poles of the sphere, the more intervals for θ are used. Then the point (θ_i, ϕ_j) in S_{ij} is chosen as follows

$$\theta_i = i \frac{2\pi}{m_{\theta}}, \quad 1 \le i \le m_{\theta}, \tag{2.2.28}$$

$$\phi_j = j \frac{\pi}{m_\phi + 1}, \quad 1 \le j \le m_\phi.$$
 (2.2.29)

Note that there are many different ways to distribute collocation points. However, the one that we describe here will guarantee convergence to the solution to (2.2.27) with fewer collocation points used from our experiment. Furthermore, one should be careful when choosing the distribution of collocation points on a sphere. If one chooses $\phi_j = j \frac{\pi}{m_{\phi}}, 1 \leq j \leq m_{\phi}$, then when $j = m_{\phi}, \phi_j = \pi$ and thus there is only one point for this ϕ regardless of the value of θ as shown in (2.2.30). The position of a point in each S_{ij} can be computed by

$$(x, y, z)_{ij} = a(\cos\theta_i \sin\phi_j, \sin\theta_i \sin\phi_j, \cos\phi_j), \qquad (2.2.30)$$

and the outward-pointing unit normal vector N to S at this point is

$$N_{ij} = N(\theta_i, \phi_j) = (\cos \theta_i \sin \phi_j, \sin \theta_i \sin \phi_j, \cos \phi_j).$$
(2.2.31)

For a star-shaped body with a different shape, only the normal vector N needs to be recomputed. Rewrite the integral equation (2.2.27) as

$$\frac{J(s)}{2} + \int_{S} \nabla_{s} g(s,t) N_{s} \cdot J(t) dt - \int_{S} \frac{\partial g(s,t)}{\partial N_{s}} J(t) dt = -[N_{s}, E_{0}].$$
(2.2.32)

This integral equation can be discretized as follows

$$J(i) + 2\sum_{j \neq i}^{P} [\nabla_s g(i,j) N_s(i) \cdot J(j) - J(j) \nabla_s g(i,j) \cdot N_s(i)] \Delta_j = F(i), \quad 1 \le i \le P, \quad (2.2.33)$$

in which by *i* the point (x_i, y_i, z_i) is denoted, $F(i) := -2[N_s, E_0](i)$, and Δ_j is the surface area of the subdomain *j*. This is a linear system with unknowns $J(i) := (X_i, Y_i, Z_i), 1 \le i \le P$. This linear system can be rewritten as follows

$$X_{i} + \sum_{j \neq i}^{P} a_{ij} X_{j} + b_{ij} Y_{j} + c_{ij} Z_{j} = F_{x}(i), \qquad (2.2.34)$$

$$Y_i + \sum_{j \neq i}^{P} a'_{ij} X_j + b'_{ij} Y_j + c'_{ij} Z_j = F_y(i), \qquad (2.2.35)$$

$$Z_i + \sum_{j \neq i}^{P} a_{ij}'' X_j + b_{ij}'' Y_j + c_{ij}'' Z_j = F_z(i), \qquad (2.2.36)$$

where by the subscripts x, y, z the corresponding coordinates are denoted, e.g. $F(i) = (F_x, F_y, F_z)(i)$, and

$$a_{ij} := 2[\nabla g(i,j)_x N_x(i) - \nabla g(i,j) \cdot N(i)]\Delta_j, \qquad (2.2.37)$$

$$b_{ij} := 2\nabla g(i,j)_x N_y(i)\Delta_j, \qquad (2.2.38)$$

$$c_{ij} := 2\nabla g(i,j)_x N_z(i)\Delta_j, \qquad (2.2.39)$$

for $i \neq j$; when i = j: $a_{ii} = 1, b_{ii} = 0$, and $c_{ii} = 0$,

$$a'_{ij} := 2\nabla g(i,j)_y N_x(i)\Delta_j, \qquad (2.2.40)$$

$$b'_{ij} := 2[\nabla g(i,j)_y N_y(i) - \nabla g(i,j) \cdot N(i)]\Delta_j, \qquad (2.2.41)$$

$$c'_{ij} := 2\nabla g(i,j)_y N_z(i)\Delta_j, \qquad (2.2.42)$$

for $i \neq j$; when i = j: $a'_{ii} = 0, b'_{ii} = 1$, and $c'_{ii} = 0$,

$$a_{ij}'' := 2\nabla g(i,j)_z N_x(i)\Delta_j, \qquad (2.2.43)$$

$$b_{ij}'' := 2\nabla g(i,j)_z N_y(i) \Delta_j,$$
 (2.2.44)

$$c_{ij}'' := 2[\nabla g(i,j)_z N_z(i) - \nabla g(i,j) \cdot N(i)]\Delta_j, \qquad (2.2.45)$$

 $\text{for } i\neq j; \text{ when } i=j; \; a_{ii}^{\prime\prime}=0, b_{ii}^{\prime\prime}=0, \text{ and } c_{ii}^{\prime\prime}=1.$

2.2.2 Error analysis

Recall the boundary integral equation (2.2.8)

$$\frac{J(s)}{2} + \int_{S} [N_s, [\nabla_s g(s, t), J(t)]] dt = -[N_s, E_0].$$
(2.2.46)

Integrate both sides of this equation over S and get

$$Q + \Gamma Q = -|D|\nabla \times E_0, \qquad (2.2.47)$$

see Section 2.2. Once J is found from solving (2.2.46), Q can be computed by $Q = \int_S J(t)dt$. Then one can validate the values of J and Q by checking the following things

• Is J tangential to S as shown in Section 2.2? One needs to check $J(s) \cdot N_s$.

• Is $Q = \int_S J(t) dt$ correct? The relative error of Q can be computed as follows

$$\operatorname{Error} = \frac{|Q + \Gamma Q - RHS|}{|RHS|}, \qquad (2.2.48)$$

where $RHS := -|D|\nabla \times E_0$. This will give the error of the numerical method for the case of one body.

Furthermore, one can also compare the value of the asymptotic Q_a in formula (2.2.26) with the exact Q_e defined in (2.2.12) by

$$\operatorname{Error} = \frac{|Q_e - Q_a|}{|Q_e|},\tag{2.2.49}$$

and check the difference between the asymptotic E_a in (2.2.17) and the exact E_e defined in (2.2.7) by computing this relative error

Error
$$= \frac{|E_e - E_a|}{|E_e|}.$$
 (2.2.50)

2.2.3 General method for solving EM wave scattering by one perfectly conducting body

In this section, we present a general method for solving the EM wave scattering problem by one perfectly conducting body, whose surface is parametrized by f(u, v) = (x(u, v), y(u, v), z(u, v)).

- Step 1: One needs to partition the surface of the body into P non-intersecting subdomains. In each subdomain, choose a collocation point. The position of the collocation points can be computed using f(u, v) = (x(u, v), y(u, v), z(u, v)), see for example (2.2.28)-(2.2.30).
- Step 2: Find the unit normal vector N of the surface from the function f.
- Step 3: Solve the linear system (2.2.34)-(2.2.36) for X_i, Y_i , and $Z_i, 1 \le i \le P$. Then

vector J in the boundary integral equation (2.2.8) is computed by $J(i) := (X_i, Y_i, Z_i)$ at the point i on the surface.

• Step 4: Compute the electric field E using (2.2.7).

2.3 EM wave scattering by many small perfectly conducting bodies

Consider a bounded domain Ω containing M small bodies D_m , $1 \leq m \leq M$, and S_m are their corresponding smooth boundaries. Let $D := \bigcup_{m=1}^{M} D_m \subset \Omega$ and D' be the complement of D in \mathbb{R}^3 . We assume that $S = \bigcup_{m=1}^{M} S_m$ is C²-smooth. ϵ is the dielectric permittivity constant and μ is the magnetic permeability constant of the medium. Let E and H denote the electric and magnetic fields, respectively. E_0 is the incident field and v is the scattered field. The problem of electromagnetic wave scattering by many small perfectly conducting bodies involves solving the following system

$$\nabla \times E = i\omega\mu H$$
, in $D' := \mathbb{R}^3 \setminus D$, $D := \bigcup_{m=1}^M D_m$, (2.3.1)

$$\nabla \times H = -i\omega\epsilon E, \quad \text{in } D', \tag{2.3.2}$$

$$[N, [E, N]] = 0, \quad \text{on } S, \tag{2.3.3}$$

$$E = E_0 + v, (2.3.4)$$

$$E_0 = \mathcal{E}e^{ik\alpha \cdot x}, \quad \mathcal{E} \cdot \alpha = 0, \quad \alpha \in S^2.$$
(2.3.5)

where v satisfies the radiation condition (2.2.6), $\omega > 0$ is the frequency, $k = 2\pi/\lambda$ is the wave number, $ka \ll 1$, $a := \frac{1}{2} \max_{m} \operatorname{diam} D_{m}$, and α is a unit vector that indicates the direction of the incident wave E_0 . Furthermore,

$$\epsilon = \epsilon_0, \quad \mu = \mu_0 \quad \text{in } \Omega' := \mathbb{R}^3 \setminus \Omega.$$
 (2.3.6)

Assume that the distribution of small bodies D_m , $1 \le m \le M$, in Ω satisfies the following formula

$$\mathcal{N}(\Delta) = \frac{1}{a^3} \int_{\Delta} N(x) dx [1 + o(1)], \quad a \to 0,$$
 (2.3.7)

where $\mathcal{N}(\Delta)$ is the number of small bodies in Δ , Δ is an arbitrary open subset of Ω , and N(x) is the distribution function

$$N(x) \ge 0, \quad N(x) \in C(\Omega). \tag{2.3.8}$$

Note that E solves this equation

$$\nabla \times \nabla \times E = k^2 E, \quad k^2 = \omega^2 \epsilon \mu, \tag{2.3.9}$$

if $\mu = \text{const.}$ Once we have E, then H can be found from this relation

$$H = \frac{\nabla \times E}{i\omega\mu}.$$
 (2.3.10)

From (2.3.10) and (2.3.9), one can get (2.3.2). Thus, we need to find only E which satisfies the boundary condition (2.3.3). It was proved in [50] that under the radiation condition and the assumptions $a \ll d \ll \lambda$, the problem (2.3.1)-(2.3.5) has a unique solution and its solution is of the form

$$E(x) = E_0(x) + \sum_{m=1}^{M} \nabla \times \int_{S_m} g(x, t) J_m(t) dt,$$
 (2.3.11)

where J_m are unknown continuous functions that can be found from the boundary condition. Let

$$Q_m := \int_{S_m} J_m(t) dt. \tag{2.3.12}$$

When $a \to 0$, the asymptotic solution for the electric field is given by

$$E(x) = E_0(x) + \sum_{m=1}^{M} [\nabla g(x, x_m), Q_m], \quad a \to 0.$$
 (2.3.13)

Therefore, instead of finding $J_m(t), \forall t \in S, 1 \leq m \leq M$, to get the solution E, one can just find Q_m . This allows one to solve the EM scattering problem with a very large number of small bodies which is impossible to do before. The analytic formula for Q_m can be derived by using formula (2.2.26) and replacing E_0 in this formula by the effective field $E_e(x_m)$ acting on the m-th body

$$Q_m = -|D_m|(I+\Gamma)^{-1}\nabla \times E_e(x_m), \quad 1 \le m \le M, \quad x_m \in D_m,$$
(2.3.14)

where the effective field acting on the m-th body is defined as

$$E_e(x_m) = E_0(x_m) + \sum_{j \neq m}^{M} [\nabla g(x_m, x_j), Q_j] \quad 1 \le m \le M.$$
(2.3.15)

When $a \to 0$, the effective field $E_e(x)$ is asymptotically equal to the field E(x) in (2.3.13) as proved in [50] and [51].

Let $E_{em} := E_e(x_m)$, where x_m is a point in D_m . From (2.3.14), and (2.3.15), one gets

$$E_{em} = E_{0m} - \sum_{j \neq m}^{M} [\nabla g(x_m, x_j), (I + \Gamma)^{-1} \nabla \times E_{ej}] |D_j|, \quad 1 \le m \le M.$$
(2.3.16)

2.3.1 Numerical method for solving EM wave scattering by many small perfectly conducting bodies

For finding the solution to EM wave scattering in the case of many small perfectly conducting bodies, we need to find E_{em} in (2.3.16). Apply the operator $(I + \Gamma)^{-1} \nabla \times$ to both sides of (2.3.16) and let $A_m := (I + \Gamma)^{-1} \nabla \times E_{em}$. Then

$$A_m = A_{0m} - (I + \Gamma)^{-1} \sum_{j \neq m}^M |D_j| \left(\nabla_x \times [\nabla g(x, x_j), A_j] \right)|_{x = x_m}, \quad 1 \le m \le M, \qquad (2.3.17)$$

Solving this system yields A_m , for $1 \le m \le M$. Then E can be computed by

$$E(x) = E_0(x) + \sum_{m=1}^{M} [\nabla g(x, x_m), Q_m], \qquad (2.3.18)$$

where

$$Q_m = -|D_m|A_m, \quad 1 \le m \le M.$$
(2.3.19)

Equation (2.3.17) can be rewritten as follows

$$A_m = A_{0m} - \sum_{j \neq m}^M \tau [k^2 g(x_m, x_j) A_j + (A_j \cdot \nabla_x) \nabla g(x, x_j)|_{x = x_m}] |D_j|, \qquad (2.3.20)$$

where $1 \le m \le M$, $\tau := (I + \Gamma)^{-1}$, and A_m are vectors in \mathbb{R}^3 .

Let $A_i := (X_i, Y_i, Z_i)$ then one can rewrite the system (2.3.20) as

$$X_{i} + \sum_{j \neq i}^{M} a_{ij} X_{j} + b_{ij} Y_{j} + c_{ij} Z_{j} = F_{x}(i), \qquad (2.3.21)$$

$$Y_i + \sum_{j \neq i}^{M} a'_{ij} X_j + b'_{ij} Y_j + c'_{ij} Z_j = F_y(i), \qquad (2.3.22)$$

$$Z_i + \sum_{j \neq i}^{M} a_{ij}'' X_j + b_{ij}'' Y_j + c_{ij}'' Z_j = F_z(i), \qquad (2.3.23)$$

in which by the subscripts x, y, z the corresponding coordinates are denoted, e.g. $F(i) = (F_x, F_y, F_z)(i)$, where $F(i) := A_{0i}$ and

$$a_{ij} := [k^2 g(i,j) + \partial_x \nabla g(i,j)_x] |D_j| \tau(1,1), \qquad (2.3.24)$$

$$b_{ij} := \partial_y \nabla g(i,j)_x |D_j| \tau(1,1),$$
 (2.3.25)

$$c_{ij} := \partial_z \nabla g(i,j)_x |D_j| \tau(1,1), \qquad (2.3.26)$$

for $i \neq j$, here $\tau(1, 1)$ is the entry (1,1) of matrix τ in (2.3.20); when i = j: $a_{ii} = 1, b_{ii} = 0$, and $c_{ii} = 0$;

$$a'_{ij} := \partial_x \nabla g(i, j)_y |D_j| \tau(2, 2), \qquad (2.3.27)$$

$$b'_{ij} := [k^2 g(i,j) + \partial_y \nabla g(i,j)_y] |D_j| \tau(2,2), \qquad (2.3.28)$$

$$c'_{ij} := \partial_z \nabla g(i,j)_y |D_j| \tau(2,2), \qquad (2.3.29)$$

 $\text{for } i\neq j; \text{ when } i=j; \ a_{ii}^{\prime}=0, b_{ii}^{\prime}=1, \text{ and } c_{ii}^{\prime}=0;$

$$a_{ij}'' := \partial_x \nabla g(i,j)_z |D_j| \tau(3,3), \qquad (2.3.30)$$

$$b_{ij}'' := \partial_y \nabla g(i,j)_z |D_j| \tau(3,3), \tag{2.3.31}$$

$$c_{ij}'' := [k^2 g(i,j) + \partial_z \nabla g(i,j)_z] |D_j| \tau(3,3), \qquad (2.3.32)$$

 $\text{for } i\neq j; \text{ when } i=j; \; a_{ii}^{\prime}=0, b_{ii}^{\prime}=0, \text{ and } c_{ii}^{\prime}=1.$

2.3.2 Error analysis

The error of the solution to the EM wave scattering problem by many small perfectly conducting bodies can be estimated as follows. From the solution E of the electromagnetic scattering problem by many small bodies given in (2.3.11)

$$E(x) = E_0(x) + \sum_{m=1}^{M} \nabla \times \int_{S_m} g(x, t) J_m(t) dt,$$
(2.3.33)

we can rewrite it as

$$E(x) = E_0(x) + \sum_{m=1}^{M} [\nabla g(x, x_m), Q_m] + \sum_{m=1}^{M} \nabla \times \int_{S_m} [g(x, t) - g(x, x_m)] J_m(t) dt. \quad (2.3.34)$$

Comparing this with the asymptotic formula for E when $a \to 0$ given in (2.3.13)

$$E(x) = E_0(x) + \sum_{m=1}^{M} [\nabla g(x, x_m), Q_m], \qquad (2.3.35)$$

we have the error of this asymptotic formula is

$$\operatorname{Error} = \left| \sum_{m=1}^{M} \nabla \times \int_{S_m} [g(x,t) - g(x,x_m)] J_m(t) dt \right| \sim \frac{1}{4\pi} \left(\frac{ak^2}{d} + \frac{ak}{d^2} + \frac{a}{d^3} \right) \sum_{m=1}^{M} |Q_m|,$$
(2.3.36)

where $d = \min_m |x - x_m|$ and

$$Q_m = -|D_m|(I+\Gamma)^{-1}\nabla \times E_e(x_m), \quad 1 \le m \le M, \quad x_m \in D_m, \quad a \to 0,$$
(2.3.37)

because

$$|\nabla[g(x,t) - g(x,x_m)]| = O\left(\frac{ak^2}{d} + \frac{ak}{d^2} + \frac{a}{d^3}\right), \quad a = \max_m |t - x_m|.$$
(2.3.38)

2.4 Experiments

2.4.1 EM wave scattering by one perfectly conducting spherical body

To illustrate the idea of the numerical method, we use the following physical parameters to solve the EM wave scattering problem by one small perfectly conducting sphere, i.e solving the linear system (2.2.34)-(2.2.36)

- Speed of wave, c = (3.0E + 10) cm/sec.
- Frequency, $\omega = (5.0E + 14)$ Hz.
- Wave number, $k = (1.05E + 05) \text{ cm}^{-1}$.
- Wave length, $\lambda = (6.00E 05)$ cm.

- Direction of incident plane wave, $\alpha = (0, 1, 0)$.
- Magnetic permeability, $\mu = 1$.
- Vector $\mathcal{E} = (1, 0, 0)$.
- Incident field vector, E_0 : $E_0(x) = \mathcal{E}e^{ik\alpha \cdot x}$.
- The body is a sphere of radius *a*, centered at the origin.

We use GMRES iterative method, see [26], to solve the linear system (2.2.34)-(2.2.36). For a spherical body, matrix Γ in (2.2.24) can be computed analytically as follows. Recall that

$$\Gamma_{pq}(t) := \int_{S} \frac{\partial g(s,t)}{\partial s_p} N_q(s) ds, \quad 1 \le p, q \le 3,$$
(2.4.1)

where

$$N = (\cos\theta\sin\phi, \sin\theta\sin\phi, \cos\phi) \tag{2.4.2}$$

and

$$\frac{\partial g(s,t)}{\partial s_p} \simeq \frac{\partial g_0(s,t)}{\partial s_p} = -\frac{s_p - t_p}{4\pi |s - t|^3}, \quad g_0(s,t) := \frac{1}{4\pi |s - t|}.$$
 (2.4.3)

We choose a coordinate system centered at the center of the sphere such that t = (0, 0, a)and s = aN. Then

$$\Gamma_{pq}(t) := -\frac{a^2}{4\pi} \int_0^{2\pi} d\theta \int_0^{\pi} d\phi \sin \phi \frac{(s_p - t_p)N_q}{a^{38} \sin^3 \frac{\phi}{2}}, \quad 1 \le p, q \le 3.$$
(2.4.4)

When

$$p = q = 1$$
: $\Gamma_{11}(t) = -1/3,$ (2.4.5)

$$p = q = 2$$
: $\Gamma_{22}(t) = -1/3,$ (2.4.6)

$$p = q = 3: \quad \Gamma_{33}(t) = 1/6,$$
 (2.4.7)

$$p \neq q: \qquad \Gamma_{pq}(t) = 0. \tag{2.4.8}$$

Therefore, matrix Γ is

$$\Gamma \simeq \begin{bmatrix} -1/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 1/6 \end{bmatrix}$$
(2.4.9)

For example, Table 2.1 shows the exact and asymptotic vector Q when the radius of the body is a = (1.0E - 09) cm and the number of collocation points used to solve the integral equation (2.2.27) is P = 766. Note that a = (1.0E - 09) cm satisfies $ka \ll 1$. The point x_1 in (2.2.17) is taken at the center of the body, the origin. Table 2.2 and 2.3 show the exact and asymptotic vector $E = (E_x, E_y, E_z)$, the electric field, at the point x outside of the body, respectively. The distance $|x - x_1|$ is measured in cm in these tables.

Table 2.1: Vector Q_e and Q_a when P = 766 collocation points and a = (1.0E - 09) cm.

P = 760, a = 1.0E - 09				
1.0E-21 *				
Q_e	0.0000 + 0.0000i	0.0000 + 0.0000i	0.0000 + 0.3925i	
Q_a	0.0000 + 0.0000i	0.0000 + 0.0000i	0.0000 + 0.3760i	

Table 2.2: Vector E_e for one perfectly conducting body with a = (1.0E - 09) cm and P = 766 collocation points.

$ x-x_1 $		$E_e(x)$	
1.73E-08	1.0000 + 0.0010i	0.0001 + 0.0000i	0.0004 + 0.0000i
1.73E-07	0.9999 + 0.0105i	0.0000 + 0.0000i	0.0000 + 0.0000i
1.73E-06	0.9945 + 0.1045i	0.0000 + 0.0000i	0.0000 + 0.0000i

Table 2.3: Vector E_a for one perfectly conducting body with a = (1.0E - 09) cm and P = 766 collocation points.

$ x - x_1 $		$E_a(x)$	
1.73E-08	1.0000 + 0.0010i	0.0000 + 0.0000i	0.0000 + 0.0000i
1.73E-07	0.9999 + 0.0105i	0.0000 + 0.0000i	0.0000 + 0.0000i
1.73E-06	0.9945 + 0.1045i	0.0000 + 0.0000i	0.0000 + 0.0000i

In this case, we also verify the following things:

a) Is J tangential to S?

Table 2.4: Relative errors between the asymptotic and exact formulas for E when P = 766 collocation points and a = (1.0E - 09) cm.

$ x - x_1 $	E_e vs E_a
1.73E-08	4.67E-04
1.73E-07	$4.67 \text{E}{-}07$
1.73E-06	4.70E-10

In fact, this vector J is tangential to the surface S of the body, $J \cdot N_s = O(10^{-14})$.

b) How accurate is the asymptotic formula (2.2.26) for Q?

We check the accuracy of the asymptotic formula for Q in (2.2.26) by comparing it with the exact formula (2.2.12), see Section 2.2.2, and the relative error is 4.21E - 02. The more collocation points used, the little this relative error is.

c) How accurate is the asymptotic formula (2.2.17) for E?

The accuracy of the asymptotic formula for E in (2.2.17) can be checked by comparing it with the exact formula (2.2.7) at several points x outside of the body, $|x - x_1| \gg a$ where x_1 is the center of the body, see the error analysis in Section 2.2.2. The relative errors are given in Table 2.4.

Table 2.5: Relative errors of the asymptotic E and Q when P = 1386 collocation points. $P = 1386 |x - x_1| = 1.73E - 05$

$1 = 1500, x - x_1 = 1.15D = 0.5$				
a	1.00E-07	1.00E-08	1.00E-09	1.00E-10
E_e vs E_a	1.08E-06	1.08E-09	1.08E-12	1.12E-15
Q_e vs Q_a	1.96E-02	1.96E-02	1.96E-02	1.89E-02

Table 2.5 compares the asymptotic Q_a versus exact Q_e and asymptotic E_a versus exact E_e , when P = 1386 collocation points, $|x - x_1| = 1.73E - 05$ cm, and with various a. The errors shown in this table are relative errors, see the error analysis in Section 2.2.2. As one can see from this table, the smaller the radius a is, compared to the distance from the point of interest to the center of the body, the more precise the asymptotic formulas of E and Q are.

Furthermore, the numerical results also depend on the number of collocation points used. The more collocation points used, the more accurate the results is.

2.4.2 EM wave scattering by one perfectly conducting ellipsoid body

In this section, we consider the EM wave scattering problem by a small perfectly conducting ellipsoid body. The method for solving the problem in this setting is the same as that of Section 2.2.1 except that one needs to recompute the unit normal vector N.

To get the solution of this problem, one can follow the steps in Section 2.2.1. In particular, one needs to solve the linear system (2.2.34)-(2.2.36).

To illustrate the idea, we use the same physical parameters as described in Section 2.4.1, except that the body now is an ellipsoid. Let S be its smooth surface. The way we partition S into many subdomains S_{ij} is the same as the way we partition a spherical body as described in section 2.2.1. Then, the position of the collocation point in each subdomain S_{ij} is defined by

$$(x, y, z)_{ij} = (a\cos\theta_i\sin\phi_j, b\sin\theta_i\sin\phi_j, c\cos\phi_j), \qquad (2.4.10)$$

where a, b, and c are the lengths of the semi-principal axes of the ellipsoid. The outwardpointing normal vector n to S at this point is

$$n_{ij} = n(\theta_i, \phi_j) = 2\left(\frac{\cos\theta_i \sin\phi_j}{a}, \frac{\sin\theta_i \sin\phi_j}{b}, \frac{\cos\phi_j}{c}\right), \qquad (2.4.11)$$

and the corresponding unit normal vector N is

$$N_{ij} = N(\theta_i, \phi_j) = n_{ij} / |n_{ij}|.$$
(2.4.12)

Table 2.6: Vector E_e for one perfectly conducting ellipsoid body with a = (1.0E - 08) cm, b = (1.0E - 09) cm, c = (1.0E - 09) cm, and P = 1052 collocation points.

$ x - x_1 $		$E_e(x)$	
1.01E-07	0.9998 + 0.0010i	-0.0000 + 0.0000i	-0.0000 - 0.0000i
1.01E-06	0.9999 + 0.0105i	-0.0000 + 0.0000i	-0.0000 - 0.0000i
1.01E-05	0.9945 + 0.1045i	-0.0000 + 0.0000i	-0.0000 - 0.0000i

$ x - x_1 $		$E_a(x)$	
1.01E-07	1.0000 + 0.0010i	-0.0000 + 0.0000i	0.0000 - 0.0000i
1.01E-06	0.9999 + 0.0105i	-0.0000 + 0.0000i	0.0000 - 0.0000i
1.01E-05	0.9945 + 0.1045i	-0.0000 + 0.0000i	0.0000 - 0.0000i

Table 2.7: Vector E_a for one perfectly conducting ellipsoid body with a = (1.0E - 08) cm, b = (1.0E - 09) cm, c = (1.0E - 09) cm, and P = 1052 collocation points.

For example, Tables 2.6 and 2.7 show the exact and asymptotic vector $E = (E_x, E_y, E_z)$, the electric field, got from solving this EM wave scattering problem with one perfectly conducting ellipsoid body, when the semi-principle axes of the body are a = (1.0E - 08) cm, b = (1.0E - 09) cm, c = (1.0E - 09) cm, and the number of collocation points is P = 1052. Note that a, b, and c satisfy $k \max(a, b, c) \ll 1$. The point x_1 in (2.2.17) is taken at the center of the ellipsoid body. Each row in Tables 2.6 and 2.7 shows the exact and asymptotic $E = (E_x, E_y, E_z)$, respectively, at the point x outside of the body. The distance $|x - x_1|$ is measured in cm in these tables.

As for the case of one body, we need to verify the following things:

a) Is J tangential to S?

In fact, this vector J is tangential to the surface S of the body, $J \cdot N_s = O(10^{-13})$.

b) Are Q and J correct? We check the relative error described in Section 2.2.2, Error = $\frac{|Q+\Gamma Q-RHS|}{|RHS|} = 14\%$. The more collocation points used, the smaller this error is, for example, with P = 1762 collocation points, this error is only 3.6%.

c) How accurate is the asymptotic formula (2.2.17) for E?

The accuracy of the asymptotic formula for E in (2.2.17) can be checked by comparing it with the exact formula (2.2.7) at several points x outside of the body, $|x - x_1| \gg \max(a, b, c)$ where x_1 is the center of the body. The relative errors are given in Table 2.8.

Table 2.9 shows the relative errors between the asymptotic E versus exact E, when P = 1052 collocation points, $|x - x_1| = 1.73E - 07$ cm, and with various semi-principle axes a, b, and c. As one can see from this table, the smaller the semi-principle axes are, compared to the distance from the point of interest to the center of the body, the more accurate the asymptotic formulas of E is.

Table 2.8: Relative errors between the asymptotic and exact formulas for E when P = 1052 collocation points, a = (1.0E - 08) cm, b = (1.0E - 09) cm, and c = (1.0E - 09) cm.

$ x - x_1 $	E_e vs E_a
1.01E-07 1.01E-06	1.73E-04 1.73E-07
1.01E-05	1.73E-10

Table 2.9: Relative errors of the asymptotic E when P = 1052 collocation points.

	P = 1052,	$ x - x_1 = 1$	1.73E - 07	
a	1.00E-07	1.00E-08	1.00E-09	1.00E-10
b	1.00E-08	1.00E-09	1.00E-10	1.00E-11
c	1.00E-08	1.00E-09	1.00E-10	1.00E-11
E_e vs E_a	2.65 E-02	2.76E-05	2.76E-08	2.76E-11

2.4.3 EM wave scattering by one perfectly conducting cubic body

In this section, we consider the EM wave scattering problem by a small perfectly conducting cubic body. Again, the method for solving the problem in this setting is the same as that of Section 2.2.1 except that one needs to recompute the unit normal vector N.

One can follow the steps outlined in Section 2.2.1 to solve this problem. That means, one needs to solve the linear system (2.2.34)-(2.2.36).

For illustration purpose, we use the same physical parameters as described in Section 2.4.1, except that the body now is a cube. Suppose the cube is placed in the first octant where the origin is one of its vertices, one can use the standard unit vectors in \mathbb{R}^3 as the unit normal vectors to the surfaces of the cube.

Table 2.10: Vector E_e for one perfectly conducting body with a = (1.0E - 07) cm and M = 600 collocation points.

$ x - x_1 $		$E_e(x)$	
1.73E-04	-0.5000 - 0.8660i	-0.0000 + 0.0000i	-0.0000 + 0.0000i
1.73E-05	0.5000 + 0.8660i	0.0000 + 0.0000i	0.0000 + 0.0000i
1.73E-06	0.9945 + 0.1045i	0.0006 + 0.0000i	0.0006 + 0.0000i

For example, Tables 2.10 and 2.11 show the exact and asymptotic vector $E = (E_x, E_y, E_z)$, the electric field, got from solving this EM wave scattering problem with one perfectly con-

$ x - x_1 $	$E_a(x)$				
1.73E-04	-0.5000 - 0.8660i	0.0000 - 0.0000i	0.0000 + 0.0000i		
1.73E-05	0.5000 + 0.8660i	-0.0000 + 0.0000i	-0.0000 - 0.0000i		
1.73E-06	0.9945 + 0.1045i	-0.0000 + 0.0000i	-0.0000 - 0.0000i		

Table 2.11: Vector E_a for one perfectly conducting body with a = (1.0E - 07) cm and M = 600 collocation points.

ducting cubic body, when the half side of the body is a = (1.0E - 07) cm and the number of collocation points is M = 600. Note that a = 1.0E - 07 cm satisfies $ka \ll 1$. The point x_1 in (2.2.17) is taken at the center of the cubic body. Each row in Tables 2.10 and 2.11 shows the exact and asymptotic $E = (E_x, E_y, E_z)$, respectively, at the point x outside of the body. The distance $|x - x_1|$ is measured in cm in these tables.

As before, for the case of one body, we need to verify the following things:

a) Is J tangential to S?

In fact, this vector J is tangential to the surface S of the body, $J \cdot N_s = O(10^{-13})$.

b) How accurate is the asymptotic formula (2.2.26) for Q?

We check the relative error described in Section 2.2.2, Error = $\frac{|Q+\Gamma Q-RHS|}{|RHS|} = 1.13\%$.

c) How accurate is the asymptotic formula (2.2.17) for E?

The accuracy of the asymptotic formula for E in (2.2.17) can be checked by comparing it with the exact formula (2.2.7) at several points x outside of the body, $|x - x_1| \gg a$ where x_1 is the center of the body. The relative errors are given in Table 2.12.

Table 2.12: Relative errors between the asymptotic and exact formulas for E when M = 600 collocation points and a = (1.0E - 07) cm.

E_e vs E_a
1.19E-08
1.19E-07
1.52E-06
8.64E-04

Table 2.13 shows the relative errors between the asymptotic E versus exact E, when M = 600 collocation points, $|x - x_1| = (1.73E - 06)$ cm, and with various a. From this table, we can see that the smaller the side of the cube is, compared to the distance from the

 M = 600, $|x - x_1| = 1.73E - 06$
 $M = 600, |x - x_1| = 1.73E - 06$
 $E_e \text{ vs } E_a$

 8.64E-04
 6.49E-07

 6.32E-10

point of interest to the center of the body, the more accurate the asymptotic formula of E is.

2.4.4 EM wave scattering by many small perfectly conducting bodies

To illustrate the idea, consider a domain Ω as a unit cube placed in the first octant such that the origin is one of its vertices. This domain Ω contains M small bodies. Suppose these small bodies are particles. We use GMRES iterative method, see [26], to solve the linear system (2.3.21)-(2.3.23). The following physical parameters are used to solve the EM wave scattering problem

- Speed of wave, c = (3.0E + 10) cm/sec.
- Frequency, $\omega = (5.0E + 14)$ Hz.
- Wave number, $k = (1.05E + 05) \text{ cm}^{-1}$.
- Wave length, $\lambda = (6.00E 05)$ cm.
- Direction of incident plane wave, $\alpha = (0, 1, 0)$.
- Magnetic permeability, $\mu = 1$.
- Volume of the domain Ω that contains all the particles, $|\Omega| = 1 \text{ cm}^3$.
- The distance between two neighboring particles, d = (1.00E 07) cm.
- Vector $\mathcal{E} = (1, 0, 0)$.
- Vector A_0 : $A_{0m} := (I + \Gamma)^{-1} \nabla \times E_0(x)|_{x=x_m} = (I + \Gamma)^{-1} \nabla \times \mathcal{E}e^{ik\alpha \cdot x}|_{x=x_m}$.

Note that the distance d satisfies the assumption $d \ll \lambda$. The radius a of the particles is chosen variously so that it satisfies the assumption $ka \ll 1$. For illustration purpose, the problem of EM wave scattering by many small perfectly conducting bodies is solved with M = 27 and 1000 particles.

	1 / (/
M = 2	7, $d = 1.0E - 07$, $a = 1$.	0E - 09
1.00E+00+1.01E-14i	5.69E-17-1.01E-14i	0.00E+00+0.00E+00i
1.00E + 00 + 1.19E - 14i	0.00E + 00 + 0.00E + 00i	0.00E + 00 + 0.00E + 00i
1.00E + 00 + 1.01E - 14i	-5.69E-17+1.01E-14i	0.00E+00+0.00E+00i
1.00E + 00 + 1.05E - 02i	1.24E-16-1.19E-14i	-1.36E-29-5.20E-36i
1.00E + 00 + 1.05E - 02i	0.00E + 00 + 0.00E + 00i	-4.80E-30-5.20E-36i
1.00E + 00 + 1.05E - 02i	-1.24E-16+1.19E-14i	-1.22E-30-5.20E-36i
1.00E + 00 + 2.09E - 02i	1.54E-16-1.01E-14i	-3.40E-30-1.04E-35i
1.00E + 00 + 2.09E - 02i	0.00E + 00 + 0.00E + 00i	-2.43E-30-1.04E-35i
1.00E + 00 + 2.09E - 02i	-1.54E-16+1.01E-14i	-1.20E-30-1.04E-35i
1.00E + 00 + 1.19E - 14i	6.63E-17-1.19E-14i	0.00E + 00 + 0.00E + 00i
1.00E + 00 + 1.40E - 14i	4.80E-30+0.00E+00i	0.00E + 00 + 0.00E + 00i
1.00E+00+1.19E-14i	-6.63E-17+1.19E-14i	0.00E + 00 + 0.00E + 00i
1.00E + 00 + 1.05E - 02i	1.47E-16-1.40E-14i	-4.80E-30-5.20E-36i
1.00E + 00 + 1.05E - 02i	2.61E-30+0.00E+00i	-2.61E-30-5.20E-36i
1.00E + 00 + 1.05E - 02i	-1.47E-16+1.40E-14i	-9.24E-31-5.20E-36i
1.00E + 00 + 2.09E - 02i	1.82E-16-1.19E-14i	-2.43E-30-1.04E-35i
1.00E+00+2.09E-02i	9.24E-31+0.00E+00i	-1.85E-30-1.04E-35i
1.00E+00+2.09E-02i	-1.82E-16+1.19E-14i	-1.01E-30-1.04E-35i
1.00E+00+1.01E-14i	5.69E-17-1.01E-14i	0.00E + 00 + 0.00E + 00i
1.00E+00+1.19E-14i	2.43E-30+0.00E+00i	0.00E + 00 + 0.00E + 00i
1.00E+00+1.01E-14i	-5.69E-17+1.01E-14i	0.00E + 00 + 0.00E + 00i
1.00E+00+1.05E-02i	1.24E-16-1.19E-14i	-1.22E-30-5.20E-36i
1.00E+00+1.05E-02i	1.85E-30+0.00E+00i	-9.24E-31-5.20E-36i
1.00E + 00 + 1.05E - 02i	-1.24E-16+1.19E-14i	-5.03E-31-5.20E-36i
1.00E + 00 + 2.09E - 02i	1.54E-16-1.01E-14i	-1.20E-30-1.04E-35i
1.00E+00+2.09E-02i	9.98E-31+0.00E+00i	-1.01E-30-1.04E-35i
1.00E + 00 + 2.09E - 02i	-1.54E-16+1.01E-14i	-6.54E-31-1.04E-35i

Table 2.14: Vector E when M = 27 particles, d = (1.0E - 07) cm and a = (1.0E - 09) cm.

For example, Tables 2.14 show the result of solving the EM wave scattering problem with M = 27 particles in the unit cube in which the distance between neighboring particles is d = (1.0E - 07) cm and the radius of the particles is a = (1.0E - 09) cm. Each row in Tables 2.14 is a vector $E(i) = (E_x, E_y, E_z)(i)$ at the point *i* in the cube. The norm of this asymptotic solution E is 5.20E + 00 and the error of the solution is 8.16E - 10. This error is computed using (2.3.36).

Table 2.15 shows the relative errors of E when there are M = 27 particles in the cube, the distance between neighboring particles is d = (1.0E - 07) cm, and with various radius a. Figure 2.1 shows the relative error of the asymptotic E. From this figure, one can see that when the ratio a/d decreases from 1.0E - 01 to 1.0E - 04, the error of the asymptotic solution decreases linearly and rapidly from 8.16E - 06 to about 8.16E - 18. The smaller the ratio a/d is, the better the asymptotic formula (2.3.13) approximates E.

Table 2.15: Error of the asymptotic solution E when M = 27 and d = (1.0E - 07) cm.

M=27, d=1.0E-07							
a	1.00E-08	1.00E-09	1.00E-10	1.00E-11			
a/d	1.00E-01	1.00E-02	1.00E-03	1.00E-04			
Norm of E	5.20E + 00	5.20E + 00	5.20E + 00	5.20E + 00			
Error of E	8.16E-06	8.16E-10	8.16E-14	8.16E-18			



Figure 2.1: Error of the asymptotic solution E when M = 27 and d = (1.0E - 07) cm.

Table 2.16 and Figure 2.2 show the results of solving the problem with M = 1000 particles, when the distance between neighboring particles is d = (1.0E - 07) cm, and with different radius a. From these table and figure, one can see that the relative error of the asymptotic solution in this case is also very small, less than 3.02E - 04, when the ratio a/d < 1.0E - 01. In this case, the error of the asymptotic E is greater than that of the



Table 2.16: Error of the asymptotic solution E when M = 1000 and d = (1.0E - 07) cm.

Figure 2.2: Error of the asymptotic solution E when M = 1000 and d = (1.0E - 07) cm.

previous case when M = 27. However, this time, the error is also decreasing quickly and linearly when the ratio a/d decreases from 1.0E - 01 to 1.0E - 04. Therefore, the asymptotic formula (2.3.13) for the solution E is applicable when $a \ll d$.

2.5 Conclusions

In this paper, we present a numerical method for solving the EM wave scattering by one and many small perfectly conducting bodies. One of the advantages of this method is that it is relatively easy to implement. Furthermore, one can get an asymptotically exact solution to the problem when the characteristic size of the bodies tends to zero. To illustrate the applicability and efficiency of the method, we use it to solve the EM wave scattering problem by one and many small perfectly conducting bodies. Numerical results of these experiments are presented and error analysis of the asymptotic solutions for the case of one and many bodies are also discussed. For the case of one small body, one can always find the exact solution using the described method. For the case of many small bodies, the accuracy of our method is high if $a \ll d \ll \lambda$.

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