A fast, direct algorithm for the Lippmann-Schwinger integral equation in two dimensions

Yu Chen
Courant Institute of Mathematical Sciences, New York University

Feb, 2001

Abstract. State-of-the-art, large-scale numerical simulations of the scattering problem for the Helmholtz equation in two dimensions rely on iterative solvers for the Lippmann-Schwinger integral equation, with an optimal CPU time $O(m^3 \log(m))$ for an m-by-m wavelength problem. We present a method to solve the same problem directly, as opposed to iteratively, with the obvious advantage in efficiency for multiple right hand sides corresponding to distinct incident waves. Analytically, this direct method is a hierarchical, recursive scheme consisting of the so-called splitting and merging processes. Algebraically, it amounts to a recursive matrix decomposition, for a cost of $O(m^3)$, of the discretized Lippmann–Schwinger operator. With this matrix decomposition, each back substitution requires only $O(m^2 \log(m))$; therefore, a scattering problem with m incident waves can be solved, altogether, in $O(m^3 \log(m))$ flops.

1 Introduction

The subject of this paper is the rapid numerical solution of the scattering problem for the Helmholtz equation. Existing fast algorithms [1] – [6] for the scattering problem are iterative in nature. Like all iterative methods, they are inefficient in solving problems with multiple right hand sides, each corresponding to an individual incident wave. We will develop in this article a direct method for the Helmholtz equation in two dimensions which will be $O(m)$ times faster than the iterative solvers for an m-by-m wavelength problem with $O(m)$ incident waves.

This fast, direct method solves the Lippmann-Schwinger integral equation by dividing the entire computational domain into sufficiently small, non-overlapping subdomains, referred to as the bottom-level subdomains. The scattering problem for each subdomain on the bottom level is first solved separately, with no regard to multiple scatterings among the subdomains. Then the multiple scattering interactions among the subdomains are taken into account by merging, recursively, the subdomains in a hierarchical manner: two subdomains on a hierarchical level are merged to form a solution of scattering problem on a bigger, parent subdomain, which is the union of the two child subdomains, and which lives on a hierarchy one level higher than that of the children. In fact, the algorithm constructs scattering matrices for the bottom-level

subdomains, and then merge them recursively to obtain the scattering matrices for the parents in higher levels, all in $O(m^3)$ steps.

The paper is organized as follows. The scattering matrix is introduced in Section 2. The merging process of scattering matrices of non-overlapping scatterers is developed in Section 3. Finally, in Section 4, we present a fast algorithm for the Lippmann-Schwinger integral equation.

Remark 1.1 *There are two basic versions of the fast algorithm: (i) Divide the scatterer into the bottom-level subdomains, each of which is still undiscretized. Then calculate and merge the scattering matrices, discretizing when necessary (ii) Discretize the Lippmann-Schwinger equation first and then regroup the discrete mesh points into "subdomains" for which a set of merging rules are required for the "scattering matrices" associated with these discrete "subdomains". In this paper, we present the first version without giving details about its discretization. The second version has been implemented and a Fortran program is available; the details will be presented in a separate paper.*

2 The Scattering matrix

The scattering matrix is a convenient tool to specify the complete scattering behavior of a scatterer. It is essential to describing, analyzing the multiple scattering process, and in the efficient numerical solution of the Lippmann-Schwinger equation

$$\sigma(x) + k^2 q(x) \int_D G(x,\xi)\sigma(\xi)d\xi = -k^2 q(x)\phi(x) \tag{1}$$

Here $G = -(i/4)H_0(k|x-\xi|)$ is the Green's function; q is a continuous function compactly supported in D representing the scatterer; ϕ is an incident field from sources outside D; σ is the charge density induced by ϕ which gives rise to the scattered field

$$\psi(x) = \int_D G(x,\xi)\sigma(\xi)d\xi. \tag{2}$$

According to Green's formula, ϕ is uniquely determined in D by the Green's data: the value of ϕ and its normal derivative on the boundary ∂D,

$$\phi(x) = \int_{\partial D} \left(\frac{\partial \phi(\xi)}{\partial n} G(x,\xi) - \phi(\xi) \frac{\partial G(x,\xi)}{\partial n(\xi)} \right) ds(\xi), \quad x \in D. \tag{3}$$

Furthermore, the corresponding scattered field ψ is uniquely determined by the incident field; in particular, the Green's data of ψ on the boundary ∂D are uniquely determined by the Green's data of ϕ. Finally, ψ outside D is in turn uniquely determined by its Green's data on the boundary,

$$\psi(x) = -\int_{\partial D} \left(\frac{\partial \psi(\xi)}{\partial n} G(x,\xi) - \psi(\xi) \frac{\partial G(x,\xi)}{\partial n(\xi)} \right) ds(\xi), \quad x \in R^2 \setminus D. \tag{4}$$

Therefore, letting $W(\partial D) = C(\partial D) \times C(\partial D)$, there is a linear operator - the scattering matrix $S : W(\partial D) \mapsto W(\partial D)$, defined by the formula

$$\left(\psi, \frac{\partial \psi}{\partial n}\right) = S\left(\phi, \frac{\partial \phi}{\partial n}\right). \tag{5}$$

The remainder of this section is devoted to the calculation of the scattering matrix via the solutions of the Lippmann-Schwinger equation (1), and the following three linear operators will be required.

(I) Let $G^{(v,b)} : W(\partial D) \mapsto C^{\infty}(D)$ be defined by

$$\phi(x) = G^{(v,b)}(u, v) =: \int_{\partial D} \left(v(\xi) G(x, \xi) - u(\xi) \frac{\partial G(x, \xi)}{\partial n(\xi)} \right) ds(\xi), \tag{6}$$

which is to be used as the interior Green's formula, mapping from boundary to volume.

(II) Let $P : C(D) \mapsto C(D)$ be defined by

$$P(\sigma)(x) = \sigma(x) + k^2 q(x) \int_D G(x, \xi) \sigma(\xi) d\xi \tag{7}$$

so that (1) can be rewritten

$$P(\sigma) = -k^2 q \phi. \tag{8}$$

(III) $G^{(b,v)} : L_2(D) \mapsto W(\partial D)$ is defined by

$$\left(\psi(x), \frac{\partial \psi(x)}{\partial n}\right) = G^{(b,v)}(\sigma)(x) =: \int_D \left(G(x, \xi), \frac{\partial G(x, \xi)}{\partial n(x)} \right) \sigma(\xi) d\xi, \tag{9}$$

mapping the charge density σ in D to the boundary data of the scattered field $\psi(x)$ generated by the charges.

Lemma 2.1 *The scattering matrix S corresponding to the scatterer q in D can be obtained by the solution of (8),*

$$S = -k^2 G^{(b,v)} \cdot P^{-1} \cdot q \cdot G^{(v,b)}. \tag{10}$$

3 Multiple scattering

Multiple scattering among non-overlapping scatterers is essential to forward and inverse problems. In this section, we present such a theory in terms of the scattering matrices which will lead to an efficient algorithm for the solution of the forward scattering problem. A similar analysis was first presented in [7] for the numerical solution of the Laplace equation; here we follow that line and extend it to the more natural environment for the use of scattering matrix – the scattering problem.

3.1 Analytical machinery

In this subsection, we develop necessary analytical tools for a systematic treatment of the multiple scattering process. Suppose that there are altogether m non-overlapping scatterers D_i enclosed in a bounded domain D. Suppose further that these domains have piecewise smooth boundaries ∂D_i and ∂D. Denote by $S : W(\partial D) \mapsto W(\partial D)$ the scattering matrix of the scatterer D, and by $S_i : W(\partial D_i) \mapsto W(\partial D_i)$ the scattering matrix of the scatterer D_i. Let ϕ be an arbitrary incident field on D.

The scattering matrix S can be obtained via (10). This procedure is efficient only when D is small since the direct inversion of P on a large domain D is expensive: $O(m^6)$ for an m-by-m wavelength problem. On the other hand, if we restrict (6), (7), and (9) to a sub-domain of D and define $G_i^{(v,b)} : W(\partial D_i) \mapsto C^\infty(D_i)$, $P_i : L_2(D_i) \mapsto L_2(D_i)$, and $G_i^{(b,v)} : L_2(D_i) \mapsto W(\partial D_i)$ via the formulae

$$G_i^{(v,b)}(u,v)(x) = \int_{\partial D_i} \left(v(\xi) G(x,\xi) - u(\xi) \frac{\partial G(x,\xi)}{\partial n(\xi)} \right) ds(\xi), \tag{11}$$

$$P_i(\sigma)(x) = \sigma(x) + k^2 q(x) \int_{D_i} G(x,\xi)\sigma(\xi) d\xi, \tag{12}$$

$$G_i^{(b,v)}(\sigma)(x) = \int_{D_i} \left(G(x,\xi), \frac{\partial G(x,\xi)}{\partial n(x)} \right) \sigma(\xi) d\xi, \tag{13}$$

we may first solve the sub-problems

$$P_i(\sigma) = -k^2 q \phi, \tag{14}$$

in each sub-domain D_i and obtain the scattering matrices S_i

$$S_i = -k^2 G_i^{(b,v)} \cdot P_i^{-1} \cdot q \cdot G_i^{(v,b)}. \tag{15}$$

We then merge the scattering matrices S_i in order to calculate S, and finally obtain P^{-1} in the form of a matrix decomposition. To this end, we will further require the three operators

Restriction $R_i : W(\partial D) \mapsto W(\partial D_i)$, to map the Green's data of an incident field ϕ on ∂D to the Green's data on ∂D_i

Extension $E_i : W(\partial D_i) \mapsto W(\partial D)$, to map the Green's data on ∂D_i of a scattered field ψ from D_i to its Green's data on ∂D

Translation $T_{ji} : W(\partial D_i) \mapsto W(\partial D_j)$, $i \neq j$, same as E_i except that it maps to ∂D_j

defined by the formulae

$$R_i(u,v)(x) = \int_{\partial D} \left[v(\xi) \left(G, \frac{\partial G}{\partial n_x} \right) - u(\xi) \left(\frac{\partial G(x,\xi)}{\partial n_\xi}, \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi} \right) \right] ds(\xi) \tag{16}$$

$$E_i(u,v)(x) = -\int_{\partial D_i} \left[v(\xi) \left(G, \frac{\partial G}{\partial n_x} \right) - u(\xi) \left(\frac{\partial G(x,\xi)}{\partial n_\xi}, \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi} \right) \right] ds(\xi) \tag{17}$$

$$T_{ji}(u,v)(x) = -\int_{\partial D_i} \left[v(\xi) \left(G, \frac{\partial G}{\partial n_x} \right) - u(\xi) \left(\frac{\partial G(x,\xi)}{\partial n_\xi}, \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi} \right) \right] ds(\xi) \tag{18}$$

Definition 3.1 *A function u is said to be a radiation field in a bounded, open domain Ω if ϕ is a solution of the homogeneous Helmholtz equation $\Delta u + k^2 u = 0$ inside Ω; u is said to be a radiation field outside Ω if ϕ is a solution of the homogeneous Helmholtz equation in $\mathbb{R}^2 \setminus \bar{\Omega}$, subject to the Sommerfeld radiation condition.*

Definition 3.2 *A radiation field $\phi_i \in C^\infty(D_i)$ is referred to as the total incident field upon the scatterer D_i if*

$$P_i(\sigma|_{D_i})(x) = -k^2 q(x)\phi_i(x). \tag{19}$$

Therefore, an efficient method for calculating the total incident field ϕ_i will reduce the solution of the Lippmann-Schwinger equation in a larger domain to its smaller subdomains where the equation can be solved independently and thus more efficiently for the charge density σ restricted in each of the subdomains.

3.2 Multiple scattering in non-overlapping scatterers

We first examine the case of two non-overlapping scatterers; the Lippmann-Schwinger equation (8) can be reformulated as

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix} = \begin{bmatrix} -k^2 q_1 \phi_{01} \\ -k^2 q_2 \phi_{02} \end{bmatrix}, \tag{20}$$

with $\sigma_i = \sigma|_{D_i}$, $q_i = q|_{D_i}$, $\phi_{0i} = \phi|_{D_i}$, $P_{ii} = P_i$, $P_{ji} : L_2(D_i) \mapsto L_2(D_j)$ defined via

$$P_{ji}(\sigma)(x) = k^2 q_j(x) \int_{D_i} G(x,\xi)\sigma(\xi)d\xi. \tag{21}$$

It follows from (2) that

$$\psi_{ji}(x) = \int_{D_i} G(x,\xi)\sigma(\xi)d\xi, \ x \in D_j \tag{22}$$

is the radiation field in D_j produced by the total charges $\sigma_i = \sigma|_{D_i}$ in D_i; on the other hand it follows from Definition 3.2 that ψ_{ji} is the scattered field from D_i corresponding to the total incident field ϕ_i which induced the charge density σ. We therefore conclude, as expected, that

Lemma 3.3 *Suppose that the two non-overlapping scatterers D_1 and D_2 are subjected to the incident field ϕ. Then because of multiple scattering, the total incident field ϕ_j upon D_j is the superposition of the original incident field ϕ and the scattered field ψ_{ji} from the other scatterer D_i, that is,*

$$\phi_j = \phi + \psi_{ji}. \tag{23}$$

Proof. It follows from the first equation of (20) that

$$P_1(\sigma|_{D_1})(x) = -k^2 q(x)(\phi(x) + \psi_{12}(x)). \tag{24}$$

For $j = 1$, (23) follows immediately from Definition 3.2. □

Corollary 3.4 *Generalizing the lemma to the case of m scatterers D_j, we obtain that the total incident field upon D_i is the superposition of the original incident field ϕ and all the scattered fields ψ_{ij} from the other scatterers D_j,*

$$\phi_i = \phi + \sum_{j \neq i} \psi_{ji}. \tag{25}$$

Corollary 3.5 *The total scattered field (2) induced by ϕ incident upon D is the superposition of all the scattered fields ψ_i induced by ϕ_i incident upon D_i; namely,*

$$\psi(x) = \sum_{i=1}^{m} \psi_i(x), \quad x \in \mathbb{R}^2. \tag{26}$$

3.3 Splitting the incident field

Assume as we did in Section 3.1 that there are m non-overlapping scatterers D_i inside a bounded domain D, and that ϕ is the (total) incident field on D, ϕ_i is the total incident field on D_i, $i = 1, 2, \ldots m$. The procedure of determining ϕ_i from ϕ is said to be *splitting*. This operation is essential for the treatment of multiple scattering, for fast algorithms for the Lippmann-Schwinger equation or an elliptic partial differential equations formulated as integral equations via classical potential theory.

For the original incident field ϕ on D and the corresponding scattered field ψ from D, and for the total incident field ϕ_i upon D_i and the corresponding scattered field ψ_i from D_i, we denote their respective Green's data on the boundaries ∂D or ∂D_i by

$$\Phi = \left(\phi, \frac{\partial \phi}{\partial n}\right)_{\partial D}, \tag{27}$$

$$\Psi = \left(\psi, \frac{\partial \psi}{\partial n}\right)_{\partial D_i}. \tag{28}$$

$$\Phi_i = \left(\phi_i, \frac{\partial \phi_i}{\partial n}\right)_{\partial D_i}, \tag{29}$$

$$\Psi_i = \left(\psi_i, \frac{\partial \psi_i}{\partial n}\right)_{\partial D_i}. \tag{30}$$

Restricted on ∂D_i, (25) can be reformulated as

$$\Phi_i = R_i \Phi + \sum_{j \neq i} T_{ij} \Psi_j. \tag{31}$$

By the definition of the scattering matrix,

$$\Psi_i = S_i \Phi_i; \tag{32}$$

therefore,

$$\Phi_i = R_i \Phi + \sum_{j \neq i} T_{ij} S_j \Phi_j. \tag{33}$$

Definition 3.6 *The operator*

$$S_p : C(\partial D) \mapsto \begin{bmatrix} C(\partial D_1) \\ C(\partial D_2) \\ \vdots \\ C(\partial D_m) \end{bmatrix} \tag{34}$$

defined by the formula

$$S_p = \begin{bmatrix} I & -T_{12}S_2 & \cdots & -T_{1m}S_m \\ -T_{21}S_1 & I & \cdots & -T_{2m}S_m \\ \vdots & \vdots & \cdots & \vdots \\ -T_{m1}S_1 & -T_{m2}S_2 & \cdots & I \end{bmatrix}^{-1} \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{bmatrix} \tag{35}$$

will be referred to as the splitting matrix, provided that the inverse exists.

Using (33) and this definition we immediately conclude:

Theorem 3.7 *(***Splitting the incident field***) Suppose that Φ is the Green's data of the incident field ϕ upon D, and that Φ_i is the Green's data of the total incident field ϕ_i upon the non-overlapping sub-domain D_i. Then*

$$\begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_m \end{bmatrix} = S_p \cdot \Phi. \tag{36}$$

3.4 Merging scattering matrices

We now present the scheme for merging non-overlapping scatterers; namely, how to calculate the scattering matrix S of D given the scattering matrices S_i of its non-overlapping parts D_i.

Theorem 3.8 *(***Merging scattering matrices***) Given the scattering matrices S_i for the scatterers D_i, the scattering matrix S for D can be calculated via the formula*

$$S = [E_1S_1 \;\; E_2S_2 \;\; \cdots \;\; E_mS_m] \cdot S_p. \tag{37}$$

Proof. It follows from (26), (32) and Theorem 3.7 that

$$\Psi = \sum_{i=1}^{m} E_iS_i\Phi_i = \sum_{i=1}^{m} E_iS_i(S_p\Phi)_i = ([E_1S_1 \;\; E_2S_2 \;\; \cdots \;\; E_mS_m] \cdot S_p)\,\Phi, \tag{38}$$

for an arbitrary incident field Φ. The theorem follows immediately from (5). □

4 A fast algorithm for the Lippmann-Schwinger equation

In this section, we present a fast, direct algorithm for the scattering problem by making a number of remarks on the merging and splitting schemes, as specified by Theorems 3.7 and 3.8. We will also comment on the implementation of the schemes and on the complexity analysis of the algorithm.

4.1 Merging and splitting on a hierarchy

Definition 4.1 *The domain D will be referred to as the parent of the non-overlapping sub-domains D_i whereas the domains D_i will be referred to as the children of D.*

Remark 4.2 *Once the total incident field ϕ_i is obtained for a child D_i, the scattering problem defined by the Lippmann-Schwinger equation (1) in the parent D can be solved independently in the children D_i to obtain $\sigma|_{D_i}$, see (19). And the parent solution is obviously given by the formula*

$$\sigma = \sum_i \sigma|_{D_i}. \tag{39}$$

Remark 4.3 *The merging operation on the scattering matrices goes upwards from the children to the parent, whereas the splitting operation on the incident field goes downwards from the parent to the children.*

It turns out (see Remark 4.8) that it is more efficient to executed the merging and splitting operations in a recursive manner moving up and down in a hierarchy of levels of sub-domains. A simple example for such a hierarchy is when the original domain D is a square - that is the level 0. The first level has 4 squares of the same size, the second level has 4^2 squares, and so on, so that a square on any level except level 0 is one of the four children of a parent, whereas a square on any level except the bottom level is a parent of four children.

In the following we assume that for a fixed wave number k the cost of solving the Lippmann-Schwinger equation (1) in D with a straightforward method such as Gaussian elimination is proportional to the cubic of the area of D (more precisely, the cubic of the number of mesh points in D).

Remark 4.4 *Since the solution of the scattering problem in a smaller domain is much faster than in a larger one, a fast direct solver (as opposed to an iterative approach) can be constructed by (i) Dividing D into a collection of sufficiently small non-overlapping sub-domains $\{B_j\}$ on the bottom level (ii) Evaluating the total incident field to each B_j with the splitting operation (iii) Solving each sub-problem directly, for example, with Gaussian elimination (iv) Adding up the solutions, provided that the second step can be implemented efficiently.*

The need for efficient computation required in the second step brings us to the following points.

Remark 4.5 *In order to split the incident field to the bottom level where the sub-domains $\{B_j\}$ reside, the scattering matrices must first be available for each sub-domain, see Theorem 3.7. This is done in a bottom-up motion to merge the scattering matrices (i) On the bottom level the scattering matrices of $\{B_j\}$ are calculated directly via formula (15) where inverting P_j in each B_j is required (ii) Merge recursively upwards along the hierarchy of levels, obtaining the scattering matrix of a parent from those of its children.*

4.2 Design principles for a hierarchy

The design of a hierarchy follows several simple principles outlined below. For simplicity, we assume that the original domain D is a unit square. Furthermore, we assume that the sub-domains $\{B_j\}$ on the bottom level are squares of size 2^{-L}-by-2^{-L}, with L given as the number of levels. Finally, we assume that when properly discretized the dimensions of the linear operators

$$S_i,\ T_{ij},\ R_i,\ E_i, \tag{40}$$

maps from boundary to boundary required in the merging and splitting schemes, are proportional to the arclength of the boundary; for example, $R_i : \partial D \mapsto \partial D_i$ has dimension $m \times n$ where $m \propto |\partial D_i|$ and $n \propto |\partial D|$ with the same proportionality constant.

Remark 4.6 *The first general principle for merging and splitting is that it is inefficient to merge domains of different sizes, or to split a domain into its sub-domains of different sizes.*

The size is defined as the arclength of the boundary. This principle follows directly from the operational count on the formulae (35), (36), and (37). Therefore, suppose a square Q has three children $Q_1,\ Q_2,\ Q_3$ where $Q_1,\ Q_2$ are squares of the same size filling the top half of Q whereas Q_3 is the bottom half of Q. It is easy to verify and conclude that the best way is to first merge $Q_1,\ Q_2$ and then merge the result with Q_3 to get the scattering matrix for Q. Similarly, the best way to split the incident field on Q to the total incident fields on $Q_1,\ Q_2,\ Q_3$ is to split it down to Q_3 and $Q_1 \cup Q_2$, and then to split $Q_1 \cup Q_2$ down to Q_1 and Q_2.

Remark 4.7 *The second principle for merging and splitting is that each child D_i as well as its parent should be as convex as possible so as to minimize the ratio $|\partial D_i|/|D_i|$, in order to minimize the number of merges or splits and to reduce the operational counts for each procedure.*

Remark 4.8 *The third principle is the necessity for a hierarchy where the merging and splitting are performed on its levels. To minimize the cost of evaluating the splitting matrix (35), merging from or splitting into as few children (of the same or similar size) as possible.*

An extreme example would be to merge from $\{B_j\}$ in a single step to the unit square. Then S_p itself requireis inversion of a matrix of dimension $O(M^2)$-by-$O(M^2)$ and therefore to form S_p costs $O(M^6)$. Another example is the case of merging four non-overlapping squares whose union is a larger square. We can either merge the four in a single step or accomplish the same in two stages: (i) two merges to form two rectangles - the upper and lower half of the larger square (ii) a merge of the two rectangles to get the larger square. It turns out, on the assumption made on the linear operators (40), that the ratio of costs is about $212/178 = 1.19$ in favor of the second approach. In the remainder of the discussion, however, we assume that the first approach is the choice just to simplify our exposition.

The next lemma specifies the hierarchy of levels for efficient merging and splitting; it is s a direct consequence of the preceding three principles (see Remarks 4.6, 4.7, 4.8).

Lemma 4.9 *Suppose that the original domain D, in which the Lippmann-Schwinger equation (1) is to be solved, is the unit square. Suppose further that the sub-domains $\{B_j\}$ on the bottom level are squares of size 2^{-L}-by-2^{-L}. Then for an efficient implementation of the merging and splitting schemes as specified by Theorems 3.7 and 3.8, the hierarchy of levels should be such that*

(i) Each level consists of squares of the same size whose union is the original domain, the unit square D.

(ii) Let L be the number of levels to be determine, see Remark 4.12; on the ℓ-th level for $0 \leq \ell \leq L$, there are 4^ℓ squares each of which is of the size $2^{-\ell}$-by-$2^{-\ell}$, with the unit square D residing at level zero, and 4^L small squares $\{B_j\}$ residing at the level L.

(iii) Merging and splitting is accomplished between each parent and its four children across two adjacent levels.

4.3 The fast direct algorithm

We summarize the main steps of the fast direct solver for the Lippmann-Schwinger equation (1), and provide further technical details for its discretization.

Lemma 4.10 *(***Fast algorithm for integral equation***) The main body of the fast algorithm consists of two sweeps: bottom up through all levels to merge scattering matrices and top down across all levels to split the incident fields. More specifically, it is divided into four steps.*

(i) At the bottom level L and for all $1 \leq j \leq 4^L$, invert the operator P_j defined in B_j (see (14)), and obtain the 4^L scattering matrices S_j of B_j directly (see (15)) via the formula

$$S_j = -k^2 G_j^{(b,v)} \cdot P_j^{-1} \cdot q \cdot G_j^{(v,b)}. \tag{41}$$

(ii) The bottom-up sweep. For $\ell = L, L-1, \ldots, 1$, merge the 4^ℓ scattering matrices on level ℓ to $4^{\ell-1}$ parents on level $\ell - 1$, each receiving from its four children (the scattering

matrix at level 0 will not be used for the fast solver but it is the scattering matrix for the whole scatterer and thus may itself be useful for other applications).

(iii) The top-down sweep. For $\ell = 1, 2, \ldots, L$, split the $4^{\ell-1}$ total incident fields (actually their Green's data) upon each of the $4^{\ell-1}$ squares on level $\ell - 1$ to 4^{ℓ} total incident fields (again the Green's data) upon 4^{ℓ} squares on level ℓ.

(iv) Finally back to the bottom level L, solve in the square B_j the Lippmann-Schwinger equation

$$P_i(\sigma|_{B_j})(x) = -k^2 q(x) G_j^{(v,b)} \cdot \Phi_j, \tag{42}$$

where Φ_j is the Green's data on ∂B_j of the total incident field obtained at the end of the preceding step.

The four assumptions will be required for discretizing the Lippmann-Schwinger equation and for the complexity analysis of the fast algorithm.

(I) The entire scatterer, the unit square domain D, is discretized with equispaced mesh of $M \times M$ points over which the integral equation is approximated with a high order quadrature. For example, for a smooth scatterer q compactly supported in D, it is not difficult to design a fourth or sixth order quadrature formula discretizing on the equispaced mesh the integral equation with the singular kernel G.

(II) The linear operators (40), which are required in the merging and splitting operations, all map from boundary to boundary. The number of points required to discretize them on the respective boundaries are assumed proportional to the arclength of the boundary. These points on the boundary need not to coincide with the mesh points in the domain discretizing the integral equation. They are assumed to have the same density as that of the points in the domain. Therefore, if there are m points on each side of a square sub-domain D_i, the number of points in the square is m^2; this is denoted by

$$\|\partial D_i\| = 4m, \quad \|D_i\| = m^2. \tag{43}$$

Remark 4.11 *The assumption (43) turns out to be realistic and feasible based on which an effective strategy for accurately discretizing the four linear operators (40) exists. A Fortran implementation is available.*

(III) The standard LU factorization will be used to solve the linear systems and in effect to apply the inverse to a vector. It costs $N^3/3$ to factor and N^2 to apply.

(IV) The linear operators T_{ij}, R_i, E_i used for merging and splitting are given independently of a particular scattering problem. Therefore, they can be and will be pre-computed at a cost proportional to N^3 where N is the dimension of the respective discretized operator. Moreover, this pre-computation costs only a fraction of that required for the inversion for S_p (see (35)), and therefore will be neglected in the complexity analysis.

Let M be the number of the equispaced points in each dimension of the unit square D for the discretization of the integral equation, N be the total number of unknowns,

z be the number of points on each side of a square B_j on the bottom level so that $n = 4(z-1)$ is the total number of points on the four sides and $s = z^2$ is the number of points on $\overline{B_j}$. In other words,

$$N = M^2, \quad z = 2^{-L}M. \tag{44}$$

Remark 4.12 *Our numerical experience shows that the integer z should be chosen from the interval $[5,\ 15]$ which in turn requires possible adjustment of M and determines L.*

Let us examine the dimensions of the linear operators (40).

Remark 4.13 *At any level $0 \le \ell < L$ of the hierarchy, a square sub-domain Q has four children $\{Q_i\}$ residing at the next lower level. In the merging or splitting process between the parent Q and its four children $\{Q_i\}$, R_i maps from the boundary of the parent square to that of the child square Q_i. If there are $2n$ points discretizing ∂Q, there will n points discretizing ∂Q_i according to Assumption II given above. Therefore, R_i is of dimension $p \times 2p$ where $p = 2n$ is the number of rows of the matrix R_i (the factor of 2 in front of n is due to the fact that R_i maps the Green's data–not only the function but also its normal derivative on ∂Q to the Green's data on ∂Q_i; see (16)). Similarly, we can determine the dimensions of the other three discretized operators*

$$S_i \in \mathbb{C}^{p\times p},\ T_{ij} \in \mathbb{C}^{p\times p},\ R_i \in \mathbb{C}^{p\times 2p},\ E_i \in \mathbb{C}^{2p\times p}. \tag{45}$$

with

$$p = 2n, \quad n = 4 \cdot 2^{-\ell} \cdot M \tag{46}$$

where n is the number of points on the boundary of Q_i at level ℓ.

4.4 The complexity analysis

Now we come to the mechanical process for counting flops required in each of the four steps of the fast algorithm, accompanied by remarks further revealing the natures of the operations.

Remark 4.14 *Step 1. This is the initialization for the bottom-up sweep, and is the only level of the merging sweep where the scatterer q is referenced, and where the volume nature (as opposed to surface, in 3-D) of the scattering problem is treated. In all other higher levels of the merging steps, only surface-to-surface (in 2-D, curve-to-curve) linear maps are required and inverted.*

Remark 4.15 *Cost of Step 1. At the bottom level L, there are 4^L squares B_j; there are $n = 4(z-1)$ points on ∂B_j, and $s = z^2$ points on $\overline{B_j}$. Therefore, the dimensions of the matrices required in (41) are, $P_j \in \mathbb{C}^{s\times s}$, $G_j^{(v,b)} \in \mathbb{C}^{s\times 2n}$, $G_j^{(b,v)} \in \mathbb{C}^{2n\times s}$. The cost of (41) via LU decomposition is*

$$\begin{aligned} c_1 &= 4^L \cdot \{cost(LU) + cost(P_j^{-1} \cdot q \cdot G_j^{(v,b)}) + cost(G_j^{(b,v)} \times \cdots)\} \\ &= 4^L \cdot (2s^3 + 1.5s^2 \cdot 2n + 2n \cdot s \cdot 2n) \\ &= 2z^2(32 + 4z + z^2/3)N. \end{aligned} \tag{47}$$

If $z = 2^{-L}M$ is kept a (small) constant, the cost of the first step is proportional to the the number of unknows. We know we cannot do better than that, up to a constant.

Remark 4.16 *Step 2. The bottom-up merging operations through all levels are devoid of the volume feature of the integral equation. The merging procedure is totally independent of a particular scattering problem to be solved; it depends only on the hierarchical structure. Here we are dealing, managing, and assembling the multiple scattering between the non-overlapping sub-domains on each level. We know that these interactions take place across the boundaries of these sub-domains, and can be represented and calculated strictly through operators that map from boundary to boundary (surface to surface in 3-D) as opposed to from domain to domain (volume to volume in 3-D) which is needed in the direct solution of the integral equation without the use of the scattering matrices. Great savings are realized here.*

Remark 4.17 *Cost of Step 2. Here we only consider the case of merging the four child squares on level ℓ to their parent square on level $\ell - 1$. The merging formula (37) is divided into five stages whose costs we list below using the dimensions specified in (45), (46).*

1. $8p^3 = 4 \cdot (2p^3)$ *flops to form* $[E_1S_1 \;\; E_2S_2 \;\; E_3S_3 \;\; E_4S_4] \in \mathbb{C}^{2p\times 4p}$.

2. $12p^3$ *flops to form* $T_{ij}S_j \in \mathbb{C}^{p\times p}$.

3. $(64/3)p^3 = (4p)^3/3$ *for* LU *decomposition of* $\mathbb{C}^{4p\times 4p}$ *required in (35).*

4. $32p^3 = 4p \cdot 4p \cdot 2p$ *to multiply* $(LU)^{-1} \in \mathbb{C}^{4p\times 4p}$ *and* $[R_1 \; R_2 \; R_3 \; R_4]^T \in \mathbb{C}^{4p\times 2p}$.

5. $16p^3 = 2p \cdot 4p \cdot 2p$ *to multiply* $[E_1S_1 \;\; E_2S_2 \;\; E_3S_3 \;\; E_4S_4] \in \mathbb{C}^{2p\times 4p}$ *and* $S_p \in \mathbb{C}^{4p\times 2p}$ *to obtain* $S \in \mathbb{C}^{2p\times 2p}$.

In total, the five stages require $90p^3$ flops. With $p = 8 \cdot 2^{-\ell} \cdot M$ and since there $4^{\ell-1}$ parent squares on level ℓ, the cost for Step 2 on this level is

$$c_{2,\ell} = 4^{\ell-1} \cdot (90p^3) = 2 \cdot 8^2 \cdot 90 \cdot 2^{-\ell}M^3 = 11520 \cdot 2^{-\ell}M^3, \tag{48}$$

and the total cost for Step 2 is bounded by

$$c_2 = \sum_{\ell\geq 0} c_{2,\ell} = 11520 \cdot M^3. \tag{49}$$

This is the leading cost of the algorithm which is on the order of $N^{1.5}$ where N is the number of unknowns.

Remark 4.18 *It is possible to reduce the coefficient 11520 to about 8000 or less by use of symmetry for the square domains. It is further possible to reduce p by a factor of 2 via a compression of the Green's data (27)–(30). Then the flops required for the first two steps will be*

$$c_1 = 2z^2(8 + 2z + z^2/3), \quad c_2 = (10M)^3. \tag{50}$$

Remark 4.19 *Steps 3 and 4. These two steps in the top-down sweep are similar in structure to the first two steps. From the linear algebra point of view, if Step 2 is regarded as some type of matrix decomposition for the entire discretized integral operator, then Step 3 is the corresponding back substitution. Therefore, the computational cost for Step 3 is an order of magnitude lower than that for Step 2. Step 4 costs much less than Step 1 for the same reason.*

Remark 4.20 *Cost of Steps 3 and 4. For $\ell > 0$ and for each square on level $\ell - 1$, the Green's data of the total incident field is of dimension $\Phi \in \mathbb{C}^{2p}$ with p defined in (46); therefore for each square on level $\ell - 1$, the splitting (36) is to apply $S_p \in \mathbb{C}^{4p \times 2p}$ to $\Phi \in \mathbb{C}^{2p}$ now that S_p has been obtain in Step 2; the splitting requires $8p^2 = 4p \cdot 2p$ flops for each square, and*

$$c_{3\ell} = 4^{\ell-1} \cdot (8p^2) = 128M^2, \tag{51}$$

on level ℓ. The total cost for Step 3 is bounded by, and taken as

$$c_3 = \sum_{\ell=1}^{\log_2 M} c_{3\ell} = 128M^2 \cdot \log_2 M. \tag{52}$$

Finally, solution of (42) in Step 4 is similar to (41) of Step 1, except that the LU factorization and $G_j^{(b,v)}$ multiplication are not required. It follows from (47) that

$$c_4 = 4^L \cdot \{cost(P_j^{-1} \cdot q \cdot (G_j^{(v,b)} \cdot \Phi_j)\} = 4^L \cdot s^2 = z^2 N. \tag{53}$$

Again, it is possible to reduce p by a factor of 2 via a reduction of the size of the Green's data. Moreover, within a thousand-by-thousand wavelength problem and with 10 points per wavelength, M is on the order of $10,000$, and $\log_2(M)$ is about 15. Consequently, the cost of Step 3 will be no more than $480M^2$ flops, and M right hand sides will cost $480M^3$ which is about $(6M)^3$ flops.

Lemma 4.21 *Let $z = 2^{-L}M$. Then solving the integral equation on an $M \times M$ mesh with L levels, the four steps of the fast algorithm cost*

$$\begin{aligned} c_1 &= 2z^2(32 + 4z + z^2/3)M^2, && (54)\\ c_2 &= 11520 \cdot M^3, && (55)\\ c_3 &= 128M^2 \cdot \log_2 M, && (56)\\ c_4 &= z^2 M^2 && (57) \end{aligned}$$

where c_3, c_4 are the flops required for each right hand side.

One of the applications of this fast solver is the inverse scattering problem for which M forward problems may be solved for a given wave number. Each of these M right hand sides corresponds to an incident, probing wave. In this context, we recast Lemma 4.21 in more practical terms.

Lemma 4.22 *Suppose that reductions are made as specified in Remark 4.18, and that* $M \leq 10^6$, $z = 10$. *Then the flops required to solve* M *forward problems will be*

$$c_1 = 12267M^2, \tag{58}$$
$$c_2 \sim (10M)^3, \tag{59}$$
$$c_3 \sim (8M)^3, \tag{60}$$
$$c_4 = 100M^3. \tag{61}$$

References

[1] J. H. Lin and W. C. Chew, *Solution of the three-dimensional electromagnetic inverse problem by the local shape function and the conjugate gradient fast Fourier transform methods,* J. Opt. Soc. Am., vol. 14, no. 11, pp. 3037- 3045, Nov. 1997.

[2] Song JM, Lu CC, Chew WC, et al. Fast Illinois Solver Code (FISC) IEEE ANTENNAS PROPAG 40: (3) 27-34 JUN 1998

[3] W. W. Symes: Iterative Procedures for Wave Propagation in The Frequency Domain Technical Reports, Rice University, 1996

[4] Zhao JS, Chew WC Three-dimensional multilevel fast multipole algorithm from static to electrodynamic MICROW OPT TECHN LET 26: (1) 43-48 JUL 5 2000

[5] Chen YH, Chew WC, Zeroug S Fast multipole method as an efficient solver for 2D elastic wave surface integral equations COMPUT MECH 20: (6) 495-506 NOV 1997

[6] L. Greengard, J. Huang, and S. Wandzura, V. Rokhlin, *Accelerating Fast Multipole Methods For Low Frequency Scattering,* IEEE Computational Science and Engineering, v. 5, No. 3, July-September 1998.

[7] J. Ma, V. Rokhlin, and P. Jones (1994) *A Fast Direct Algorithm for the Solution of the Laplace Equation on Regions with Fractal Boundaries, Journal of Computational Physics*, Vol 113, No. 1, July 1994.