

Acoustic multiple scattering using recursive algorithms



Feruza A. Amirkulova*, Andrew N. Norris

Mechanical and Aerospace Engineering, Rutgers University, 98 Brett Road, Piscataway, NJ 08854, United States

ARTICLE INFO

Article history:

Received 24 December 2014

Received in revised form 8 July 2015

Accepted 9 July 2015

Available online 21 July 2015

Keywords:

Acoustics

Multiple scattering

Wave propagation

Recursive algorithms

Computation methods

Parallel computation

OpenMP

ABSTRACT

Acoustic multiple scattering by a cluster of cylinders in an acoustic medium is considered. A fast recursive technique is described which takes advantage of the multilevel Block Toeplitz structure of the linear system. A parallelization technique is described that enables efficient application of the proposed recursive algorithm for solving multilevel Block Toeplitz systems on high performance computer clusters. Numerical comparisons of CPU time and total elapsed time taken to solve the linear system using the direct LAPACK and TOEPLITZ libraries on Intel FORTRAN, show the advantage of the TOEPLITZ solver. Computations are optimized by multi-threading which displays improved efficiency of the TOEPLITZ solver with the increase of the number of scatterers and frequency.

© 2015 Elsevier Inc. All rights reserved.

1. Introduction

Multiple scattering (MS) and radiation of waves by a system of scatterers is of great theoretical and practical importance. MS is required in a wide variety of physical contexts such as the implementation of “invisibility” cloaks, the characterization of effective parameters of heterogeneous media, and the fabrication of dynamically tunable structures, i.e. superlenses and waveguides, etc. Our interest here is with examining acoustic MS from 2D cylindrical structures, although the method may be extended to 3D to include elastodynamic [1] or electromagnetic material properties. A broad review of the literature on single and MS and of the concepts of MS is given in [2]; a survey of more recent findings on MS from obstacles in acoustic and elastic media is provided in [1]. The development of numerically efficient techniques and algorithms that are appropriate for a wide range of problems is one of the main challenges in wave propagation research. The expensive costs of direct matrix inversion of a linear system motivates development of alternative numerically efficient methods [31]. Here we consider a recursive technique that is not limited by physical parameters such as the frequency or spacing between the scatterers, but is based on the structure of the MS formulation. The exact approach described in this paper takes advantage of multilevel Block Toeplitz structure of the linear system to speed up the matrix solution in a manner suitable for parallel computation. The recursive algorithm is robust, and resistant to machine errors.

* Corresponding author. Current address: Physics and Astronomy Department, Vassar College, 124 Raymond Ave., Poughkeepsie, NY 12604, United States. Tel.: +1 845 437 5972.

E-mail addresses: feamirkulova@vassar.edu (F.A. Amirkulova), norris@rutgers.edu (A.N. Norris).

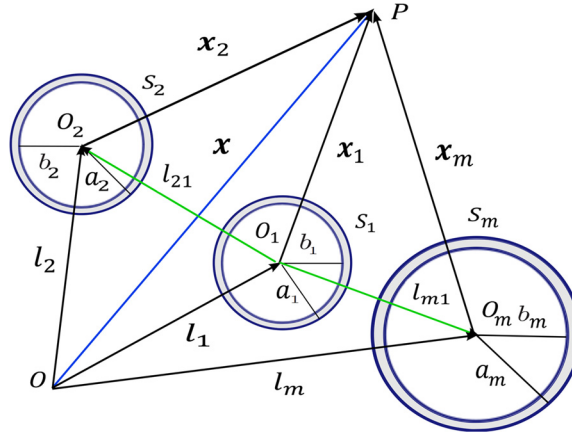


Fig. 1. An arbitrary planar configuration of M cylinders S_m with outer radius a_m and inner radius b_m , $m = \overline{1, M}$.

1.1. Problem definition

The two-dimensional (2D) MS problem may be reduced using Graf's addition theorem [3, eq. (9.1.79)] to an infinite linear system of equations which can be truncated to the finite dimensional system of the form:

$$\mathbb{X} \mathbf{b} = \mathbf{a}. \quad (1.1)$$

In this equation $\mathbf{a}$ is the column vector of the known coefficients of the excitation field, $\mathbf{b}$ is the column vector of the unknown scattering coefficients, and $\mathbb{X}$ is the interaction matrix that defines the coupling between each scatterer of the configuration (see Appendix A for details):

$$\mathbb{X} = \begin{bmatrix} \mathbf{I} & -\mathbf{T}^{(1)} \mathbf{p}^{1,2} & -\mathbf{T}^{(1)} \mathbf{p}^{1,3} & \dots & -\mathbf{T}^{(1)} \mathbf{p}^{1,M} \\ -\mathbf{T}^{(2)} \mathbf{p}^{2,1} & \mathbf{I} & -\mathbf{T}^{(2)} \mathbf{p}^{2,3} & \dots & -\mathbf{T}^{(2)} \mathbf{p}^{2,M} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathbf{T}^{(M)} \mathbf{p}^{M,1} & -\mathbf{T}^{(M)} \mathbf{p}^{M,2} & -\mathbf{T}^{(M)} \mathbf{p}^{M,3} & \dots & \mathbf{I} \end{bmatrix}. \quad (1.2)$$

The matrix $\mathbf{T}^{(j)}$ is the transition or T-matrix for scatterer j . The matrix $\mathbf{p}^{j,m} = [\mathbf{p}_{ql}^{j,m}]$ is a Toeplitz matrix; it depends on the position vector $\mathbf{l}_{jm}$ depicted in Fig. 1, and takes into account the interaction between the scatterers, whereas the transition matrix $\mathbf{T}^{(j)}$ depends on the shape and the physical properties of the material of cylinder, as well as the boundary conditions on the interfaces.

Here we consider 2-dimensional configurations of circularly cylindrical scatterers, for which the T-matrices become diagonal, see [1] for specific details. In particular, $\mathbf{p}^{j,m} = [\mathbf{p}_{ql}^{j,m}]$ ($q, l \in \mathbb{Z}$), where $\mathbf{p}_{ql}^{j,m} = V_{l-q}^+(\mathbf{l}_{jm})$ ($q = -N_j, N_j, l = -N_m, N_m$) ($j, m = \overline{1, M}, j \neq m$), where the functions $V_n^\pm(\mathbf{x})$ are

$$V_n^\pm(\mathbf{x}) = H_n^{(1)}(k|\mathbf{x}|)e^{\pm i n \arg \mathbf{x}}. \quad (1.3)$$

Here $H_n^{(1)}$ is the Hankel function of the first kind of order n , $\mathbf{x}$ is the position vector of point P (see Fig. 1), $k = \omega/c$ is the wavenumber, c is the acoustic speed, ω is the frequency with time dependence $e^{-i\omega t}$ assumed. The vectors in eq. (1.1) then have the structure

$$\mathbf{a} = \begin{pmatrix} \mathbf{T}^{(1)} \mathbf{a}^{(1)} \\ \mathbf{T}^{(2)} \mathbf{a}^{(2)} \\ \vdots \\ \mathbf{T}^{(M)} \mathbf{a}^{(M)} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} \mathbf{b}^{(1)} \\ \mathbf{b}^{(2)} \\ \vdots \\ \mathbf{b}^{(M)} \end{pmatrix}, \quad \mathbf{a}^{(j)} = \begin{pmatrix} A_{-N}^{(j)} \\ A_{-N+1}^{(j)} \\ \vdots \\ A_N^{(j)} \end{pmatrix}, \quad \mathbf{b}^{(j)} = \begin{pmatrix} B_{-N}^{(j)} \\ B_{-N+1}^{(j)} \\ \vdots \\ B_N^{(j)} \end{pmatrix} \quad (j = \overline{1, M}), \quad (1.4)$$

where $\mathbf{a}^{(j)}$ ($j = \overline{1, M}$) is the vector of coefficients of the excitation field around cylinder S_j (see Fig. 1).

The matrix $\mathbb{X}$ is a complex valued dense $N \times N$ matrix, and N is proportional to the number of scatterers M multiplied by $2N + 1$ where N is the mode number. For high frequencies and a large number of scatterers, the system (1.1) becomes an extremely large linear system. The computational complexity of inverting $\mathbb{X}$ by direct methods is $O(N^3)$, i.e. the Gauss–Jordan method requires N^3 multiplication operations and N^3 addition–subtraction operations, the Gauss method using LU decomposition requires $N^3/3$ multiplication and $N^3/3$ addition–subtraction operations. The memory requirements to solve (1.1) by direct methods grow as $O(N^2)$. This is prohibitive for many realistic multiple scattering problems at high frequencies and a large number of scatterers. For large N and required number of iterations, the most widely used Krylov Space

methods such as GMRES, BICGSTAB, etc. can lead to excessive run times [4,5]. The computational complexity of the problem can be reduced if the $\mathbb{X}$ matrix has some specific characteristics. When the $\mathbb{X}$ matrix has Toeplitz structure, its inversion requires $O(N^2)$ arithmetic operations using Levinson and Trench algorithms [6,7]. The inverse of a Toeplitz matrix can be decomposed into the sum of two multiplications of triangular Toeplitz matrices using fast recursive algorithms [8–11]. These algorithms have a simple description and use minimal storage; they require $O(N \log_2 N)$ arithmetic operations and the memory of order $O(N)$. There is a correspondence between the scalar algorithms [8,10,11] for Toeplitz matrix and their block analogs [9,7,12] according to which block multiplications and additions in block algorithms correspond to multiplications and additions in the scalar case. Specifically, for some planar configuration of cylindrical structures, $\mathbb{X}$ has a Block Toeplitz structure which allows the use of such algorithms and greatly reduces simulation run time. This aspect is investigated in detail here.

1.2. Background review

Before considering the new recursive technique, we briefly review the literature on relevant numerical methods. Auger and Stout [13] proposed a set of numerically stable recursive relations to solve MS equations for a configuration of N dielectric spheres taking into account full interaction between the spheres. The recursive relations are based on the N -centered T-matrix concept, and allow the calculation of the total T-matrix of the N particles' system from the known 'total T-matrix of the $N - 1$ particles' system and the multiple T-matrix of the N th sphere' [13]. Barrowes et al. [14,15] presented a Fast Fourier Transform method to speed up a matrix–vector product involving multi-level BT matrices. The method was applied to solve an electromagnetic 3D scattering problem [15] using a discretized integral formulation. Antoine et al. [16] studied an acoustic multiple scattering by circular obstacles at high frequencies and large number of obstacles and proposed fast iterative numerical methods for solving a large complex-valued dense linear system using its Toeplitz block structure. These methods yield a large memory saving; the efficiency of the method was shown for several general configurations by studying the convergence rate with respect to different geometrical parameters. They performed calculations considering GMRES and BICGSTAB iterative solvers and GMRES(η) with a restart parameter η and combined with optimized memory storage techniques. Antoine et al. [17,18] studied the numerical solution of integral equations for multiple scattering by circular cylinders for a large band of frequencies and large number of obstacles. They proposed a solution procedure via projection method based on Fourier series using an iterative solver (GMRES) with preconditioners. The same authors took advantage of the Toeplitz structure of off-diagonal blocks of the linear system and stored a compressed version of the system using a root vector for the Toeplitz matrix. Two preconditioners were proposed to increase the convergence.

Villamizar and Acosta [19] presented a grid generation algorithm for 2D multiply connected regions with multiple holes of complex geometry. They applied the algorithm to generate a grid for a finite difference scheme, and to numerically solve acoustic MS problems and estimate the pressure field over geometrically complex configurations. Pashaev and Yilmaz [20] studied the hydrodynamic interaction between an arbitrary number of cylinders and vortices. The problem is formulated using a Laurent series expansion with unknown coefficients which are found using a standard LU decomposition and the convergence properties of the infinite system was investigated. Genechten et al. [21] proposed a numerical 'multilevel' 2D modeling method for a solution of steady-state low- and mid-frequency time-harmonic acoustic MS and radiation problems for a configuration of well separated scatterers of arbitrary shape in both bounded and unbounded problem domains. Each level considers the reflection and scattering from a single scatterer using the so-called wave based method for unbounded problems. Geuzaine et al. [22] provided an open source finite element solver based on domain decomposition methods; the open source solver software available online, is suitable for solution of high frequency time-harmonic electromagnetic wave problems. Challa and Sini [23] studied the acoustic MS problem by many small rigid scatterers of arbitrary shapes using the Foldy–Lax approximation; they solved the inverse problem of scattering by the small obstacles. Thierry et al. [24] proposed a new efficient Matlab toolbox, so-called ' μ -diff' suitable for a large class of 2D MS problems with any deterministic or random distribution of cylinders. The toolbox is developed based on integral equation methods, and includes the integral operators and post-processing facilities (near- and far-fields); it can use either direct solvers or iterative Krylov subspace solvers to solve Block Toeplitz linear systems. Draine and Flatau [25] developed an open-source FORTRAN-90 software package DDSCAT 7.3, the DDA (discrete dipole approximation) code to calculate scattering and absorption of electromagnetic waves by isolated or periodic arrays of particles. The code can be compiled on Unix using MKL library and parallelized using OpenMP and MPI to achieve an efficient fast computation. Koyama [26] showed a convergence of Parallel Schwarz Method for a solution of MS problems and developed techniques of acceleration of the convergence of the Schwarz method. Gallivan et al. [27] developed a high performance library based on several high performance variants of Schur algorithms to factor symmetric positive definite and indefinite Block Toeplitz matrices. Chen [28] proposed a fast algorithm for matrix vector product involving Toeplitz matrices by employing Fast Fourier Transform tricks.

In this work, we solve an MS problem that includes full interactions between closely spaced scatterers, allowing us to find the scattering coefficients and far-field behavior. We start in Section 2 with a review of Toeplitz matrices, and categorize some associated matrix types. Specifically, we study the structure of multilevel matrices and consider illustrative examples. The high performance recursive algorithms for solving the MS linear systems are described in Section 3. In Section 3.1, we review some properties of biorthogonal and orthogonal polynomials, and use them for matrix inversion. The recursive technique for Block Toeplitz matrices of level 1 and 2 are described in Section 3.2. Numerical results are presented in Section 4. The theoretical predictions are verified through Matlab and FORTRAN implementations using different direct and

iterative solvers. Numerical results are also given for the CPU time taken to solve the linear system by varying values of M and d where M is the number of the scatterers and d is the distance between the centers of two cylinders (see Fig. 2).

2. Matrix types

In this section we classify and define matrix types. General matrices are denoted by the symbol $\mathbb{G}$, Toeplitz matrices by $\mathbb{T}$, and Circulant matrices by $\mathbb{C}$. We start with the definition and properties of Toeplitz and Circulant matrices in Section 2.1. The general type of matrices and multilevel matrices are considered in more detail in Section 2.2.

2.1. Toeplitz and Circulant matrices

Toeplitz matrices or Toeplitz forms are named after O. Toeplitz [29], honoring his work in 1911 on bilinear L-forms in relation to Laurent series. A Toeplitz matrix has a specific structure such that its each descending diagonal from the left to the right is constant. In the early 1920s, Szegő [30] studied the distribution of eigenvalues of Toeplitz forms and introduced a new class of closely related polynomials. As we will see, the special features of the Toeplitz matrix allow us to apply the fast iterative algorithms for Block Toeplitz systems [7,9].

The Toeplitz matrix $\mathbf{P}^{j,m} = [\mathbf{P}_{ql}^{j,m}] = [P_{q-l}^{j,m}]$ has each of its subdiagonals, which are parallel to the main diagonal, equal to a constant:

$$\mathbf{P} = [P_{q-l}] = \begin{bmatrix} P_0 & P_{-1} & P_{-2} & \dots & P_{-2N} \\ P_1 & P_0 & P_{-1} & \dots & P_{-2N+1} \\ P_2 & P_1 & P_0 & \dots & P_{-2N+2} \\ \dots & \dots & \dots & \ddots & \dots \\ P_{2N} & P_{2N-1} & P_{2N-2} & \dots & P_0 \end{bmatrix}, \quad (2.5)$$

where $1 \leq q, l \leq 2N+1$, $N = N_j = N_m$. Here we drop upper indices j and m of matrix $\mathbf{P}^{j,m}$ for simplicity of notation. Matrix $\mathbf{P}$ of order $2N+1$ with elements P_{ql} will have Toeplitz structure if and only if [9]:

$$P_{q_1 l_1} = P_{q_2 l_2}, \quad \text{with } q_1 - l_1 = q_2 - l_2. \quad (2.6)$$

A special form of Toeplitz matrix where each column vector is rotated one element upward relative to the preceding column vector is called a Circulant matrix. In particular, if [9]

$$P_{q_1 l_1} = P_{q_2 l_2}, \quad \text{with } q_1 - l_1 = (q_2 - l_2) \bmod (2N+1), \quad (2.7)$$

then such a matrix will have Circulant structure, and will be called a Circulant matrix of order $2N+1$ and denoted by $\mathbf{C}$:

$$\mathbf{C} = \begin{bmatrix} P_0 & P_{-1} & P_{-2} & \ddots & P_{-2N} \\ P_{-2N} & P_0 & P_{-1} & \ddots & P_{-2N+1} \\ P_{-2N+1} & P_{-2N} & P_0 & \ddots & P_{-2N+2} \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ P_{-1} & P_{-2} & P_{-3} & \ddots & P_0 \end{bmatrix}. \quad (2.8)$$

The Circulant matrices that have upper triangular or lower triangular form are called semicirculant matrices. For example, the elements of upper triangular semicirculant matrix $\mathbf{C}^U$ can be formed from elements of matrix $\mathbf{P}$ of order $2N+1$:

$$C_{ql}^U = \begin{cases} P_{q-l}, & q \leq l, \\ 0, & q > l, \end{cases} \quad \text{for } 1 \leq q, l \leq 2N+1. \quad (2.9)$$

The Toeplitz matrix $\mathbf{P}$ of order $2N+1$ can be defined by its first row and first column and can be generated by the root vector

$$\mathbf{p} = (P_{-2N}, P_{-2N+1}, \dots, P_{-1}, P_0, P_1, \dots, P_{2N-1}, P_{2N})^T, \quad (2.10)$$

whereas the Circulant matrix $\mathbf{C}$ of order $2N+1$ can be generated by its first column:

$$\mathbf{c} = (P_0, P_{-2N}, P_{-2N+1}, \dots, P_{-1})^T, \quad (2.11)$$

or its first row:

$$\mathbf{c}' = (P_0, P_{-1}, \dots, P_{-2N+1}, P_{-2N}). \quad (2.12)$$

As we can see, the Circulant matrix $\mathbf{C}$ requires fewer elements to store as compared to the Toeplitz matrix.

In some cases P_i elements of Toeplitz matrix $\mathbf{P}$, eq. (2.5), can be treated as square matrices that can have Toeplitz structure. Furthermore, these block matrices can themselves consist of blocks of Toeplitz structure leading to the construction of multilevel block matrices that will be addressed next.

2.2. Multilevel matrices

The concept of multilevel matrices was proposed by Voevodin and Tyrtshnikov [9]. For some fixed values $\alpha_{ij}^{(q)}$ and $\gamma^{(q)}$ ($1 \leq i \leq m$, $1 \leq j \leq n$, $1 \leq q \leq Q$) consider a class of matrices of size $m \times n$ with elements a_{ij} that satisfy the condition [9]:

$$\sum_{i,j} \alpha_{ij}^{(q)} a_{ij} = \gamma^{(q)}, \quad 1 \leq q \leq Q. \quad (2.13)$$

If $\mathbb{K}$ is one of such matrix class and $\mathbf{A} \in \mathbb{K}$ then the matrix $\mathbf{A} = [a_{ij}]$ is called $\mathbb{K}$ type. The general type of matrices $\mathbb{G}$ can be defined by eq. (2.13) when this identity is only satisfied by $\alpha_{ij}^{(q)} = 0$ and $\gamma^{(q)} = 0$.

Equation (2.13) is a linear system with respect to the elements of matrix $\mathbf{A} = [a_{ij}]$. It can be written in a matrix form as

$$\boldsymbol{\alpha} \text{vec}(\mathbf{A}) = \boldsymbol{\gamma}, \quad (2.14)$$

where

$$\boldsymbol{\alpha} = \begin{pmatrix} \text{vec}(\boldsymbol{\alpha}^{(1)})^T \\ \text{vec}(\boldsymbol{\alpha}^{(2)})^T \\ \vdots \\ \text{vec}(\boldsymbol{\alpha}^{(Q)})^T \end{pmatrix}, \quad \boldsymbol{\gamma} = \begin{pmatrix} \gamma^{(1)} \\ \gamma^{(2)} \\ \vdots \\ \gamma^{(Q)} \end{pmatrix}, \quad (2.15)$$

$\boldsymbol{\alpha}^{(q)} = [\alpha_{ij}^{(q)}]$ is an $m \times n$ matrix, and $\boldsymbol{\gamma}^{(q)}$ is an $m \times 1$ vector ($1 \leq i \leq m$, $1 \leq j \leq n$, $1 \leq q \leq Q$); $\text{vec}(\mathbf{A})$ defines the vectorization of matrix $\mathbf{A}$ that is constructed by packing consecutively the columns of matrix $\mathbf{A}$ into a single column vector:

$$\text{vec}(\mathbf{A}) = [a_{11} \dots a_{m1} a_{12} \dots a_{m2} a_{13} \dots \dots a_{mn-1} a_{1n} \dots a_{mn}]^T. \quad (2.16)$$

Similarly, $\text{vec}(\boldsymbol{\alpha}^{(q)})$ is formed by stacking the columns of matrix $\boldsymbol{\alpha}^{(q)}$. Let $\mathbb{K}$ type matrix $\mathbf{A}$ satisfy the system (2.14), then the block type matrix $\mathbf{A} \in \mathbb{K}_{gl}$ is defined by the system:

$$(\mathbf{I}_l \otimes \boldsymbol{\alpha} \otimes \mathbf{I}_k) \text{vec}(\mathbf{A}) = \mathbf{g}_l \otimes \boldsymbol{\gamma} \otimes \mathbf{g}_k, \quad (2.17)$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{g}$ is the vector with all entries equal to 1, the subindices denote the order of matrix or vector, and $\otimes$ symbolizes the (associative) Kronecker tensor product defined as:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \dots & a_{1n}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \dots & a_{2n}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & a_{m2}\mathbf{B} & \dots & a_{mn}\mathbf{B} \end{bmatrix}. \quad (2.18)$$

Let $\mathbb{K}_1, \dots, \mathbb{K}_s$ be different classes of matrices admitting such classification. We can construct new composite types based on these, e.g. $\mathbb{K}_1\mathbb{K}_2$, $\mathbb{K}_1\mathbb{K}_2\mathbb{K}_3$, ..., $\mathbb{K}_1 \dots \mathbb{K}_s$. The matrices of composite type are called multilevel matrices and characterized by block partitioning of different levels. We will denote blocks as follows. The matrix $\mathbf{A}$ itself is a single block of level 0. If the matrix $\mathbf{A}$ has a composite type $\mathbb{K}_1 \dots \mathbb{K}_s$ and class $\mathbb{K}_k$ consists of matrices of sizes $m_k \times n_k$ ($1 \leq k \leq s$) then the matrix $\mathbf{A}$ comprises $m_1 \times n_1$ blocks $a_{i_1 j_1}$ of size $m_2 \dots m_k \times n_2 \dots n_k$ that form the level 1 ($1 \leq i_1 \leq m_1$, $1 \leq j_1 \leq n_1$). Next, $\forall a_{i_1 j_1}$ blocks consist of $m_2 \times n_2$ blocks $a_{i_1 j_1, i_2 j_2}$ that construct the level 2. For $1 \leq k < s$, each of $a_{i_1 j_1, \dots, i_k j_k}$ blocks of level k consists of $m_k \times n_k$ blocks of level $k+1$. The last level s is formed by the elements that cannot be partitioned, and assumed to contain only complex numbers. In general, an s -level block matrix has a composite type $\mathbb{G}_{m_1 n_1} \dots \mathbb{G}_{m_s n_s}$. When each block is square, we can use one index: $\mathbb{G}_{m_1} \dots \mathbb{G}_{m_s}$. Multilevel partitioning is of interest if the level blocks have some structure. In the next section we will consider the matrices of composite types $\mathbb{T}_{m_1} \mathbb{G}_{m_2}$ and $\mathbb{T}_{m_1, m_2} \mathbb{G}_{m_3}$. The former defines a two-level block matrix, i.e. a block Toeplitz (BT) matrix of level 1 with general type subblocks of order m_2 embedded in Toeplitz blocks of order m_1 ; the latter type characterizes a three-level block matrix with level orders m_1 , m_2 and m_3 that is a BT matrix of level 2 with general type subblocks, here the general type subblocks of order m_3 are embedded in Toeplitz blocks of order m_2 that are nested inside of another Toeplitz block of order m_1 .

2.2.1. Examples of multilevel matrices

Consider a planar configuration consisting of M_y rows and M_x columns of scatterers in an infinite acoustic medium. Each scatterer is a cylinder of the same radius and material properties and hence characterized by the same T-matrix for each cylinder, i.e. $\mathbf{T}^{(j)} = \mathbf{T}$ ($j = \overline{1, M}$) where $M = M_x M_y$. The matrix $\mathbb{X}$ defined by eq. (1.2) has BT structure for this configuration of M scatterers. Fig. 2 shows examples of such an array of scatterers.

Example of BT matrix of level 1. The matrix $\mathbb{X} \in T_M \mathbb{G}_{2N+1}$ becomes a BT matrix of level 1 with $M = M_x$ for a single row of cylinders ($M_y = 1$), and $M = M_y$ for a single column of cylinders ($M_x = 1$), see Fig. 2(a). The matrix $\mathbb{X}$ is square of order

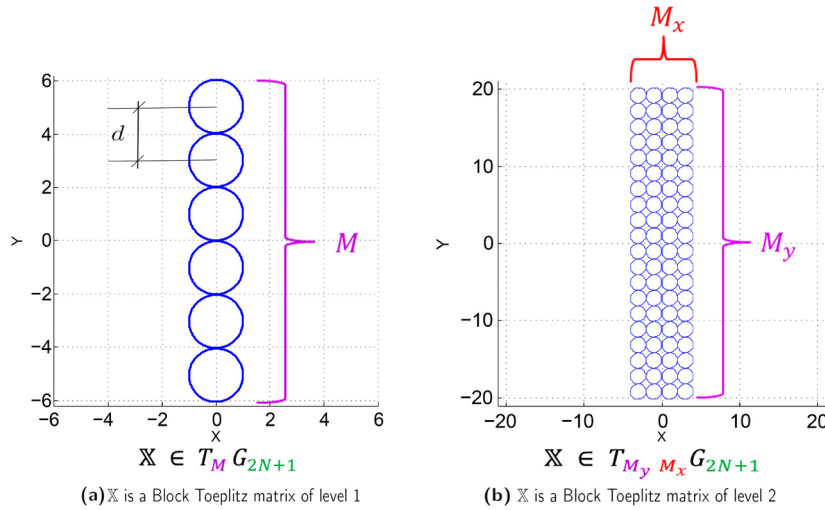


Fig. 2. Examples of configurations that lead to Block Toeplitz matrices of level 1, $\mathbb{X} \in T_M G_{2N+1}$, and level 2, $\mathbb{X} \in T_{M_y, M_x} G_{2N+1}$, where $M_x M_y = M$. On the left, d is the distance between the centers of two cylinders, here $d = 2a \times 1.01$ where a is the cylinder outer radius.

$M(2N + 1)$, where N is the number of azimuthal modes considered. As a two-level block matrix, the BT matrix $\mathbb{X}$ has order M and consists of square blocks $\mathbf{X}_{ij}^1 = \mathbf{X}_{i-j}^1$ where $1 \leq i, j \leq M$, and in general, every block can be a non-symmetric complex valued matrix of order $(2N + 1)$:

$$\mathbb{X} = \begin{bmatrix} \mathbf{X}_0^1 & \mathbf{X}_{-1}^1 & \mathbf{X}_{-2}^1 & \cdots & \mathbf{X}_{-M+1}^1 \\ \mathbf{X}_1^1 & \mathbf{X}_0^1 & \mathbf{X}_{-1}^1 & \cdots & \mathbf{X}_{-M+2}^1 \\ \mathbf{X}_2^1 & \mathbf{X}_1^1 & \mathbf{X}_0^1 & \cdots & \mathbf{X}_{-M+3}^1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mathbf{X}_{M-1}^1 & \mathbf{X}_{M-2}^1 & \mathbf{X}_{M-3}^1 & \cdots & \mathbf{X}_0^1 \end{bmatrix}. \quad (2.19)$$

Here $\mathbf{X}_0^1$ is the block identity matrix of order $2N + 1$.

Example of BT matrix of level 2. Consider a planar configuration of M_y rows and M_x columns of cylinders with identical transition matrices $\mathbf{T}^{(j)} = \tilde{\mathbf{T}} \ (j = \overline{1, M})$, see Fig. 2(b). The matrix $\mathbb{X}$ is now a three-level block matrix, i.e. $\mathbb{X} \in T_{M_y, M_x} G_{2N+1}$, with BT structure of level 2. Again, the matrix $\mathbb{X}$ is of order $M(2N + 1)$. At the same time, as a BT matrix, $\mathbb{X}$ has order M_y (see eq. (2.20)). Each block $\mathbf{X}_{i-j}^1$ has order $M_x(2N + 1)$ and appears in $\mathbb{X}$ again in BT form (2.21). The block entries $\mathbf{X}_{i-j}^1 \in T_{M_x} G_{2N+1} \ (1 \leq i, j \leq M_y)$ are BT matrices of order M_x with individual entries $\mathbf{X}_{i-j}^2 \in G_{2N+1} \ (1 \leq i, j \leq M_x)$, where block $\mathbf{X}_{i-j}^2$ is of general type and of order $2N + 1$. In other words, a general type matrix $\mathbf{X}_{i-j}^2$ of order $(2N + 1)$ is embedded in a Toeplitz block $\mathbf{X}_{i-j}^1$ of order M_x that is nested inside of another Toeplitz block of order M_y , i.e. the matrix $\mathbb{X}$:

$$\mathbb{X} = \begin{bmatrix} \mathbf{X}_0^1 & \mathbf{X}_{-1}^1 & \mathbf{X}_{-2}^1 & \cdots & \mathbf{X}_{-M_y+1}^1 \\ \mathbf{X}_1^1 & \mathbf{X}_0^1 & \mathbf{X}_{-1}^1 & \cdots & \mathbf{X}_{-M_y+2}^1 \\ \mathbf{X}_2^1 & \mathbf{X}_1^1 & \mathbf{X}_0^1 & \cdots & \mathbf{X}_{-M_y+3}^1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mathbf{X}_{M_y-1}^1 & \mathbf{X}_{M_y-2}^1 & \mathbf{X}_{M_y-3}^1 & \cdots & \mathbf{X}_0^1 \end{bmatrix}, \quad (2.20)$$

where

$$\mathbf{X}_{ij}^1 = \mathbf{X}_{i-j}^1 = \begin{bmatrix} \mathbf{X}_0^2 & \mathbf{X}_{-1}^2 & \mathbf{X}_{-2}^2 & \cdots & \mathbf{X}_{-M_x+1}^2 \\ \mathbf{X}_1^2 & \mathbf{X}_0^2 & \mathbf{X}_{-1}^2 & \cdots & \mathbf{X}_{-M_x+2}^2 \\ \mathbf{X}_2^2 & \mathbf{X}_1^2 & \mathbf{X}_0^2 & \cdots & \mathbf{X}_{-M_x+3}^2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \mathbf{X}_{M_x-1}^2 & \mathbf{X}_{M_x-2}^2 & \mathbf{X}_{M_x-3}^2 & \cdots & \mathbf{X}_0^2 \end{bmatrix}, \quad (2.21)$$

with $\mathbf{X}_{i-j}^2 \in G_{2N+1}$; here $\mathbf{X}_0^2$ is the block identity matrix of order $2N + 1$.

3. High performance recursive algorithms for solving linear system of equations

Numerical resolution of the complex-valued linear system of equations (1.1) is considered in this section. We take advantage of the structure of matrix $\mathbb{X}$ defined by eq. (1.2): its block diagonals are identity matrices, and off-diagonal blocks are obtained by multiplying the matrix $\mathbf{T}^{(j)}$ by $\mathbf{P}^{j,m}$, which allows us to solve eq. (1.1) using direct linear solvers. Nonetheless, for a large number of scatterers, especially at high frequencies, eq. (1.1) becomes a large-scale complex-valued linear system with complexity growing as the frequency and number of scatterers increase. Solution by direct methods needs excessive computational time and memory to store the system, requiring the development of iterative and recursive algorithms. Here we describe some recursive techniques suitable for parallel computing.

To be specific, we consider a planar configuration of large number of cylindrical scatterers at high frequencies leading to a large scale complex valued linear system, eq. (1.1) is a complex-valued, full, non-symmetric matrix of order $(2N + 1) \cdot M$ with $N = N_j = N_m$. Each cylinder has to have the same physical properties and radius, i.e. the transition matrices $\mathbf{T}^{(j)} = \mathbf{T}$ ($j = \overline{1, M}$) should be the same. The method does not work for a configuration of scatterers with randomly distributed boundary conditions. It also cannot be employed if the distances between the neighboring cylinders, located in one row or one column of cluster, change. The approach works for a row or column of cylindrical rods and shells of the same radius; for quadratic, rectangular and triangular lattice of 2D phononic crystals. It can also be applied to 3D phononic crystals with cubic lattice structure.

3.1. Recursive algorithms for linear Toeplitz systems

3.1.1. Orthogonal polynomials and Hermitian Toeplitz matrices

An Hermitian positive definite Toeplitz matrix $\mathbf{P}_n$ and the Szegő orthogonal polynomials $\varphi_n(\mathbf{z})$ [33] defined on the unit circle $|\mathbf{z}| = 1$ satisfy the orthogonality condition [43]

$$\begin{bmatrix} \bar{\varphi}_{00} & \bar{\varphi}_{01} & \bar{\varphi}_{02} & \cdots & \bar{\varphi}_{0n} \\ \bar{\varphi}_{10} & \bar{\varphi}_{11} & \bar{\varphi}_{12} & \cdots & \bar{\varphi}_{1n} \\ \bar{\varphi}_{20} & \bar{\varphi}_{21} & \bar{\varphi}_{22} & \cdots & \bar{\varphi}_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \bar{\varphi}_{n0} & \bar{\varphi}_{n1} & \bar{\varphi}_{n2} & \cdots & \bar{\varphi}_{nn} \end{bmatrix} \mathbf{P}_n \begin{bmatrix} \varphi_{00} & \varphi_{01} & \varphi_{02} & \cdots & \varphi_{0n} \\ \varphi_{11} & \varphi_{12} & \cdots & \varphi_{1n} \\ \varphi_{22} & \cdots & \varphi_{2n} \\ \mathbf{0} & \ddots & \vdots \\ \varphi_{nn} \end{bmatrix} = \mathbf{I}. \quad (3.22)$$

This is equivalent to the inverse form of Cholesky decomposition of $\mathbf{P}_n$ [43]. The last column of the upper triangular matrix multiplied by $\bar{\varphi}_{nn}$ is the last column of $\mathbf{P}_n^{-1}$. The Szegő polynomials can be written explicitly as [30]:

$$\varphi_0(\mathbf{z}) = D_0^{-\frac{1}{2}} = P_0^{-\frac{1}{2}},$$

$$\varphi_n(\mathbf{z}) = (D_{n-1} D_n)^{-\frac{1}{2}} \det \begin{bmatrix} P_0 & P_{-1} & P_{-2} & \cdots & P_{-n} \\ P_1 & P_0 & P_{-1} & \cdots & P_{-n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ P_{n-1} & P_{n-2} & P_{n-3} & \cdots & P_{-1} \\ 1 & \mathbf{z} & \mathbf{z}^2 & \cdots & \mathbf{z}^n \end{bmatrix}, \quad n \geq 1, \quad (3.23)$$

where $D_n = \det(P_{q-l})_0^n$ is the determinant of the Toeplitz matrix $\mathbf{P}_n = [P_{q-l}]_{q,l=0}^n$.

Szegő [32,30,33] introduced the theory of orthogonal polynomials on a unit circle while studying the spectrum of Hermitian Toeplitz matrices in the 1920s. Hermitian Toeplitz matrices and operators and associated orthogonal polynomials on a unit circle were also studied by Geronimus [34], Krein [35], and others [36–38]. The idea of orthogonality can be extended to the notion of biorthogonality [39]. Generalizations to biorthogonal polynomials that correspond to non-Hermitian Toeplitz matrices and operators were investigated by Baxter [40,8,41], Trench [6], Gohberg and Semencul [10], Kailath et al. [42], Voevodin and Tyrtshnikov [9], Tyrtshnikov [43], Brezinski [44], Heinig and Rost [11], Freund et al. [45], etc.

3.1.2. Biorthogonal polynomials for inverting non-Hermitian Toeplitz matrices

Baxter [40] generalized the above results to non-Hermitian Toeplitz matrices. Let $\mathbf{P}_n$ be non-Hermitian Toeplitz, then the biorthogonal Szegő polynomials $\varphi_n(\mathbf{z})$ and $\psi_n(\mathbf{z})$ defined on the unit circle $|\mathbf{z}| = 1$ satisfy [43]

$$\begin{bmatrix} \psi_{00} & & & & \\ \psi_{01} & \psi_{11} & & & \mathbf{0} \\ \psi_{02} & \psi_{12} & \psi_{22} & & \\ \vdots & \vdots & \vdots & \ddots & \\ \psi_{0n} & \psi_{1n} & \psi_{2n} & \cdots & \psi_{nn} \end{bmatrix} \mathbf{P}_n \begin{bmatrix} \varphi_{00} & \varphi_{01} & \varphi_{02} & \cdots & \varphi_{0n} \\ & \varphi_{11} & \varphi_{12} & \cdots & \varphi_{1n} \\ & & \varphi_{22} & \cdots & \varphi_{2n} \\ \mathbf{0} & & & \ddots & \vdots \\ & & & & \varphi_{nn} \end{bmatrix} = \mathbf{I}. \quad (3.24)$$

Here, φ_{nn} multiplied by the last row of the lower triangular matrix defines the last row of the inverse matrix $\mathbf{P}_n^{-1}$, and the last column of the upper triangular matrix multiplied by ψ_{nn} is the last column of $\mathbf{P}_n^{-1}$. Note the equality of coefficients $\varphi_{nn} = \psi_{nn}$ in eq. (3.24) which is required to uniquely determine (to within a plus or minus sign) $\varphi_n(\mathbf{z})$ and $\psi_n(\mathbf{z})$ [40].

If the leading principal minors of matrix $\mathbf{P}_n$ are nonzero, then the elements of the inverse matrix $\mathbf{P}_n^{-1}$ can be reproduced using Christoffel–Darboux formulae [33] as

$$[\mathbf{P}_n^{-1}]_{ql} = [\mathbf{P}_n^{-1}]_{q-1, l-1} + \psi_{n-q} \varphi_{n-l} - \varphi_{q-1} \psi_{l-1} \quad (0 \leq q, l \leq n). \quad (3.25)$$

This formula is analogous to Trench's [6] Levinson-type recursion algorithm for the inverse of $\mathbf{P}_n$. Summing up the increments $[\mathbf{P}_n^{-1}]_{ql} - [\mathbf{P}_n^{-1}]_{q-1, l-1}$, the inverse matrix can be written explicitly in the matrix form:

$$\mathbf{P}_n^{-1} = \begin{bmatrix} \psi_{nn} & & & 0 \\ \psi_{n-1, n} & \psi_{nn} & & \\ \vdots & \vdots & \ddots & \\ \psi_{0, n} & \psi_{1, n} & \cdots & \psi_{nn} \end{bmatrix} \begin{bmatrix} \varphi_{nn} & \varphi_{n-1, n} & \cdots & \varphi_{0, n} \\ & \varphi_{nn} & \cdots & \varphi_{1, n} \\ & & \ddots & \vdots \\ 0 & & & \varphi_{n, n} \end{bmatrix} - \begin{bmatrix} 0 & & & 0 \\ \varphi_{0, n} & 0 & & \\ \vdots & \ddots & \ddots & \\ \varphi_{n-1, n} & \cdots & \varphi_{0, n} & 0 \end{bmatrix} \begin{bmatrix} 0 & \psi_{0, n} & \cdots & \psi_{n-1, n} \\ & \ddots & \ddots & \vdots \\ & & 0 & \psi_{0, n} \\ 0 & & & 0 \end{bmatrix}. \quad (3.26)$$

This formula represents the inverse of the Toeplitz matrix as the difference of products of two semicirculant matrices, i.e. the lower and upper triangular Toeplitz matrices. An alternative derivation was given by Baxter and Hirschman [41]; they showed that the inverse of the non-Hermitian Toeplitz matrix $\mathbf{P}_n$ can be uniquely defined by the solutions of the system [10]

$$\sum_{l=0}^n P_{q-l} x_l = \delta_{q,0}, \quad \sum_{l=0}^n P_{q-l} y_{l-n} = \delta_{q,n} \quad (q = 0, 1, \dots, n) \quad (3.27)$$

if the polynomials

$$\chi(\mathbf{z}) = \sum_{q=0}^n x_q \mathbf{z}^q, \quad \gamma(\mathbf{z}) = \sum_{q=0}^n y_{-q} \mathbf{z}^q \quad (3.28)$$

are not zero in $|\mathbf{z}| \leq 1$. For $x_0 \neq 0$, Gohberg and Semencul [10] showed that if the system (3.27) has solutions then the matrix $\mathbf{P}_n$ is nondegenerate, and derived an explicit formula for its inverse:

$$\mathbf{P}_n^{-1} = x_0^{-1} \left\{ \begin{bmatrix} x_0 & 0 & \cdots & 0 \\ x_1 & x_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ x_n & x_{n-1} & \cdots & x_0 \end{bmatrix} \begin{bmatrix} y_0 & y_{-1} & \cdots & y_{-n} \\ 0 & y_0 & \cdots & y_{-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & y_0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ y_{-n} & 0 & 0 & \cdots & 0 & 0 \\ y_{-n+1} & y_{-n} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ y_{-1} & y_{-2} & y_{-3} & \cdots & y_{-n} & 0 \end{bmatrix} \begin{bmatrix} 0 & x_n & x_{n-1} & \cdots & x_1 \\ 0 & 0 & x_n & \cdots & x_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & x_n \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix} \right\}. \quad (3.29)$$

Thus, $\mathbf{P}_n^{-1}$ can be constructed by elements of its first and last columns. As we mentioned earlier, the scalar algorithms (3.25) and (3.29) for non-Hermitian Toeplitz matrices correspond to their block analogs [7,9], and block multiplications and additions in block algorithms correspond to multiplications and additions in the scalar case. If the matrix $\mathbf{P}_n$ has a block Toeplitz structure, its inverse $\mathbf{P}_n^{-1}$ can be formed analogously by elements of its first and last block columns, and first and last block rows [9]. Further details are given next.

3.2. Recursive algorithms for Block Toeplitz systems

3.2.1. Algorithms for BT matrix of level 1

For a configuration of one row or column of cylinders, the matrix $\mathbb{X}$ given by eq. (2.19) is a BT matrix of level one, i.e. $\mathbb{X} \in T_M G_{2N+1}$. Finding the inverse of a matrix that has a specific structure does not always require finding all elements of the inverse matrix. Instead it requires the development of algorithms that ensure the compact form of the inverse matrix and allow its fast multiplication on an arbitrary vector. Such an approach was proposed by Voevodin and Tyrtshnikov [9] for BT matrices of level 1. We will use this method to find the inverse of $\mathbb{X}$ and solve the system (1.1) by adapting their notation. For $0 \leq m \leq M-1$, let us denote by $\mathbb{X}_m$ the leading submatrix consisting of blocks $\mathbf{X}_{i-j}^1$ where $1 \leq i, j \leq m+1$; particularly $\mathbb{X}_{M-1} = \mathbb{X}$ and $\mathbb{X}^{-1} = \mathbb{X}_{M-1}^{-1}$. If all leading submatrices are nondegenerate, then according to [9, Theorem 5.7], $\forall m$ the matrix $\mathbb{X}_m^{-1}$ can be restored using its first and last block columns, and first and last block rows. We will denote the block column vectors by $\mathbf{v}_i^{(m)}, \mathbf{y}_i^{(m)}$, and the block row vectors by $\mathbf{z}_i^{(m)}, \mathbf{w}_i^{(m)}$ ($0 \leq i \leq m$). Importantly, these block vectors can be calculated recursively as the index varies m from 0 to $M-1$.

Let $\mathbb{X}$ be a nondegenerate complex valued BT matrix of order M with blocks of order $2N+1$. Assume that the block vectors $\mathbf{v} = [\mathbf{v}_0 \mathbf{v}_1 \cdots \mathbf{v}_{M-1}]^T$ and $\mathbf{y} = [\mathbf{y}_0 \mathbf{y}_1 \cdots \mathbf{y}_{M-1}]^T$ satisfy

$$\mathbb{X}\mathbf{v} = \mathbf{e}, \quad \mathbb{X}\mathbf{y} = \mathbb{J}\mathbf{e}, \quad (3.30)$$

and correspond to the first and the last block columns of inverse matrix $\mathbb{X}^{-1}$, and $\mathbf{z} = [\mathbf{z}_0 \mathbf{z}_1 \cdots \mathbf{z}_{M-1}]$ and $\mathbf{w} = [\mathbf{w}_0 \mathbf{w}_1 \cdots \mathbf{w}_{M-1}]$ satisfy

$$\mathbf{z}\mathbb{X} = \mathbf{e}^T, \quad \mathbf{w}\mathbb{X} = \mathbf{e}^T \mathbb{J}, \quad (3.31)$$

and correspond to the first and the last block rows of inverse matrix $\mathbb{X}^{-1}$, where $\mathbf{e}$ is the unit block vector, and $\mathbb{J}$ is the permutation matrix:

$$\mathbf{e} = \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \mathbb{J} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{I} \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{I} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{0} & \mathbf{I} & \cdots & \mathbf{0} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} \end{bmatrix} \quad (3.32)$$

where $\mathbf{I}$ is the block identity matrix of order $2N+1$. Then, if the blocks $\mathbf{v}_0$ and $\mathbf{y}_{M-1}$ are nondegenerate, and $\mathbf{v}_0 = \mathbf{z}_0$, $\mathbf{y}_{M-1} = \mathbf{w}_{M-1}$, the matrix inverse of $\mathbb{X} = \mathbb{X}_{M-1}$ can be obtained as

$$\begin{aligned} \mathbb{X}^{-1} = & \begin{bmatrix} \mathbf{v}_0 & & & \mathbf{0} \\ \mathbf{v}_1 & \mathbf{v}_0 & & \\ \cdots & \cdots & \cdots & \\ \mathbf{v}_{M-1} & \mathbf{v}_{M-2} & \cdots & \mathbf{v}_0 \end{bmatrix} \mathbb{D}_{\mathbf{v}_0^{-1}} \begin{bmatrix} \mathbf{z}_0 & \mathbf{z}_1 & \cdots & \mathbf{z}_{M-1} \\ & \mathbf{z}_0 & \mathbf{z}_1 & \mathbf{z}_{M-2} \\ & & \cdots & \\ \mathbf{0} & & & \mathbf{z}_0 \end{bmatrix} \\ & - \begin{bmatrix} \mathbf{0} & & & \mathbf{0} \\ \mathbf{y}_0 & & & \\ \cdots & \cdots & \cdots & \\ \mathbf{y}_{M-2} & \mathbf{y}_{M-3} & \cdots & \mathbf{0} \end{bmatrix} \mathbb{D}_{\mathbf{y}_{M-1}^{-1}} \begin{bmatrix} \mathbf{0} & \mathbf{w}_0 & \cdots & \mathbf{w}_{M-2} \\ & \cdots & \cdots & \\ \mathbf{0} & \mathbf{0} & \mathbf{w}_0 & \\ & & \mathbf{0} \end{bmatrix}, \end{aligned} \quad (3.33)$$

or

$$\begin{aligned} \mathbb{X}^{-1} = & \begin{bmatrix} \mathbf{y}_{M-1} & \mathbf{y}_{M-2} & \cdots & \mathbf{y}_0 \\ & \mathbf{y}_{M-1} & \mathbf{y}_{M-2} & \cdots & \mathbf{y}_1 \\ & & \cdots & \cdots & \\ \mathbf{0} & & & \mathbf{y}_{M-1} \end{bmatrix} \mathbb{D}_{\mathbf{y}_{M-1}^{-1}} \begin{bmatrix} \mathbf{w}_{M-1} & & \mathbf{0} \\ \mathbf{w}_{M-2} & \mathbf{w}_{M-1} & \\ & \cdots & \\ \mathbf{w}_0 & \mathbf{w}_1 & \cdots & \mathbf{w}_{M-1} \end{bmatrix} \\ & - \begin{bmatrix} \mathbf{0} & \mathbf{v}_{M-1} & \cdots & \mathbf{v}_1 \\ & \cdots & \cdots & \\ \mathbf{0} & \mathbf{0} & \mathbf{v}_{M-1} & \\ \mathbf{0} & & \mathbf{0} \end{bmatrix} \mathbb{D}_{\mathbf{v}_0^{-1}} \begin{bmatrix} \mathbf{0} & & \mathbf{0} \\ \mathbf{z}_{M-1} & \mathbf{0} & \\ \cdots & \cdots & \\ \mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{0} \end{bmatrix}, \end{aligned} \quad (3.34)$$

where

$$\mathbb{D}_{\mathbf{v}_0^{-1}} = \begin{bmatrix} \mathbf{v}_0^{-1} & & \mathbf{0} \\ & \mathbf{v}_0^{-1} & \\ & & \ddots \\ \mathbf{0} & & & \mathbf{v}_0^{-1} \end{bmatrix}, \quad \mathbb{D}_{\mathbf{y}_{M-1}^{-1}} = \begin{bmatrix} \mathbf{y}_{M-1}^{-1} & & \mathbf{0} \\ & \mathbf{y}_{M-1}^{-1} & \\ & & \ddots \\ \mathbf{0} & & & \mathbf{y}_{M-1}^{-1} \end{bmatrix}. \quad (3.35)$$

Here the upper indices of blocks are dropped for convenience: $\mathbf{v}_i = \mathbf{v}_i^{M-1}$, $\mathbf{y}_i = \mathbf{y}_i^{M-1}$, $\mathbf{z}_i = \mathbf{z}_i^{M-1}$, $\mathbf{w}_i = \mathbf{w}_i^{M-1}$ for $i = 0, 1, \dots, M-1$. Thus, the inverse of the BT matrix $\mathbb{X}$ can be evaluated as the difference of products of semicirculant matrices.

We will compute the block vectors recursively using the recurrent block algorithms given in [9] for calculating block vectors $\mathbf{v}_i^{(m)}$, $\mathbf{y}_i^{(m)}$ and $\mathbf{z}_i^{(m)}$, $\mathbf{w}_i^{(m)}$ with the index m ranging from 0 to $M - 1$. To reduce the number of operations used, instead of computing these blocks directly each block was normalized such that:

$$\mathbf{v}_i^{(m)} = \tilde{\mathbf{v}}_i^{(m)} \mathbf{p}_m, \quad \mathbf{y}_i^{(m)} = \tilde{\mathbf{y}}_i^{(m)} \mathbf{q}_m, \quad 0 \leq i \leq m, \quad (3.36)$$

for column blocks, or

$$\mathbf{z}_i^{(m)} = \hat{\mathbf{p}}_m \tilde{\mathbf{z}}_i^{(m)}, \quad \mathbf{w}_i^{(m)} = \hat{\mathbf{w}}_i^{(m)} \hat{\mathbf{q}}_m, \quad 0 \leq i \leq m \quad (3.37)$$

for row blocks. Here $\tilde{\mathbf{v}}_i^{(m)}$, $\tilde{\mathbf{y}}_i^{(m)}$, $\tilde{\mathbf{z}}_i^{(m)}$ and $\tilde{\mathbf{w}}_i^{(m)}$ are normalized blocks, and $\mathbf{p}_m$, $\mathbf{q}_m$, $\hat{\mathbf{p}}_m$ and $\hat{\mathbf{q}}_m$ are non-degenerate blocks acting as normalizing multipliers.

The recursion algorithm for normalized column blocks $\tilde{\mathbf{v}}_i^{(m)}$, $\tilde{\mathbf{y}}_i^{(m)}$ is formulated as follows [9]:

$\mathbf{m} = 0$: $\mathbf{p}_0$, $\mathbf{q}_0$ – any non-degenerate blocks

$$\tilde{\mathbf{v}}_0^{(0)} = \mathbf{X}_0^{-1} \mathbf{p}_0^{-1}, \quad \tilde{\mathbf{y}}_0^{(0)} = \mathbf{X}_0^{-1} \mathbf{q}_0^{-1}; \quad (3.38)$$

$\mathbf{m} = 1, \dots, M - 1$:

$$\begin{aligned} \mathbf{s}_m &= -\mathbf{q}_{m-1} (\mathbf{X}_m \tilde{\mathbf{v}}_0^{(m-1)} + \mathbf{X}_{m-1} \tilde{\mathbf{v}}_1^{(m-1)} + \dots + \mathbf{X}_1 \tilde{\mathbf{v}}_{m-1}^{(m-1)}), \\ \mathbf{t}_m &= -\mathbf{p}_{m-1} (\mathbf{X}_{-1} \tilde{\mathbf{y}}_0^{(m-1)} + \mathbf{X}_{-2} \tilde{\mathbf{y}}_1^{(m-1)} + \dots + \mathbf{X}_{-m} \tilde{\mathbf{y}}_{m-1}^{(m-1)}), \\ \mathbf{p}_m &= (\mathbf{I} - \mathbf{t}_m \mathbf{s}_m)^{-1} \mathbf{p}_{m-1}, \quad \mathbf{q}_m = (\mathbf{I} - \mathbf{s}_m \mathbf{t}_m)^{-1} \mathbf{q}_{m-1}, \\ [\tilde{\mathbf{v}}_0^{(m)} \tilde{\mathbf{v}}_1^{(m)} \dots \tilde{\mathbf{v}}_m^{(m)}]^T &= [\tilde{\mathbf{v}}_0^{(m-1)} \dots \tilde{\mathbf{v}}_{m-1}^{(m-1)} 0]^T + [0 \tilde{\mathbf{y}}_0^{(m-1)} \dots \tilde{\mathbf{y}}_{m-1}^{(m-1)}]^T \mathbf{s}_m, \\ [\tilde{\mathbf{y}}_0^{(m)} \tilde{\mathbf{y}}_1^{(m)} \dots \tilde{\mathbf{y}}_m^{(m)}]^T &= [0 \tilde{\mathbf{y}}_0^{(m-1)} \tilde{\mathbf{y}}_1^{(m-1)} \dots \tilde{\mathbf{y}}_{m-1}^{(m-1)}]^T + [\tilde{\mathbf{v}}_0^{(m-1)} \tilde{\mathbf{v}}_1^{(m-1)} \dots \tilde{\mathbf{v}}_{m-1}^{(m-1)} 0]^T \mathbf{t}_m. \end{aligned} \quad (3.39)$$

The algorithm for normalized row blocks $\tilde{\mathbf{z}}_i^{(m)}$, $\tilde{\mathbf{w}}_i^{(m)}$ is of the following form [9]:

$\mathbf{m} = 0$: $\hat{\mathbf{p}}_0$, $\hat{\mathbf{q}}_0$ – any nondegenerate blocks

$$\tilde{\mathbf{z}}_0^{(0)} = \mathbf{X}_0^{-1} \hat{\mathbf{p}}_0^{-1}, \quad \tilde{\mathbf{w}}_0^{(0)} = \mathbf{X}_0^{-1} \hat{\mathbf{q}}_0^{-1}; \quad (3.40)$$

$\mathbf{m} = 1, \dots, M - 1$:

$$\begin{aligned} \hat{\mathbf{s}}_m &= -(\tilde{\mathbf{z}}_0^{(m-1)} \mathbf{X}_{-m} + \tilde{\mathbf{z}}_1^{(m-1)} \mathbf{X}_{-m+1} + \dots + \tilde{\mathbf{z}}_{m-1}^{(m-1)} \mathbf{X}_{-1}) \hat{\mathbf{q}}_{m-1}, \\ \hat{\mathbf{t}}_m &= -(\tilde{\mathbf{w}}_0^{(m-1)} \mathbf{X}_1 + \tilde{\mathbf{w}}_1^{(m-1)} \mathbf{X}_2 + \dots + \tilde{\mathbf{w}}_{m-1}^{(m-1)} \mathbf{X}_m) \hat{\mathbf{p}}_{m-1}, \\ \hat{\mathbf{p}}_m &= \hat{\mathbf{p}}_{m-1} (\mathbf{I} - \hat{\mathbf{s}}_m \hat{\mathbf{t}}_m)^{-1}, \quad \hat{\mathbf{q}}_m = \hat{\mathbf{q}}_{m-1} (\mathbf{I} - \hat{\mathbf{t}}_m \hat{\mathbf{s}}_m)^{-1}, \\ [\tilde{\mathbf{z}}_0^{(m)} \tilde{\mathbf{z}}_1^{(m)} \dots \tilde{\mathbf{z}}_m^{(m)}] &= [\tilde{\mathbf{z}}_0^{(m-1)} \tilde{\mathbf{z}}_1^{(m-1)} \dots \tilde{\mathbf{z}}_{m-1}^{(m-1)} 0] + \hat{\mathbf{s}}_m [0 \tilde{\mathbf{w}}_0^{(m-1)} \tilde{\mathbf{w}}_1^{(m-1)} \dots \tilde{\mathbf{w}}_{m-1}^{(m-1)}], \\ [\tilde{\mathbf{w}}_0^{(m)} \tilde{\mathbf{w}}_1^{(m)} \dots \tilde{\mathbf{w}}_m^{(m)}] &= [0 \tilde{\mathbf{w}}_0^{(m-1)} \tilde{\mathbf{w}}_1^{(m-1)} \dots \tilde{\mathbf{w}}_{m-1}^{(m-1)}] + \hat{\mathbf{t}}_m [\tilde{\mathbf{z}}_0^{(m-1)} \tilde{\mathbf{z}}_1^{(m-1)} \dots \tilde{\mathbf{z}}_{m-1}^{(m-1)} 0]. \end{aligned} \quad (3.41)$$

Each of the algorithms require $2(2N + 1)^3 M^2$ operations of multiplication and the same number of addition and subtraction operations.

3.2.2. Recursive technique for BT matrix of level 2

We cannot directly apply eq. (3.34) to BT matrices of level 2, $\mathbb{X} \in T_{M_y, M_x} G_{2N+1}$. However, a block matrix $\mathbb{X} \in T_{M_y, M_x} G_{2N+1}$ can also be written as a BT matrix of level 1: $\mathbb{X} \in T_{M_y} G_{M_x(2N+1)}$, i.e. the block matrix $\mathbb{X}$ can be written in the form of eq. (2.20) with $\mathbf{X}_{ij}^1 = \mathbf{X}_{i-j}^1 \in G_{M_x(2N+1)}$ and $\mathbf{X}_0^1$ is the identity matrix of order $M_x(2N + 1)$. Therefore, we can still use eq. (3.34) to solve a linear system with $\mathbb{X} \in T_{M_y} G_{M_x(2N+1)}$ for configurations of M_x rows and M_y columns of cylinders.

Another possibility for solving a linear system (1.1) with a BT matrix of level 2, $\mathbb{X} \in T_{M_y, M_x} G_{2N+1}$, is to use the GMRES solver with a fast algorithm for matrix vector product (MVP), as proposed by Barrowes et al. [15,14] for multilevel BT matrices. The method is based on a Fast Fourier Transform and expedites MVP involving multilevel BT matrices with minimal memory requirements and computational cost. The method was applied to electromagnetic 3D scattering problems [15].

4. Numerical results

We present results produced using the recursive algorithms for BT matrices of level 1 described in Section 3.2.1. This recursive technique is included in the TOEPLITZ package, a library which implements a Toeplitz matrix system solver. The TOEPLITZ package solves a variety of Toeplitz and Circulant linear systems, their block analogs, and some other more

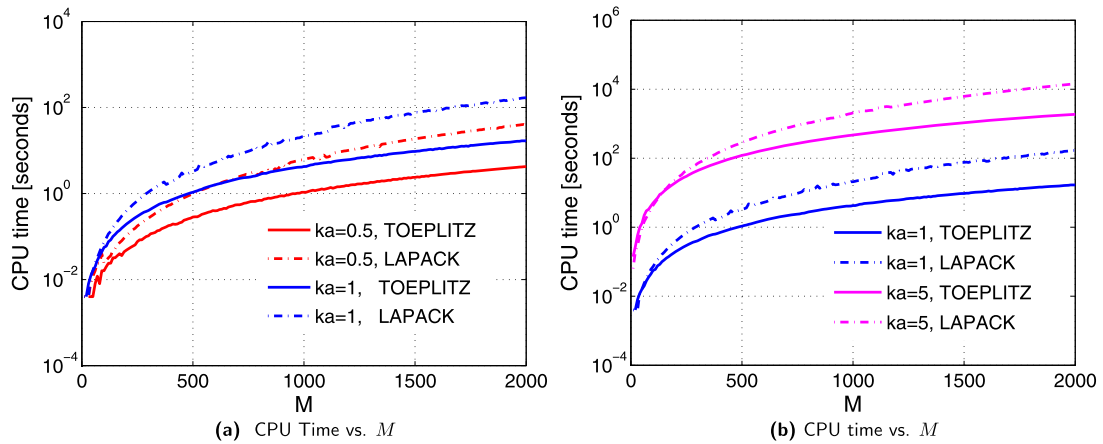


Fig. 3. Variation of CPU time taken to calculate the scattering coefficients $B_n^{(m)}$ with a number of cylinders M for selected values of ka for a cluster of rigid cylinders submerged in fluid medium using two solvers: LAPACK and the recursive algorithm described in Section 3.2.1.

complicated forms. The TOEPLITZ package was written in Fortran77 by a joint working group of American and Soviet mathematicians in the early 1980s [7]. The original version of the TOEPLITZ library is available in the TOEPLITZ subdirectory of the NETLIB web site www.netlib.org. The modified version of the TOEPLITZ package, converted to Fortran90, is provided at

http://people.sc.fsu.edu/~jburkardt/f_src/toeplitz/toeplitz.html

The TOEPLITZ package [7] is used here to solve several large acoustic MS problems. For verification and comparison, we compared the results for the TOEPLITZ package with the LAPACK (Intel MKL) library. The computations are performed in Intel FORTRAN on the Rutgers University SOE HPC Cluster which is based on Intel Sandy Bridge 2670 CPUs, 16 cores and 128 GB of RAM per node.

We consider a 2D rectangular array of very closely spaced rigid cylinders of radius a ; the distance between the centers of two neighboring cylinders is taken as $d = 2a \times 1.01$, resulting in very strong near-field interaction effects. The incident field is excited by the near-field source located at point $\mathbf{S} = (-50a, 50a)$. The proposed method can also be applied for plane wave incidence, achieved by increasing the source position distance, e.g. by considering the source at $\mathbf{S} = (-1000a, 1000a)$. The size of the matrix $\mathbb{X}$ is $M(2N+1) \times M(2N+1)$ and the number of the scattering coefficients $B_n^{(m)}$ is equal to $M(2N+1)$ where M is the total number of scatterers and N is the truncated mode number. N obviously should scale with frequency; extensive experience in single and multiple scattering has shown that $N = 2.5ka$ is more than adequate.

Note that such a strong interaction $d = 2a \times 1.01$ cannot be considered by means of the Neumann series expansion method. It is shown in [1] that for very closely spaced cluster of M rigid cylinders with $d = 2a \times 1.01$, the Neumann series converges only for $M = 2$ two rigid cylinders in the frequency range $ka = 0.1, 50$. For a cluster with $M \geq 2$ and high frequencies, the Neumann series converges slowly and depends strongly on the cylinder separation distance d and the frequency. The TOEPLITZ solver does not depend on the distance d , and works well at high and low frequency regimes, requiring less resources (computation time, RAM, CPU) than LAPACK library at high frequencies and large numbers of scatterers.

We determined the CPU time taken to calculate the scattering coefficients $B_n^{(m)}$ for the cluster of cylinders using two solvers: LAPACK and TOEPLITZ. Fig. 3 illustrates the variation of CPU time with the number of cylinders M for selected values of $ka = 0.5, 1, 5$. Figs. 4 and 5 show the CPU time dependence vs. nondimensional frequency ka . In Fig. 4, computations are performed considering $nfreq = 200$ frequency nodes for a symmetric configuration centered at the origin (see Fig. 2) at fixed values of numbers of scatterers, $M = 200$: $M_x = 10$, $M_y = 20$ and $M = 1000$: $M_x = 10$, $M_y = 100$. For $M = 1000$ at fixed value of $ka = 10$ with the size of the matrix $\mathbb{X}$: 51000×51000 , it took approximately 5 hours to evaluate the $B_n^{(m)}$ coefficients using the LAPACK library and 61 minutes using the TOEPLITZ package. The TOEPLITZ solver is clearly faster than the LAPACK solver. The advantage of the recursive approach increases with the rise of M and ka . These results together demonstrate that the recursive technique takes less time to find the scattering coefficients and is therefore more computationally efficient as compared with the direct method.

In Fig. 5, we considered a high frequency regime for a symmetric configuration centered at the origin at fixed values of numbers of scatterers, $M = 100, 150, 200, 250, 300$ with $M_x = 5$ and varying values of $M_y = 20, 60$ accordingly. We took $nfreq = 100$ frequency nodes in Fig. 5(a), and $nfreq = 50$ frequency nodes in Fig. 5(b) because of the increase of computation time with M and ka ; for instance, for $M = 150$ it took 19 days to evaluate a graph in Fig. 5(a) using LAPACK solver sequentially. The graphs in the high frequency regime again show the advantage of recursive algorithms over Gaussian elimination with the increase of number of scatterers and frequency. At $M = 100$, the LAPACK solver computes faster than the TOEPLITZ solver. However, starting with $M = 150$ the TOEPLITZ method shows better performance than LAPACK; the computation time difference grows with increasing the value of M . For $M = 300$ using the LAPACK library and requesting

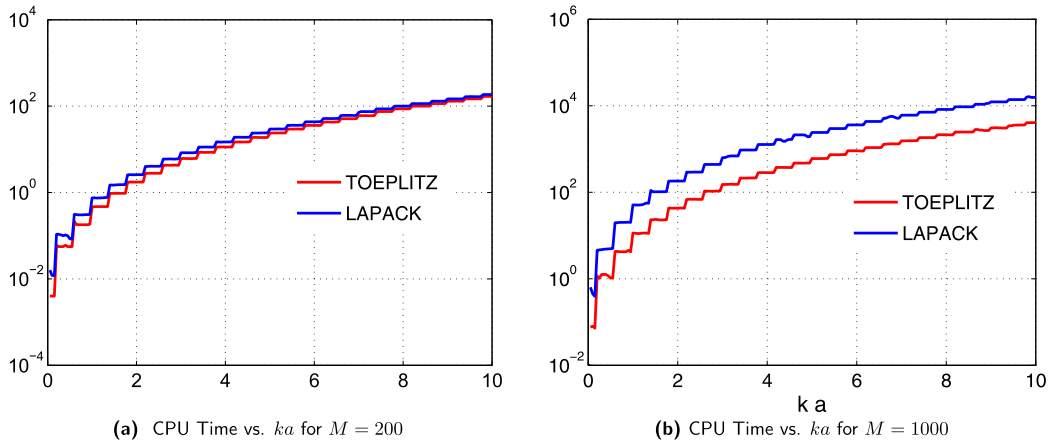


Fig. 4. Variation of CPU time taken to calculate the scattering coefficients $B_n^{(m)}$ with a nondimensional wavenumber ka ($nfreq = 200$ frequency intervals) for a cluster of rigid cylinders submerged in a fluid medium using two solvers: LAPACK and TOEPLITZ solvers.

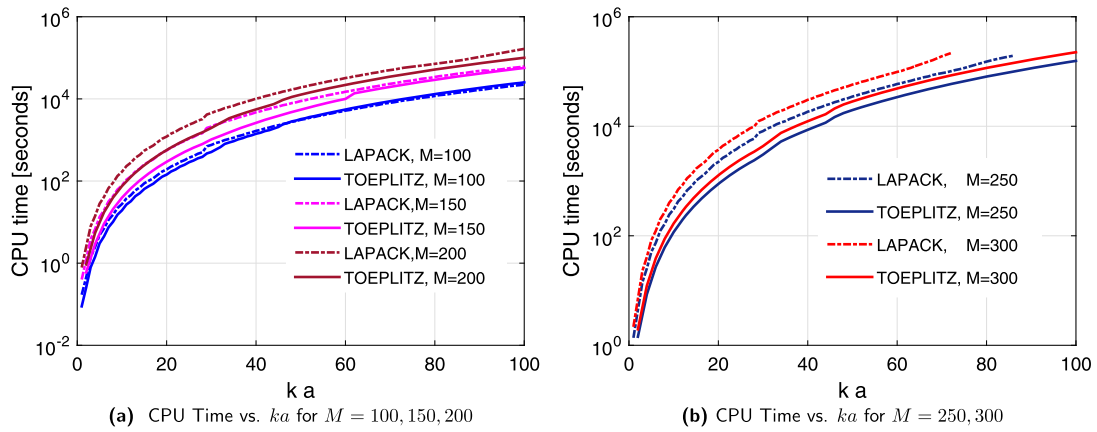


Fig. 5. Variation of CPU time taken to calculate the scattering coefficients $B_n^{(m)}$ with a nondimensional wavenumber ka for a cluster of rigid cylinders submerged in a fluid medium using two solvers: LAPACK and TOEPLITZ solvers.

Table 1

Total elapsed time to find the unknown coefficients using TOEPLITZ library for a configuration of $M = 200$ rigid cylinders with $nfreq = 200$ (frequency intervals), and OMP without scheduling.

Number of threads	Total elapsed time (min)
1	129.2
5	74.3
10	43.9
15	31.5
16	28.8

all available RAM in one node with 128 GB RAM, “insufficient virtual memory” error message was received. We were not able to get results for values of ka starting at $ka = 88$ with the size of the matrix $\mathbb{X}$: $110\,250 \times 110\,250$ for $M = 250$, and at $ka = 74$ with the size of the matrix $\mathbb{X}$: $111\,300 \times 111\,300$ for $M = 300$. Nonetheless, TOEPLITZ solver was able to evaluate the scattering coefficients at all considered values of frequency ka and number of scatterers M .

To further expedite the simulation run time, the Fortran codes are parallelized using OpenMP. OpenMP is an implementation of multithreading; it runs the section of the code in parallel by dividing a task among available threads. We performed parallel computations over the frequency intervals using “OMP dynamic scheduling”, “OMP static scheduling”, and “OMP” without scheduling by varying the chunk size and the number of threads used. The increase of number of threads reduced the total elapsed time to solve a linear system using TOEPLITZ package as expected.

Tables 1 and 2 evaluate the efficiency of parallelization using TOEPLITZ package and OpenMP compilers, for a configuration of $M_x = 10$ columns and $M_y = 20$ row of rigid cylinders at $nfreq = 200$ (frequency intervals). For a configuration of $M = 200$ cylinders the computation time reduced from 129.2 minutes using 1 thread to 14.9 minutes using 16 threads

Table 2

Total elapsed time to find the unknown coefficients using TOEPLITZ library using Dynamic and Static Schedules for a configuration of $M = 200$ rigid cylinders with $nfreq = 200$ (frequency intervals).

Number of threads	Chunk size	Total elapsed time (min)		Least value of total elapsed time (min)
		Dynamic Schedule	Static Schedule	
5	2	28.6	28.6	28.6
	3	29.7	29.0	
	5	31.9	31.6	
10	2	17.7	19.6	17.7
	3	19.1	20.7	
	5	21.6	21.6	
15	2	15.9	19.3	15.9
	3	16.3	19.5	
	5	18.7	18.7	
16	2	14.9	19.4	14.9
	3	16.5	22.5	
	5	17.1	18.6	

Table 3

Total elapsed time to find the unknown coefficients using TOEPLITZ and LAPACK libraries with Dynamic Schedule: chunk size = 2 and number of threads = 16 for a configuration of $M = 200$ and $M = 500$ rigid cylinders with $nfreq = 200$ (frequency intervals).

Number of scatterers	Total elapsed time (min)	
	TOEPLITZ solver	LAPACK solver
200	14.9	13.7
500	148.8	207.5

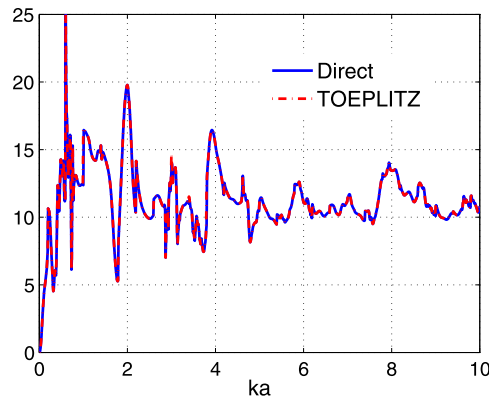


Fig. 6. Variation of total scattering cross section with a nondimensional frequency ka for a cluster of $M = 80$ rigid cylinders submerged in a fluid medium using two solvers: Direct and TOEPLITZ solvers.

with dynamic scheduling and chunk size = 2. Table 3 illustrates the comparison of total elapsed time to find the unknown coefficients using TOEPLITZ and LAPACK libraries on 16 threads with dynamic scheduling and chunk size = 2 varying the number of scatterers. As we can see for smaller number scatterers, $M = 200$ LAPACK library works faster but at larger value of scatterers, $M = 500$, TOEPLITZ solver is more effective and takes less run time and shows its advantage with increase of M and ka .

To check the accuracy of presented recursive approach, the total scattering cross section Q and the form function $|f^M|$ are evaluated by solving a linear system using Direct solver, backlash (left matrix divide) operator in Matlab, and TOEPLITZ solver in FORTRAN. The total scattering cross section Q is given by eq. (B.7) and the form function $|f^M|$ is defined by (B.5). The symmetric configuration is centered at the origin; it consists of a cluster of $M = 80$ ($M_x = 4$, $M_y = 20$) rigid cylinders with $d = 2a \times 1.01$ and submerged in a fluid medium. The source is positioned at $\mathbf{S} = (-50a, 50a)$. Figs. 6 and 7 illustrate correspondingly the variation of total scattering cross section and the backscattering form function $|f^M(\pi)|$ with respect to non-dimensional wavenumber ka . Here, we considered $nfreq = 1000$ frequency intervals. The graphs in each of these figures overlap. The results for the total scattering cross section Q and the form function $|f^M|$ show a good agreement between these two methods.

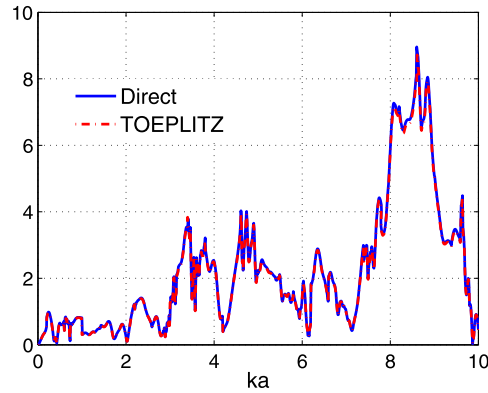


Fig. 7. Variation of backscattering form function $|f^M(\pi)|$ with a nondimensional frequency ka for a cluster of $M = 80$ rigid cylinders submerged in a fluid medium using two solvers: Direct and TOEPLITZ solvers.

5. Conclusions

The paper considers an effective implementation of a fast recursive technique for a solution of 2D MS problems. The MS problem formulation reduces to a system of linear algebraic equations using Graf's theorem; its complexity grows as the number of scatterers and frequency increases, requiring the development of techniques for parallel computing. Taking advantage of the Block Toeplitz structure of the system, the recursive algorithm is employed to increase the efficiency and reduce the computational cost. For the 2D MS problems considered, the recursive technique for BT matrix of level 1 showed computational time advantages over a direct method with the increase of nondimensional frequency ka and number of scatterers M . The numerical results show that the TOEPLITZ solver is clearly faster than the LAPACK solver. The parallelization of the FORTRAN codes using OpenMP multithreading, and Dynamic and Static Schedules reduces the simulation run time and speeds up the problem solution at high frequency regime for large number of scatterers. The approach works for a row or column of cylindrical rods and shells of the same radius; for quadratic, rectangular and triangular lattice of 2D phononic crystals. The concept employed in this work can be extended to model three-dimensional scattering problems. The considered recursive techniques can be applied to model 3D MS problems in acoustic, elastodynamic, and electromagnetic media. It can be employed to model 3D phononic crystals of cubic lattice. Preliminary work along these lines has been provided in [15] for an electromagnetic scattering by 3D spheres where the formulation leads to the linear system of BT structure of level 3 which is solved using fast MVP method. Alternatively, the recursive algorithm used in this work can be applied to BT matrix of level 3: $\mathbb{X} \in T_{M_z, M_y, M_x} G_{2N+1}$ by rearranging it as BT matrix of level 1: $\mathbb{X} \in T_{M_z} G_{M_y M_x (2N+1)}$. However, the MS problem could be solved even faster if the second BT level was taken into account. To accelerate the solution process, the approach needs to take into account a full multilevel structure of the system. Such approaches are developed for symmetric and Hermitian Toeplitz matrices and needs to be extended for non-Hermitian Block Toeplitz matrices to apply them for MS problems.

Acknowledgements

The authors would like to thank Dr. Yuriy Gulak for helpful discussions and for providing information on available solvers including the TOEPLITZ package. The authors also would like to thank referees for suggestions and helpful comments that enhanced this research.

Appendix A. Multiple scattering theory

Consider an acoustic multiple scattering by an arbitrary grating of M obstacles S_m ($m = \overline{1, M}$) of cylindrical shape. In general, each obstacle may have no rotational symmetry. We will refer to obstacles simply as cylinders but may consider elastic solid, rigid, or hollow cylinders of outer radii a_m , as well as thin, thick and multi-laminate cylindrical shells of outer a_m and inner b_m radii with and without attachments inside the shells. Let $\mathbf{x} = (x, y)$ be a position vector of a typical point in two-dimensional Cartesian coordinates with origin at O , and let us define plane polar coordinates (r_m, θ_m) at the centers O_m . An arbitrary planar configuration of cylinders is given in Fig. 1. Assume that the S_m ($m = \overline{1, M}$) cylinders have different physical properties and are located at the centers O_m , at $\mathbf{x} = \mathbf{l}_m$, the distance $|\mathbf{l}_m|$ from the origin O (see Fig. 1). Time harmonic dependence $e^{-i\omega t}$ is assumed but omitted in the following. The governing equation for the total pressure field $p(\mathbf{x})$ is the acoustic Helmholtz wave equation

$$\nabla^2 p + k^2 p = q, \quad (\text{A.1})$$

where $k = \omega/c$ is the wavenumber, c is the acoustic speed, ω is the frequency, and q represents sources. The total field $p(\mathbf{x})$ is defined as the sum of incident p_{inc} and scattered p_{sc} pressure fields:

$$p = p_{inc} + p_{sc}. \quad (\text{A.2})$$

The incident field in the neighborhood of cylinder S_m is given as

$$p_{inc}^{(m)} = \sum_{n=-\infty}^{\infty} A_n^{(m)} U_n^+(\mathbf{x}_m), \quad \mathbf{x}_m = \mathbf{x} - \mathbf{l}_m, \quad (\text{A.3})$$

where $\mathbf{x}_m$ is a position vector of point P with respect to the centers of multipoles at O_m (see Fig. 1). The function $U_n^\pm(\mathbf{x})$ is defined by

$$U_n^\pm(\mathbf{x}) = J_n(k|\mathbf{x}|)e^{\pm in \arg \mathbf{x}}, \quad (\text{A.4})$$

where $\arg \mathbf{x} \in [0, 2\pi)$ and $\arg(-\mathbf{x}) = (\arg \mathbf{x} \pm \pi) \bmod 2\pi$, and J_n is the Bessel function of the first kind of order n .

The total scattered field p_{sc} can be considered as a superposition of the scattered fields by all the cylinders in the configuration, and expanded as a sum of multipoles in the form:

$$p_{sc} = \sum_{m=1}^M p_{sc}^{(m)}, \quad p_{sc}^{(m)} = \sum_{n=-\infty}^{\infty} B_n^{(m)} V_n^+(\mathbf{x}_m), \quad (\text{A.5})$$

where $p_{sc}^{(m)}$ is the wave scattered by cylinder S_m , $B_n^{(m)}$ are the unknown coefficients, and the function $V_n^\pm(\mathbf{x})$ is defined by (1.3). In order to use boundary conditions on the surface of each cylinder S_m , we will express the total field in terms of r_m and θ_m using Graf's theorem [3, eq. (9.1.79)]:

$$V_l^+(\mathbf{x} - \mathbf{y}) = \sum_{n=-\infty}^{\infty} \begin{cases} V_n^+(\mathbf{x}) U_{n-l}^-(\mathbf{y}), & |\mathbf{x}| > |\mathbf{y}|, \\ U_n^+(\mathbf{x}) V_{n-l}^-(\mathbf{y}), & |\mathbf{x}| < |\mathbf{y}|. \end{cases} \quad (\text{A.6})$$

The functions $U_n^\pm(\mathbf{x})$ and $V_n^\pm(\mathbf{x})$ possess the properties

$$U_n^\pm(-\mathbf{x}) = (-1)^n U_n^\pm(\mathbf{x}), \quad V_n^\pm(-\mathbf{x}) = (-1)^n V_n^\pm(\mathbf{x}), \quad V_{-n}^\pm(\mathbf{x}) = (-1)^n V_n^\mp(\mathbf{x}). \quad (\text{A.7})$$

Let $\mathbf{l}_{mj} = \mathbf{l}_m - \mathbf{l}_j$ ($= -\mathbf{l}_{jm}$) be a position vector of multipole O_m with respect to multipole O_j . Since $\mathbf{x} = \mathbf{l}_m + \mathbf{x}_m = \mathbf{l}_j + \mathbf{x}_j \rightarrow \mathbf{x}_m = \mathbf{x}_j + (\mathbf{l}_j - \mathbf{l}_m)$, the total field p in the neighborhood of cylinder S_j can be written as

$$p = \sum_{n=-\infty}^{\infty} \left\{ A_n^{(j)} U_n^+(\mathbf{x}_j) + B_n^{(j)} V_n^+(\mathbf{x}_j) + \sum_{\substack{m=1 \\ m \neq j}}^M B_n^{(m)} V_n^+(\mathbf{x}_j + \mathbf{l}_{jm}) \right\}. \quad (\text{A.8})$$

Then noting the properties of $V_n^+(\mathbf{x})$, eq. (A.7), and using Graf's theorem, we obtain for $|\mathbf{x}_j| < l_j$, where $l_j = \min |\mathbf{l}_{jm}|$:

$$p = \sum_{n=-\infty}^{\infty} \left\{ B_n^{(j)} V_n^+(\mathbf{x}_j) + A_n^{(j)} U_n^+(\mathbf{x}_j) + U_n^+(\mathbf{x}_j) \sum_{\substack{m=1 \\ m \neq j}}^M \sum_{l=-\infty}^{\infty} P_{nl}(\mathbf{l}_{jm}) B_l^{(m)} \right\}, \quad (\text{A.9})$$

where

$$P_{nl}(\mathbf{x}) \equiv V_{l-n}^+(\mathbf{x}). \quad (\text{A.10})$$

Here the matrix $\mathbf{P} = [P_{nl}]$ is equal to the transpose of Martin's $\mathbf{S} = [S_{nl}]$ matrix [2], $\mathbf{P} = \mathbf{S}^T$. The total incident field impinging on the cylinder S_j is a sum of the last two terms on the right hand side of eq. (A.9), i.e.

$$p_{inc}^{(j)} + \sum_{\substack{m=1 \\ m \neq j}}^M p_{sc}^{(m)} = \sum_{n=-\infty}^{\infty} \left\{ A_n^{(j)} + \sum_{\substack{m=1 \\ m \neq j}}^M \sum_{l=-\infty}^{\infty} P_{nl}(\mathbf{l}_{jm}) B_l^{(m)} \right\} U_n^+(\mathbf{x}_j). \quad (\text{A.11})$$

The response of shell S_j to the incident field (A.11) can be obtained by incorporating the boundary conditions at the interface and the transition matrix elements $T_{nq}^{(j)}$ of cylinder S_j [46]:

$$p_{sc}^{(j)} = \sum_{n=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} T_{nq}^{(j)} \left\{ A_q^{(j)} + \sum_{\substack{m=1 \\ m \neq j}}^M \sum_{l=-\infty}^{\infty} P_{ql}(\mathbf{l}_{jm}) B_l^{(m)} \right\} V_n^+(\mathbf{x}_j). \quad (\text{A.12})$$

Thus, eqs. (A.5) and (A.12) yield a linear system of equation

$$B_n^{(j)} - \sum_{q=-\infty}^{\infty} T_{nq}^{(j)} \sum_{\substack{m=1 \\ m \neq j}}^M \sum_{l=-\infty}^{\infty} P_{ql}(\mathbf{l}_{jm}) B_l^{(m)} = \sum_{q=-\infty}^{\infty} T_{nq}^{(j)} A_q^{(j)}, \quad n \in \mathbb{Z}, \quad (\text{A.13})$$

where $T_{nq}^{(j)}$ is the component of the transition matrix of cylinder S_j in isolation given in [1]; for a rigid cylinder it reduces to the form: $T_{nq}^{(j)} = -J_n'(ka)/H_n^{(1)'}(ka)\delta_{nq}$. Equivalently,

$$\sum_{m=1}^M \sum_{l=-\infty}^{\infty} X_{jnml} B_l^{(m)} = \sum_{q=-\infty}^{\infty} T_{nq}^{(j)} A_q^{(j)}, \quad j = \overline{1, M}, \quad n \in \mathbb{Z}, \quad (\text{A.14a})$$

$$X_{jnml} = \begin{cases} \delta_{nl}, & m = j, \\ -\sum_{q=-\infty}^{\infty} T_{nq}^{(j)} P_{ql}(\mathbf{l}_{jm}), & m \neq j. \end{cases} \quad (\text{A.14b})$$

Consider now a truncated version of the infinite sum in equation (A.14a) that yields an algebraic system of equations with finite dimensions:

$$\sum_{m=1}^M \sum_{l=-N}^N X_{jnml} B_l^{(m)} = \sum_{q=-N}^N T_{nq}^{(j)} A_q^{(j)}, \quad j = \overline{1, M}, \quad n \in \mathbb{Z}, \quad (\text{A.15})$$

or in matrix form

$$\mathbb{X} \mathbf{b} = \mathbf{a}, \quad (\text{A.16})$$

where $\mathbb{X}$, $\mathbf{b}$, and $\mathbf{a}$ are given correspondingly by eqs. (1.2) and (1.4).

Appendix B. Far-field radiated response

Consider now farfield response, the scattered pressure field p^{sc} , when kr becomes very large: $kr \gg 1$. The scattered field p^{sc} is defined by eq. (A.5) as an infinite sum at the center of multipoles, $\mathbf{x}_m$ defined in eq. (A.3). To find far-field behavior of p^{sc} , we will write it in terms of position vector $\mathbf{x}$. Incorporating the Graf's theorem (A.6) for $|\mathbf{x}| \gg |\mathbf{l}_m|$ yields

$$p^{\text{sc}} = \sum_{m=1}^M \sum_{n=-\infty}^{\infty} B_n^{(m)} V_n^+(k(\mathbf{x} - \mathbf{l}_m)) = \sum_{n=-\infty}^{\infty} F_n V_n^+(k\mathbf{x}), \quad (\text{B.1})$$

where

$$F_n = \sum_{m=1}^M \sum_{l=-\infty}^{\infty} B_l^{(m)} U_{n-l}^-(k\mathbf{l}_m). \quad (\text{B.2})$$

Using the asymptotic expansion of the Hankel function for large values of argument, the far scattered field p^{sc} can be split into two parts, $g(k|\mathbf{x}|)$ and $f^M(\theta)$:

$$p^{\text{sc}} = g(k|\mathbf{x}|) f^M(\theta) \left[1 + O\left(\frac{1}{k|\mathbf{x}|}\right) \right], \quad (\text{B.3})$$

where the function $g(k|\mathbf{x}|)$ is defined as

$$g(k|\mathbf{x}|) = \sqrt{\frac{1}{k|\mathbf{x}|}} e^{ik|\mathbf{x}|}, \quad |\mathbf{x}| \rightarrow \infty, \quad (\text{B.4})$$

and the far-field amplitude function $f^M(\theta)$, has the form:

$$f^M(\theta) = \sum_{n=-\infty}^{\infty} f_n e^{in\theta}, \quad f_n = \sqrt{\frac{2}{\pi}} e^{-i(\frac{\pi}{4} + \frac{n\pi}{2})} F_n, \quad (\text{B.5})$$

with $\theta = \arg(\mathbf{x})$.

The total power radiated by the grating of cylinders is measured by the non-negative far-field flux parameter

$$\sigma_r = \int_0^{2\pi} |f^M(\theta)|^2 d\theta = 4 \sum_{n=-\infty}^{\infty} |F_n|^2. \quad (\text{B.6})$$

Then, for a configuration of cylinders with the radii $a_m = a$, the non-dimensional total scattering cross section is given by:

$$Q = \frac{4}{ka} \sum_{n=-\infty}^{\infty} |F_n|^2. \quad (\text{B.7})$$

References

- [1] F.A. Amirkulova, Acoustic and elastic multiple scattering and radiation from cylindrical structures, PhD thesis, Rutgers University, October 2014.
- [2] P.A. Martin, Multiple Scattering: Interaction of Time-Harmonic Waves with N Obstacles, Cambridge University Press, New York, 2006.
- [3] M. Abramowitz, I. Stegun, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, Dover, New York, 1974.
- [4] M.D. Pockock, S.P. Walker, The complex bi-conjugate gradient solver applied to large electromagnetic scattering problems, computational costs and cost scalings, IEEE Trans. Antennas Propag. 45 (1) (1997) 140–146.
- [5] R.J. Adams, A class of robust and efficient iterative methods for wave scattering problems, PhD thesis, Virginia Polytechnic Institute and State University, 1998.
- [6] W. Trench, An algorithm for the inversion of finite Toeplitz matrices, SIAM J. Appl. Math. 12 (3) (1964) 515–522.
- [7] O.B. Arushanian, M.K. Samarin, V.V. Voevodin, E.E. Tyrtysnikov, B.S. Garbow, J.M. Boyle, W.R. Cowell, K.W. Dritz, The Toeplitz package user guide, Technical report, Science Research Computing Center, Moscow State University and Mathematics and Computer Science Division, Argonne National Laboratory, 1983.
- [8] G. Baxter, Polynomials defined by a difference system, J. Math. Anal. Appl. 2 (1961) 223–263.
- [9] V.V. Voevodin, E.E. Tyrtysnikov, Numerical Processes with Toeplitz Matrices, Nauka, Moscow, 1987 (in Russian).
- [10] I.C. Gohberg, A.A. Semencul, On the inversion of finite Toeplitz matrices and their continuous analogs, Mat. Issled. 7 (2) (1972) 201–223 (in Russian).
- [11] G. Heinig, K. Rost, Algebraic Methods for Toeplitz-Like Matrices and Operators, Birkhäuser Verlag, Basel–Boston–Stuttgart, 1984.
- [12] J. Chen, T.L.H. Li, Parallelizing the conjugate gradient algorithm for multilevel Toeplitz systems, Proc. Comput. Sci. 18 (2013) 571–580.
- [13] J.-C. Auger, B. Stout, A recursive centered T-matrix algorithm to solve the multiple scattering equation: numerical validation, J. Quant. Spectrosc. Radiat. Transf. 79–80 (2003) 533–547.
- [14] B.E. Barrowes, F.L. Teixeira, J.A. Kong, Fast algorithm for matrix–vector multiply of asymmetric multilevel block-Toeplitz matrices, in: IEEE APS Int. Symposium, vol. 4, 2001, pp. 630–633.
- [15] B.E. Barrowes, F.L. Teixeira, J.A. Kong, Fast algorithm for matrix–vector multiply of asymmetric multilevel block-Toeplitz matrices in 3-D scattering, Microw. Opt. Technol. Lett. 31 (1) (2001) 26–32.
- [16] X. Antoine, C. Chniti, K. Ramdani, On the numerical approximation of high-frequency acoustic multiple scattering problems by circular cylinders, J. Comput. Phys. 227 (2008) 1754–1771.
- [17] X. Antoine, K. Ramdani, T. Bertrand, Étude numérique de la résolution par équations intégrales de la diffraction multiple par des disques, in: 10ème Congrès Français d'Acoustique, Lyon, 12–16 Avril 2010, hal.inria.fr/hal-00533171.
- [18] X. Antoine, K. Ramdani, B. Thierry, Wide frequency band numerical approaches for multiple scattering problems by disks, J. Algorithms Comput. Technol. 6 (2) (2012) 241–259.
- [19] V. Villamizar, S. Acosta, Generation of smooth grids with line control for scattering from multiple obstacles, Math. Comput. Simul. 79 (2009) 2506–2520.
- [20] O.K. Pashaev, O. Yilmaz, Power-series solution for the two-dimensional inviscid flow with a vortex and multiple cylinders, J. Eng. Math. 65 (2009) 157–169.
- [21] B.V. Genuchten, B. Bergen, D. Vandepitte, W. Desmet, A Trefftz-based numerical modelling framework for Helmholtz problems with complex multiple-scatterer configurations, J. Comput. Phys. 229 (2010) 6623–6643.
- [22] C. Geuzaine, B. Thierry, N. Marsic, D. Colignon, A. Vion, S. Tournier, Y. Boubendiry, M.E. Bouajajiz, X. Antoine, An open source domain decomposition solver for time-harmonic electromagnetic wave problems, in: IEEE Int. Conf. on Antenna Measurements and Applications, Antibes Juan-les-Pins, France, November 16–19, 2014.
- [23] D.P. Challa, M. Sini, On the justification of the Foldy–Lax approximation for the acoustic scattering by small rigid bodies of arbitrary shapes, Multiscale Model. Simul. 12 (1) (2014) 55–108.
- [24] C. Chniti, H. Alzubaidi, B. Thierry, X. Antoine, mu-diff: an open Matlab toolbox for computing multiple scattering problems by disks, arXiv:1409.8186, 2014.
- [25] B.T. Draine, P.J. Flatau, User guide for the discrete dipole approximation code DDSCAT 7.3, arXiv:1305.6497, 2013.
- [26] D. Koyama, A parallel Schwarz method for multiple scattering problems, in: Domain Decomposition Methods in Science and Engineering XIX, in: Lect. Notes Comput. Sci. Eng., vol. 78, 2011, pp. 351–358.
- [27] K.A. Gallivan, S. Thirumalai, P. Van Dooren, V. Vermaut, High performance algorithms for Toeplitz and block Toeplitz matrices, Linear Algebra Appl. 241 (243) (1996) 343–388.
- [28] K. Chen, Matrix Preconditioning Techniques and Applications, Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, New York, 2005.
- [29] O. Toeplitz, Zur Theorie der quadratischen und bilinearen Formen von unendlichvielen Veränderlichen, Math. Ann. 70 (1911) 351–376, <http://dx.doi.org/10.1007/BF01564502>.
- [30] U. Grenander, G. Szegő, Toeplitz Forms and Their Applications, University of California Press, 1958.
- [31] Y. Saad, Iterative Methods for Sparse Linear Systems, SIAM, 2003.
- [32] G. Szegő, Beiträge zur Theorie der Toeplitzschen Formen, Math. Z. 6 (1920) 167–202.
- [33] G. Szegő, Orthogonal Polynomials, revised edition, American Mathematical Society, Providence, Rhode Island, 1959.
- [34] L.Y.A. Geronimus, Orthogonal Polynomials, Consultant's Bureau, New York, 1961 (translation from Russian).
- [35] M.G. Krein, The continuous analogs of theorems on polynomials orthogonal on the unit circle, Dokl. Akad. Nauk SSSR 104 (1955) 637–640.
- [36] B. Simon, Orthogonal Polynomials on the Unit Circle. Part I–II, Am. Math. Soc. Colloq. Publ., vol. 54, 2005.
- [37] G. Polya, G. Szegő, Aufgaben und Lehrsätze aus der Analysis. I–II (Problems and Theorems in Analysis), Springer-Verlag, Berlin–Heidelberg, 1971. Originally published as vol. 216 of the Grundlehren der Mathematischen Wissenschaften.
- [38] G. Freud, Orthogonal Polynomials, Pergamon Press, 1971.
- [39] S. Banach, Theory of Linear Operations, Translated by F. Jellett, Dover Books on Mathematics, 1932.
- [40] G. Baxter, Polynomials defined by a difference system, Bull. Am. Math. Soc. 66 (1960) 187–190.
- [41] G. Baxter, I. Hirschman Jr., An explicit inversion formula for finite section Wiener–Hopf operators, Bull. Am. Math. Soc. 70 (1964) 820–823.
- [42] T. Kailath, A. Vieira, M. Morf, Inverses of Toeplitz operators, innovations, and orthogonal polynomials, SIAM Rev. 20 (1) (1978) 106–119.
- [43] E.E. Tyrtysnikov, Toeplitz Matrices, Some Analogs and Applications, Comput. Math. Dept., Academy of Science of USSR, 1989 (in Russian).
- [44] C. Brezinski, Bi-Orthogonality and Its Application to Numerical Analysis, Marcel Dekker, Inc., 1992.
- [45] R.W. Freund, H. Zha, Formally biorthogonal polynomials and a look-ahead Levinson algorithm for general Toeplitz systems, Linear Algebra Appl. 188–189 (1993) 255–303.
- [46] V.K. Varadan, V.V. Varadan (Eds.), Acoustic, Electromagnetic and Elastic Wave Scattering – Focus on the T-Matrix Approach, Pergamon Press Inc., 1980.