An efficient and highly accurate solver for multi-body acoustic scattering problems involving rotationally symmetric scatterers

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Abstract: A numerical method for solving the equations modeling acoustic scattering is presented. The method is capable of handling several dozen scatterers, each of which is several wavelengths long, on a personal work station. Even for geometries involving cavities, solutions accurate to seven digits or better were obtained. The method relies on a Boundary Integral Equation formulation of the scattering problem, discretized using a high-order accurate Nyström method. A hybrid iterative/direct solver is used in which a local scattering matrix for each body is computed, and then GMRES, accelerated by the Fast Multipole Method, is used to handle reflections between the scatterers. The main limitation of the method described is that it currently applies only to scattering bodies that are rotationally symmetric.

1. INTRODUCTION

The manuscript presents a robust and highly accurate numerical method for modeling frequency domain acoustic scattering on a domain external to a group of scatterers in three dimensions. The solver is designed for the special case where each scatterer is rotationally symmetric, and relies on a Boundary Integral Equation (BIE) formulation of the scattering problem.

The contribution of the manuscript is to combine several recently developed techniques to obtain a solver capable of solving scattering problems on complex multibody geometries in three dimensions to seven digits of accuracy or more. In particular, the solver is capable of resolving domains involving cavities such as, e.g., the geometry shown Figure 5(a).

The solution technique proposed involves the following steps:

(1) Reformulation. The problem is written mathematically as a BIE on the surface of the scattering bodies using the “combined field” formulation [5, 19]. See Section 2 for details.

(2) Discretization. The BIE is discretized using the Nyström method based on a high-order accurate composite Gaussian quadrature rule. Despite the fact that the kernel in the BIE is singular, high accuracy can be maintained using the correction techniques of [16, 13]. Following [20], we exploit the rotational symmetry of each body to decouple the local equations as a sequence of equations defined on a generating contour [22, 23, 17, 25, 24]. This dimension reduction technique requires an efficient method for evaluating the fundamental solution of the Helmholtz equation in cylindrical coordinates (the so called “toroidal harmonics”); we use the technique described in [26]. See Section 3 for details.

(3) Iterative solver. The dense linear system resulting from the Nyström discretization of the BIE is solved using the iterative solver GMRES [21], combined with a block-diagonal pre-conditioner, as in, e.g., [15] Sec. 6.4. This pre-conditioner exploits that a highly accurate discrete approximation to the scattering matrix for each individual scatterer can be computed efficiently. See Section 4 for details.

(4) Fast matrix-vector multiplication. The application of the coefficient matrix in the iterative solver is accelerated using the Fast Multipole Method (FMM) [10], specifically the version for the Helmholtz equation developed by Gimbutas and Greengard [8].

(5) Skeletonization. In situations where the individual scatterers are not packed very tightly, the number of degrees of freedom in the global system can be greatly reduced by exploiting rank deficiencies in the off-diagonal blocks of the coefficient matrix. Specifically, we use a variation of the scheme introduced in [3], and further developed in [18]. Randomized methods are used to accelerate the computation of low-rank approximations to large dense matrices [12]. See Section 5 for details.
The present work draws on several recent papers describing techniques for multibody scattering, including [15], which applies a very similar technique to acoustic scattering in two dimensions. [9] addresses the harder problem of electro-magnetic scattering in 3D (as opposed to the acoustic scattering considered here), but uses classical scattering matrices expressed in spherical harmonics. This is a more restrictive framework than the one used in [15] for problems in 2D, and in the present work for problems in 3D. The more general model for a compressed scattering matrix that we use here allows for larger scatterers to be handled, and also permits it to handle scatterers closely packed together. For a deeper discussion of different ways of representing compressed scattering matrices, see [2].

To describe the asymptotic cost of the method presented, let $m$ denote the number of scatterers, let $n$ denote the total number of discretization nodes on a single scatterer and let $I$ denote the number of iterations required in our pre-conditioned iterative solver to achieve convergence. The cost of building all local scattering matrices is then $O(mn^2)$, and the cost of solving the linear system consists of the time $T_{\text{FMM}}$ required for applying the coefficient matrices using the FMM, and the time $T_{\text{precond}}$ required for applying the block-diagonal preconditioner. These scale as $T_{\text{FMM}} \sim Imn$ and $T_{\text{precond}} \sim Imn^{3/2}$ (cf. Remark 4), but for practical problem sizes, the execution time is completely dominated by the FMM. For this reason, we implemented a “skeletonization” compression scheme [3] that reduces the cost of executing the FMM from $Imn$ to $Imk$, where $k$ is a numerically determined “rank of interaction”. We provide numerical examples in Section 6 that demonstrate that when the scatterers are moderately well separated, $k$ can be smaller than $n$ by one or two orders of magnitude, leading to dramatic practical acceleration.

2. Mathematical formulation of the scattering problem

Let $\{\Gamma_p\}_{p=1}^m$ denote a collection of $m$ smooth, disjoint, rotationally symmetric surfaces in $\mathbb{R}^3$, let $\Gamma = \bigcup_{p=1}^m \Gamma_p$ denote their union, and let $\Omega$ denote the domain exterior to $\Gamma$. Our task is to compute the “scattered field” $u$ generated by an incident field $v$ that hits the scattering surface $\Gamma$, see Figure 1. For concreteness, we consider the so called “sound-soft” scattering problem

$$\begin{cases}
-\Delta u(x) - \kappa^2 u(x) = 0 & x \in \Omega^c, \\
u(x) = -v(x) & x \in \Gamma, \\
\frac{\partial u(x)}{\partial r} - i\kappa u(x) = O(1/r) & r := |x| \to \infty.
\end{cases}$$

We assume that the “wave number” $\kappa$ is a real non-negative number. It is known [5] that (1) has a unique solution for every incoming field $v$.

Following standard practice, we reformulate (1) as second kind Fredholm Boundary Integral Equation (BIE) using a so called “combined field technique” [5, 19]. We then look for a solution $u$ of the form

$$u(x) = \int_{\Gamma} G_\kappa(x, x') \sigma(x') \, dA(x'), \quad x \in \Omega^c,$$

where $G_\kappa$ is a combination of the single and double layer kernels,

$$G_\kappa(x, x') = \frac{\partial \phi_\kappa(x, x')}{\partial n(x')} + i\kappa \phi_\kappa(x, x')$$

and where $\phi_\kappa$ is the free space fundamental solution

$$\phi_\kappa(x, x') = \frac{e^{i\kappa|x-x'|}}{4\pi|x-x'|}.$$ 

Equation (2) introduces a new unknown function $\sigma$, which we refer to as a “boundary charge distribution”. To obtain an equation for $\sigma$, we take the limit in (2) as $x$ approaches the boundary
Figure 1. Geometry of scattering problem. An incident field \( v \) propagates in a medium with constant wave-speed and hits a scattering surface \( \Gamma = \bigcup_{p=1}^{m} \Gamma_p \) (shown for \( m = 8 \)). A charge distribution \( \sigma \) is induced on the surface \( \Gamma \) and generates an outgoing field \( u \).

\( \Gamma \), and find that \( \sigma \) must satisfy the integral equation

\[
\frac{1}{2} \sigma(x) + \int_{\Gamma} G_\kappa(x, x') \sigma(x') \, dA(x') = -v(x), \quad x \in \Gamma.
\]

The combined field equation (5) is known to be a second kind Fredholm equation whenever \( \Gamma \) is smooth. Like the original boundary value problem (1), it is known to be well posed for every \( \kappa \), see [5, Theorem. 3.9], [19, Sec. 3.2.2] (in particular, it does not suffer from the problem of “artificial resonances” that plague many alternative formulations).

3. Discretization of rotationally symmetric scattering bodies

In Section 2 we formulated the scattering problem as the BIE (5) defined on the scattering surface \( \Gamma \). In this section, we show how to discretize (5) to obtain a system of linear algebraic equations \( A \sigma = -v \). We use a Nyström technique that combines high accuracy, and (relative) ease of implementation. Section 3.1 gives a general overview of the Nyström method, Section 3.2 describes how rotational symmetry can be exploited to relatively easily discretize a single body to high order, and then Section 3.3 describes how to generalize the procedure to a multibody scattering problem.

3.1. Nyström discretization. The Nyström method provides a way of discretizing a BIE on a surface \( \Gamma \) from a quadrature rule for the surface that is valid for smooth functions. To illustrate, suppose that we are given nodes \( \{x_i\}_{i=1}^{n} \) and weights \( \{w_i\}_{i=1}^{n} \) such that

\[
\int_{\Gamma} \varphi(x) \, dS(x) \approx \sum_{i=1}^{n} \varphi(x_i) w_i, \quad \text{for } \varphi \text{ smooth}.
\]

The idea is then to first use the discretization nodes \( \{x_i\}_{i=1}^{n} \) as collocation points; in other words, we require that

\[
\frac{1}{2} \sigma(x_i) + \int_{\Gamma} G_\kappa(x_i, x') \sigma(x') \, dA(x') = -v(x_i), \quad i = 1, 2, 3, \ldots, n.
\]

Next, suppose that we can somehow (this can require some work) construct an \( n \times n \) matrix \( A \) such that for any sufficiently smooth function \( \varphi \), the integral in (7) can be approximated from
the function values $\{\sigma(x_i)\}_{i=1}^n$

$$\frac{1}{2}\sigma(x_i) + \int_{\Gamma} G_\kappa(x_i, x') \sigma(x') \, dA(x') \approx \sum_{j=1}^n A(i, j) \sigma(x_j) \quad \text{for } \sigma \text{ smooth.}$$

Then a system of $n$ equations for the $n$ unknowns $\{\sigma(x_i)\}_{i=1}^n$ is obtained by inserting the approximation (8) into (7). Specifically, given a data vector $v \in \mathbb{C}^n$ given by $v(i) = v(x_i)$, we seek to determine a vector $\sigma \in \mathbb{C}^n$ of approximations $\sigma(i) \approx \sigma(x_i)$ by solving the linear system

$$\sum_{j=1}^n A(i, j) \sigma(j) = -v(i), \quad i = 1, 2, 3, \ldots, n.$$  

(9)

The task of constructing a matrix $A$ such that (8) holds is complicated by the fact that the kernel $G_\kappa(x, x')$ has a singularity as $x' \to x$. Had this not been the case, one could simply have applied the rule (6) to the integral in (7) to obtain

$$A(i, j) = G_\kappa(x_i, x_j) w_j.$$  

(10)

In Sections 3.2 and 3.3 we will describe how to construct a basic quadrature rule $\{x_i, w_i\}_{i=1}^n$ that is suitable for the geometry under consideration, and also how to construct a matrix $A$ such that (8) holds to high accuracy despite the singular kernel. It turns out to be possible to do so while having almost all elements of $A$ given by the simple formula (10) — only matrix elements $A(i, j)$ for which $||x_i - x_j||$ is “small” need to be modified. As we will see in Section 4 this will greatly help when forming fast algorithms for evaluating the matrix-vector product $\sigma \mapsto A\sigma$.

3.2. A single rotationally symmetric scatterer. We first consider the case where the scattering surface $\Gamma$ is a single rotationally symmetric surface. We let $\gamma$ denote a generating curve of $\Gamma$, and can then view $\Gamma$ as a tensor product between $\gamma$ and the circle $T$, so that $\Gamma = \gamma \times T$, see Figure 2. The idea is now to use a composite Gaussian rule to discretize $\gamma$, and a trapezoidal rule with equispaced nodes to discretize $T$, and then take the tensor product between these rules to obtain the global rule $\{x_i, w_i\}_{i=1}^n$ for $\Gamma$.

![Figure 2. The axisymmetric domain $\Gamma$ generated by the curve $\gamma$.](image)

**Remark 1** (Convergence order). Suppose that $\varphi$ is a smooth ($C^\infty$) function on $\Gamma$. Then since $\varphi$ is periodic in the azimuthal direction, the Trapezoidal rule converges super-algebraically fast. If we use $p$-point Gaussian quadrature on $r$ intervals to discretize the generating curve $\gamma$, then the error in (6) scales as $(1/r)^{2p-1}$ as $r, p \to \infty$. 

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The technique for constructing a matrix $A$ such that (8) holds is based on the observation that when $\Gamma$ is a rotationally symmetric surface, the equation (5) is diagonalized by the Fourier transform. The process is somewhat involved and we will here give only a brief overview of the key techniques, for details we refer to [26]. The first step is to introduce cylindrical coordinates $x = (r, \theta, z)$ with the $z$-axis being the symmetry axis of $\Gamma$, and let $v_p, \sigma_p,$ and $G_{k,p}$ denote the Fourier coefficients of the functions $v, \sigma$, and $G_k$:

\[
v(x) = \sum_{p \in \mathbb{Z}} e^{ip\theta} \frac{1}{\sqrt{2\pi}} v_p(r, z),
\]

\[
\sigma(x) = \sum_{p \in \mathbb{Z}} e^{ip\theta} \frac{1}{\sqrt{2\pi}} \sigma_p(r, z),
\]

\[
G_k(x, x') = G_k(\theta - \theta', r, z, r', z') = \sum_{p \in \mathbb{Z}} e^{ip(\theta - \theta')} \frac{1}{\sqrt{2\pi}} G_{k,p}(r, z, r', z').
\]

Then (5) is equivalent to the sequence of equations

\[
\frac{1}{2} \sigma_p(y) + \sqrt{2\pi} \int_{\gamma} G_{k,p}(y, y') \sigma_p(y') dA(y') = -v_p(y), \quad y \in \gamma, \ p \in \mathbb{Z}.
\]

Converting the BIE (5) defined on a surface $\Gamma$ to the sequence of BIEs (14) defined on the curve $\gamma$ has a crucial advantage in that constructing high-order Nyström discretizations of BIEs with weakly singular kernels is well-understood and computationally cheap for curves, but remains a challenge for surfaces. We use the modified quadrature of [16], as described in [26, 13].

Beyond ease of discretization, the other key benefit of the formulation (14) is that for each Fourier mode $p$, the coefficient matrix arising from discretization of (14) is small enough that it can often easily be inverted by brute force. For instance, for the geometries shown in Figure 3, it is sufficient to use at most a couple of hundred nodes along $\gamma$ to achieve ten digits accuracy.

To put it another way, the Fourier conversion allows to write the matrix $A$ as a product

\[
A = F^* \tilde{A} F
\]

where $F$ is the discrete Fourier transform (in the azimuthal variable), and $\tilde{A}$ is a block-diagonal matrix, where each diagonal block corresponds to one Fourier mode, and is relatively small.

We can pre-compute and store the block diagonal matrix $\tilde{A}^{-1}$, and then very rapidly apply the inverse

\[
A^{-1} = F^* \tilde{A}^{-1} F,
\]

by using the FFT to apply $F$ and $F^*$.

One complication to the procedure outlined in this section is that while the kernel $G_k$ in (5) is given by the simple formula (3), the kernels $G_{k,p}$ must be evaluated computationally. Techniques for doing so rapidly have been developed, and are described in [26].

**Remark 2** (Cost of precomputation). *To state the asymptotic cost of the algorithm, let $N_G$ ("G" for Gaussian) denote the number of points on the generating curve $\gamma$ of each scatter and let $N_F$ ("F" for Fourier) denote the number of points used to discretize $\mathbb{T}$. The total number of degrees of freedom of each scatter is $n = N_G N_F$. Under the simplifying assumption that $N_G \sim N_F$, the cost of forming the block diagonal matrix $\tilde{A}$ is $O(n^{3/2} \log n)$, while the cost of inverting $\tilde{A}$ is $O(n^2)$, see [26]. Applying $F$ and $F^*$ is done via the FFT in negligible time.*
3.3. Multibody scattering. Having described how to discretize the single-body scattering problem in Section 3.2, we now proceed to the general case of \( m \) disjoint scattering surfaces \( \Gamma = \bigcup_{p=1}^{m} \Gamma_p \). We assume that each scatterer is discretized using the tensor product procedure described in Section 3.2. For notational simplicity, we assume that each scatterer is discretized using the same \( n \) number of nodes, for a total of \( N = mn \) discretization nodes \( \{x_i\}_{i=1}^{N} \) with associated weights \( \{w_i\}_{i=1}^{N} \). We then seek to construct matrix blocks \( \{A_{p,q}\}_{p,q=1}^{m} \) such that the Nyström discretization of (5) associated with this quadrature rule takes the form

\[
\begin{bmatrix}
A_{1,1} & A_{1,2} & \cdots & A_{1,m} \\
A_{2,1} & A_{2,2} & \cdots & A_{2,m} \\
\vdots & \vdots & \ddots & \vdots \\
A_{m,1} & A_{m,2} & \cdots & A_{m,m}
\end{bmatrix}
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\vdots \\
\sigma_m
\end{bmatrix}
= -
\begin{bmatrix}
v_1 \\
v_2 \\
\vdots \\
v_m
\end{bmatrix},
\]

where each block \( A_{p,q} \) is of size \( n \times n \). The diagonal blocks \( A_{p,p} \) are constructed using the technique described in Section 3.2. Next observe that in the off-diagonal blocks, the “naive” formula (10) works well since the kernel \( G_\kappa(x, x') \) is smooth when \( x \) and \( x' \) belong to different scatterers.

Remark 3. In this paper, we avoid considering the complications of scatterers that touch or are very close. The procedure described works well as long as the minimal distance between scatterers is not small compared to the resolution of the quadrature rules used. This means that if two scatterers are moderately close, high accuracy can be maintained by discretizing these two scatterers more finely.

4. A block-diagonal pre-conditioner for the multibody scattering problem

We solve the linear system (17) using the iterative solver GMRES [21], accelerated by a block-diagonal pre-conditioner. To formalize, let us decompose the system matrix as

\[
A = D + B,
\]

where

\[
D = \begin{bmatrix}
A_{1,1} & 0 & 0 & \cdots \\
0 & A_{2,2} & 0 & \cdots \\
0 & 0 & A_{3,3} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix}
\quad \text{and} \quad
B = \begin{bmatrix}
0 & A_{1,2} & A_{1,3} & \cdots \\
A_{2,1} & 0 & A_{2,3} & \cdots \\
A_{3,1} & A_{3,2} & 0 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix}.
\]

Then we use GMRES to solve the linear system

\[
\sigma + D^{-1}B\sigma = -D^{-1}v.
\]

We apply the matrix \( B \) using the Fast Multipole Method [10, 4]; specifically the implementation [8] by Zydrunas Gimbutas and Leslie Greengard.

Remark 4. The cost of evaluating the term \( D^{-1}B\sigma \) in (18) consists of two parts: applying \( B \) to vector \( \sigma \) via FMM costs \( O(mn) \) operations and applying the block-diagonal pre-conditioner costs \( O(mn^{3/2}) \) operations. Observe that the matrix \( D^{-1} \) can be precomputed since each matrix \( A_{p,p}^{-1} \) is itself block-diagonal in the local Fourier basis, cf. formula (16). Applying \( A_{p,p}^{-1} \) to a vector \( w \in \mathbb{C}^n \) is executed as follows: (1) form \( Fw \) using the FFT at cost \( O(n\log n) \), (2) for each Fourier mode apply \( D^{-1} \) to \( Fw \) at cost \( O(n^{3/2}) \), and (3) use the FFT to apply \( F^* \) to \( D^{-1}Fw \).
5. ACCELERATED MULTIBODY SCATTERING

In situations where the scatterers are not tightly packed, it is often possible to substantially reduce the size of the linear system (18) before applying an iterative solver. We use a technique that was introduced in [3] for problems in two dimensions, which exploits that when the scatterers are somewhat separated, the off-diagonal blocks $A_{p,q}$ are typically rank deficient. Specifically, we assume that for some finite precision $\varepsilon$ (say $\varepsilon = 10^{-10}$), each such block admits a factorization

$$A_{p,q} = U_p \tilde{A}_{p,q} V_q^* + R_{p,q}$$

where $n$ is the number of nodes originally used to discretize a single scatterer, and $k$ is the numerical rank of the factorization. The remainder term $R_{p,q}$ satisfies $||R_{p,q}|| \leq \varepsilon$ in some suitable matrix norm (we typically use the Frobenius norm since it is simple to compute).

Now write the linear system (18) in block form as

$$\sigma_p + \sum_{q \neq p} \tilde{A}_{p,q}^{-1} A_{p,q} \sigma_q = -A_{p,p}^{-1} v_p, \quad p = 1, 2, 3, \ldots, m.$$  

We left multiply (20) by $V_p^*$, and insert the factorization (19) to obtain

$$V_p^* \sigma_p + \sum_{q \neq p} V_p^* \tilde{A}_{p,q}^{-1} U_p \tilde{A}_{p,q} V_q^* \sigma_q = -V_p^* A_{p,p}^{-1} v_p, \quad p = 1, 2, 3, \ldots, m.$$  

We now define quantities $\{\tilde{\sigma}_p\}_{p=1}^m$, $\{\tilde{v}_p\}_{p=1}^m$, and $\{\tilde{S}_p\}_{p=1}^m$ via

$$\tilde{\sigma}_p = V_p^* \sigma_p, \quad \tilde{v}_p = V_p^* A_{p,p}^{-1} v_p, \quad \tilde{S}_{p,p} = F_{p,p} A_{p,p}^{-1} U_p, \quad \text{for } p = 1, 2, 3, \ldots, m.$$  

Then the system (21) can be written

$$\tilde{\sigma}_p + \sum_{q \neq p} \tilde{S}_{p,q} \tilde{A}_{p,q} \tilde{\sigma}_q = -\tilde{v}_p, \quad p = 1, 2, 3, \ldots, m.$$  

To write (23) in block form, we introduce matrices

$$S = \begin{bmatrix} S_1 & 0 & 0 & \cdots \\ 0 & S_2 & 0 & \cdots \\ 0 & 0 & S_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \end{bmatrix} \quad \text{and} \quad \tilde{B} = \begin{bmatrix} 0 & \tilde{A}_{1,2} & \tilde{A}_{1,3} & \cdots \\ \tilde{A}_{2,1} & 0 & \tilde{A}_{2,3} & \cdots \\ \tilde{A}_{3,1} & \tilde{A}_{3,2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \end{bmatrix},$$

whence equation (23) takes the form, cf. (18),

$$\tilde{\sigma} + S \tilde{B} \tilde{\sigma} = -\tilde{v}.$$  

The process of first forming the linear system (25), and then solving it using GMRES is very computationally efficient when the following techniques are used:

- The matrices $\{U_p, V_p\}_{p=1}^m$ in the factorizations (19) can be computed via a purely local procedure in $O(n^2k)$ operations, independent of the number of scatterers $m$. The idea is to use representation techniques from scattering theory to construct a local basis for all possible incoming harmonic fields (to within precision $\varepsilon$), see [11 Sec. 5.1] or [7 Sec. 6.2].
- In constructing the factorization (19), the so called **interpolatory decomposition** should be used. Then each matrix $U_p$ and each matrix $V_p$ contains the $k \times k$ identity matrix $I_k$. Specifically, there exists for each $k$ an index vector $\hat{I}_p \subset \{1,2,\ldots,n\}$ such that $U(\hat{I}_p,:) = V(\hat{I}_p,:) = I_k$. Then each off-diagonal block $\tilde{A}_{p,q}$ is given as a submatrix $\tilde{A}_{p,q} = A_{p,q}(\hat{I}_p, \hat{I}_q)$. In consequence, the matrix $\tilde{B}$ is a sub-matrix of $B$ and can be rapidly applied using the FMM in $O(mk)$ operations.
In evaluating the formula $S_{p,p} = V_p^* A_{p,p}^{-1} U_p$, we exploit that $A_{p,p}^{-1}$ can be applied rapidly in Fourier space, cf. (16), to reduce the complexity of this step from $O(n^3)$ to $O(n^{3/2}k)$ if $A_{p,p}^{-1}$ was precomputed and stored and to $O(n^2k)$ if $A_{p,p}^{-1}$ is computed at this step.

Remark 5. Efficient techniques for computing interpolative decompositions are described in [3]. More recently, techniques based on randomized sampling have proven to be highly efficient on modern computing platforms, in particular for problems in potential theory where the low-rank matrices to be approximated have very rapidly decaying singular values. We use the specific technique described in [12].

6. Numerical examples

This section describes numerical experiments to assess the performance of the numerical scheme outlined in previous sections. All the experiments are carried out on a personal workstation with an Intel Xeon E-1660 3.3GHz 6-core CPU, and 128GB of RAM. The experiments explore (1) the accuracy of the algorithm, (2) the computational cost, (3) the performance of block-diagonal pre-conditioner and (4) the performance of the acceleration scheme when scatterers are separated suitably. In all the experiments below, we measure accuracy against a known analytic solution $u_{\text{exact}}$. This solution is generated by randomly placing one point source inside each scatterer, and then solving (1) with the Dirichlet data $v$ set to equal the field generated by these radiating sources. Let $u_{\text{approx}}$ and $u_{\text{exact}}$ denote the vectors holding the exact and the computed solutions at a set of 10 randomly chosen target points, located a few wave-lengths outside of the domain. The relative error, measured in $\ell^\infty$-norm, is then given by

$$E_{\text{rel}}^\infty = \frac{||u_{\text{approx}} - u_{\text{exact}}||_\infty}{||u_{\text{exact}}||_\infty}.$$ 

In addition to $E_{\text{rel}}^\infty$, we report:

- $n$: number of nodes discretizing each body (in form of $n = N_G \times N_F$)
- $N$: total degree of freedom $N = m \times n$, where $m$ is the number of scatterers
- $N_{\text{compressed}}$: number of skeleton points after applying the compression scheme
- $T_{\text{pre}}$: time (in seconds) of precomputation
- $T_{\text{solve}}$: total time to solve for the surface charges $\sigma$ via GMRES
- $T_{\text{compress}}$: time to do compression in the accelerated scheme
- $I$: number of GMRES iterations required to reduce the residual to $10^{-9}$.

All the numerical experiments in this section are executed on domains composed of the three sample scatterers shown in Figure 3.

6.1. Laplace’s equation. We first solve the Laplace equation exterior to the domain shown in Figure 4 and 5(a) (Example 1 and 2 respectively). A combination of the single and double layer kernels is chosen to represent the potential outside the domain. The integral equation to be solved is

$$\frac{1}{2} \sigma(x) + \frac{1}{4\pi} \left( \frac{1}{|x-x'|} + \frac{n(x') \cdot (x-x')}{|x-x'|^3} \right) \sigma(x') dA(x') = f(x), \quad x \in \Gamma.$$ 

6.1.1. Example 1. This example solves the exterior Laplace equation on the domain depicted in Figure 4. The domain consists of 125 ellipsoids contained in the box $[0,10.2]^3$, where each ellipse has a major axis of length 2 and a minor axis of length 1. The minimal distance between any two ellipsoids is 0.05. We did not apply the compression technique since the scatterers are packed tightly. We compare the performance of the algorithm with and without using block-diagonal pre-conditioner in Table 1 and find that for this example, the pre-conditioning does not make any real difference. The scheme quickly reaches 9 digits of accuracy with 10,100 discretization nodes per scatterer, with an overall solve time of about 40 minutes.
Figure 3. Domains used in numerical examples. All items are rotated about their symmetry axis. (a) An ellipsoid. (b) A bowl-shaped cavity. (c) A starfish-shaped cavity.

6.1.2. **Example 2.** This time the domain consists of 8 bowl-shaped cavities contained in the box $[0, 4.1]^3$ in Figure 3(a). The minimal distance between any two cavities is 0.5. Results are shown in Table 2. The scheme achieves 8 digits of accuracy with 400 discretization nodes on the generating curve and 201 Fourier modes. Again, the pre-conditioning is superfluous.

**Remark 6.** All examples described in this section involve geometries where all the scatterers are copies of the basic shapes shown in Figure 3. In our experience, this restriction on the geometry does not in any way change the overall accuracy or efficiency of the solver. The only advantage we benefit from is that the pre-computation gets faster, as only a small number of scattering matrices need to be pre-computed. However, it is clear from the numbers given that even for a fully general geometry (without repetitions), the pre-computation time would be dominated by the time required for the FMM.

6.2. **Helmholtz Equation.** We now consider the exterior Helmholtz problem (1). We represent the potential by a combination of the single and double layer kernels, see (3), and end up with the “combined field” integral equation (5).
**Figure 4.** Domain contains 125 randomly oriented ellipsoids. Distance between any two ellipsoids is 0.05.

**Table 1.** Example 1: exterior Laplace problem solved on the domain in Figure 4.

| $N$      | $n$       | $T_{\text{pre}}$ | $T_{\text{solve}}$ | $E_{\infty}^\text{rel}$ |
|----------|-----------|------------------|---------------------|--------------------------|
| 156250   | $50 \times 25$ | 1.09e+00         | 31 /33              | 9.731e-05                |
| 312500   | $100 \times 25$   | 3.44e+00         | 31 /33              | 9.203e-05                |
| 62500    | $200 \times 25$   | 1.29e+01         | 31 /34              | 9.814e-05                |
| 318750   | $50 \times 51$    | 1.53e+00         | 31 /33              | 1.571e-06                |
| 637500   | $100 \times 51$   | 4.36e+00         | 31 /34              | 1.529e-06                |
| 1275000  | $200 \times 51$   | 1.36e+01         | 32 /34              | 1.711e-06                |
| 631250   | $50 \times 101$   | 2.44e+00         | 31 /34              | 2.165e-08                |
| 1262500  | $100 \times 101$  | 6.11e+00         | 32 /34              | 1.182e-09                |

**Table 2.** Example 2: exterior Laplace problem solved on the domain in Figure 5(a).

| $N$      | $n$       | $T_{\text{pre}}$ | $I$ (precond /no precond ) | $T_{\text{solve}}$ (precond /no precond ) | $E_{\infty}^\text{rel}$ |
|----------|-----------|------------------|--------------------------|------------------------------------------|--------------------------|
| 20400    | $50 \times 51$ | 2.09e-01         | 398 /402                | 4.65e+02 /6.05e+02                       | 1.251e-04                |
| 40800    | $100 \times 51$| 4.55e-01         | 20 /23                  | 4.94e+01 /6.09e+01                       | 3.909e-05                |
| 81600    | $200 \times 51$| 9.83e-01         | 20 /23                  | 1.05e+02 /1.14e+02                       | 3.164e-05                |
| 40400    | $50 \times 101$| 2.25e-01         | 20 /23                  | 4.72e+01 /6.17e+01                       | 5.850e-05                |
| 80800    | $100 \times 101$| 4.49e-01         | 20 /23                  | 9.50e+01 /1.13e+02                       | 1.627e-05                |
| 161600   | $200 \times 101$| 1.35e+00         | 20 /24                  | 2.05e+02 /2.39e+02                       | 6.825e-06                |
| 80400    | $50 \times 201$ | 2.93e-01         | 20 /23                  | 9.13e+01 /1.12e+02                       | 5.704e-05                |
| 160800   | $100 \times 201$| 7.05e-01         | 20 /24                  | 1.96e+02 /2.40e+02                       | 8.000e-06                |
| 321600   | $200 \times 201$| 1.97e+00         | 20 /24                  | 4.43e+02 /5.25e+02                       | 1.931e-07                |
| 643200   | $400 \times 201$| 5.78e+00         | 21 /24                  | 7.68e+02 /8.19e+02                       | 1.726e-08                |

**6.2.1. Example 3.** The domain in this experiment contains 8 ellipsoids in the box $[0, 4.05]^3$, whose minimal distance between any two is 0.05. The wavelength is $10\pi$ so that the scatterers are approximately 10 wavelength in size and the whole region is about $20 \times 20 \times 20$ wavelengths in size. Results are presented in Table 3. We also compare the results without using block-diagonal
pre-conditioner in the same table. Around twice of the iteration numbers are required resulting in twice of the computation time. Table 4 reports the results from an analogous experiment, but now the wavenumber increases such that each scatterer contains 20 wavelengths.

| N    | n          | $T_{\text{pre}}$ | $I$ | $T_{\text{solve}}$ | $E_{\infty}^{\text{rel}}$ |
|------|------------|------------------|-----|--------------------|---------------------------|
| 20400 | 50 × 51    | 1.58e-01         | 35 /67 | 7.71e+02 /1.56e+03 | 1.364e-03 |
| 40800 | 100 × 51   | 4.20e-01         | 36 /67 | 1.75e+03 /3.43e+03 | 1.183e-03 |
| 81600 | 200 × 51   | 1.26e-01         | 36 /68 | 3.52e+03 /6.85e+03 | 1.639e-04 |
| 40400 | 50 × 101   | 2.64e-01         | 36 /68 | 1.71e+03 /3.35e+03 | 1.312e-03 |
| 80800 | 100 × 101  | 6.05e-01         | 36 /68 | 3.45e+03 /6.76e+03 | 1.839e-06 |
| 161600| 200 × 101  | 1.87e+00         | 37 /69 | 6.18e+03 /1.19e+04 | 5.126e-08 |
| 80400 | 50 × 201   | 4.61e-01         | 36 /69 | 3.40e+03 /6.70e+03 | 1.312e-03 |
| 160800| 100 × 201  | 1.09e+00         | 37 /69 | 6.07e+03 /1.18e+04 | 1.851e-06 |
| 321600| 200 × 201  | 3.11e+00         | 37 /69 | 1.20e+04 /1.97e+04 | 1.039e-09 |

Table 3. Example 3: exterior Helmholtz problem solved on the domain in Figure 5(b). Each ellipsoid is 10 wavelength in diameter.

6.2.2. **Example 4.** This example solves the exterior Helmholtz problem on the cavity domain in Figure 5(a). Tables 5 and 6 show the results from experiments involving cavities of diameters 2 and 5 wavelengths, respectively. In this case, computing the actual scattering matrix for each scatterer was essential, without using these to pre-condition the problem, we did not observe any convergence in GMRES.

6.3. **Accelerated scheme.**
| $N$  | $n$    | $T_{\text{pre}}$ (precond /no precond) | $I$ (precond /no precond) | $T_{\text{solve}}$ (precond /no precond) | $E_{\text{rel}}^\infty$ |
|------|--------|---------------------------------|-----------------|---------------------------------|------------------|
| 20400 | 50 × 51 | 2.03e-01                        | 58 /119          | 3.59e+03 /8.10e+03              | 4.362e+00        |
| 40800 | 100 × 51 | 4.44e-01                        | 39 /102          | 3.98e+03 /1.11e+04              | 1.071e+00        |
| 81600 | 200 × 51 | 1.36e+00                        | 39 /106          | 6.72e+03 /1.92e+04              | 1.008e+00        |
| 40400 | 50 × 101 | 2.78e-01                        | 54 /94           | 5.43e+03 /1.02e+04              | 5.039e+00        |
| 80800 | 100 × 101| 6.18e-01                        | 36 /82           | 6.11e+03 /1.46e+04              | 8.919e-04        |
| 161600| 200 × 101| 1.93e+00                        | 36 /83           | 9.44e+03 /2.32e+04              | 5.129e-07        |
| 80400 | 50 × 201 | 4.28e-01                        | 55 /95           | 9.19e+03 /6.41e+04              | 5.031e+00        |
| 160800| 100 × 201| 1.07e+00                        | 36 /83           | 9.49e+03 /2.31e+04              | 8.916e-04        |
| 321600| 200 × 201| 3.10e+00                        | 37 /83           | 1.45e+04 /3.57e+04              | 8.781e-09        |

Table 4. Example 3: exterior Helmholtz problem solved on the domain in Figure 5(b). Each ellipsoid is 20 wavelength in diameter.

| $N$  | $n$    | $T_{\text{pre}}$ (precond /no precond) | $I$ (precond /no precond) | $T_{\text{solve}}$ (precond /no precond) | $E_{\text{rel}}^\infty$ |
|------|--------|---------------------------------|-----------------|---------------------------------|------------------|
| 40800 | 100 × 51 | 4.29e-01                        | 59 /181          | 2.17e+03 /6.73e+03              | 1.127e-02        |
| 81600 | 200 × 51 | 1.28e+00                        | 60 / –           | 4.23e+03 / –                    | 1.131e-02        |
| 80800 | 100 × 101| 6.83e-01                        | 60 / –           | 4.18e+03 / –                    | 3.953e-03        |
| 161600| 200 × 101| 1.90e+00                        | 60 / –           | 8.93e+03 / –                    | 3.802e-04        |
| 323200| 400 × 101| 6.07e+00                        | 61 / –           | 1.91e+04 / –                    | 3.813e-04        |
| 160800| 100 × 201| 1.09e+00                        | 60 / –           | 8.35e+03 / –                    | 4.788e-05        |
| 321600| 200 × 201| 3.07e+00                        | 61 / –           | 1.88e+04 / –                    | 5.488e-06        |
| 643200| 400 × 201| 9.61e+00                        | 61 / –           | 4.03e+04 / –                    | 8.713e-08        |

Table 5. Example 4: exterior Helmholtz problem solved on the domain in Figure 5(a). Each cavity is 2 wavelength in diameter.

| $N$  | $n$    | $T_{\text{pre}}$ (precond /no precond) | $I$ (precond /no precond) | $T_{\text{solve}}$ (precond /no precond) | $E_{\text{rel}}^\infty$ |
|------|--------|---------------------------------|-----------------|---------------------------------|------------------|
| 80800 | 100 × 101| 6.54e-01                        | 62 /304          | 5.17e+03 /2.64e+04              | 1.555e-03        |
| 161600| 200 × 101| 1.82e+00                        | 63 / –           | 9.88e+03 / –                    | 1.518e-04        |
| 323200| 400 × 101| 6.46e+00                        | 64 / –           | 2.19e+04 / –                    | 3.813e-04        |
| 160800| 100 × 201| 1.09e+00                        | 63 / –           | 9.95e+03 / –                    | 1.861e-03        |
| 321600| 200 × 201| 3.00e+00                        | 64 / –           | 2.19e+04 / –                    | 2.235e-05        |
| 643200| 400 × 201| 1.09e+01                        | 64 / –           | 4.11e+04 / –                    | 8.145e-06        |
| 641600| 200 × 401| 5.02e+00                        | 64 / –           | 4.07e+04 / –                    | 2.485e-05        |
| 1283200| 400 × 401| 1.98e+01                        | 65 / –           | 9.75e+04 / –                    | 6.884e-07        |

Table 6. Example 4: exterior Helmholtz problem solved on the domain in Figure 5(a). Each cavity is 5 wavelength in diameter.

6.3.1. Example 5. We apply the accelerated scheme in Section 5 to solve the Laplace’s equation on the domain exterior to the bodies depicted in Figure 6. This geometry contains 50 different shaped scatterers (ellipsoids, bowls, and rotated “starfish”) and is contained in the box $[0, 18] \times [0, 18] \times [0, 6]$. The minimal distance between any two bodies is 4.0. We compare the results shown in Table 7 with the ones without applying accelerated scheme shown in Table 8. We see
that the compression did not substantially alter either the convergence speed of GMRES, or the final accuracy, and therefore led to improvements in the solve time of between one and two orders of magnitude.

![Figure 6](image)

**Figure 6.** Domain contains 50 randomly oriented scatters.

6.3.2. *Example 6.* The accelerated scheme is applied to solve Helmholtz equation on domain containing 64 randomly placed ellipsoids depicted in Figure 8. The minimal distance between any two bodies is 6.0. Each ellipsoid is 5 wavelength in diameter. We compare the results with

![Figure 7](image)

**Figure 7.** Example of skeletonization of three different scatterers before and after compression. With 10 100 original discretization points (denoted by black dots), after compression (a) for an ellipsoid, only 435 points survive (denoted by red dots); (b) for a bowl-shaped cavity domain, only 826 points survive; (c) for a starfish-shaped cavity, only 803 points survive.
Table 7. Example 5: exterior Laplace problem solved on the domain in Figure 6 using accelerated scheme.

Table 8. Example 5: exterior Laplace problem solved on the domain in Figure 6 without using accelerated scheme.

and without accelerated scheme in Table 9 and 10. Again, we see that the acceleration scheme leads to very substantial improvements in the solve time.
| $N$     | $n$     | $N_{\text{compressed}}$ | $k$     | $T_{\text{compressed}}$ | $I$     | $T_{\text{solve}}$ | $E_{\infty}^\text{rel}$ |
|---------|---------|--------------------------|---------|--------------------------|---------|---------------------|--------------------------|
| 80 000  | 50 × 25 | 61 184                   | 956     | 1.92e+01                 | 28      | 4.42e+03            | 2.339e-02                |
| 160 000 | 100 × 25| 75 648                   | 1182    | 6.58e+01                 | 29      | 4.79e+03            | 8.656e-03                |
| 163 200 | 50 × 51 | 87 744                   | 1371    | 8.50e+02                 | 29      | 4.92e+03            | 2.798e-04                |
| 326 400 | 100 × 51| 100 288                  | 1567    | 2.83e+03                 | 30      | 5.25e+03            | 5.892e-05                |
| 652 800 | 200 × 51| 105 216                  | 1644    | 9.06e+02                 | 30      | 5.51e+03            | 6.056e-05                |
| 323 200 | 50 × 101| 91 648                   | 1432    | 2.40e+02                 | 30      | 5.09e+03            | 9.485e-06                |
| 646 400 | 100 × 101| 102 400               | 1552    | 8.55e+02                 | 31      | 5.50e+03            | 2.150e-07                |
| 1 292 800| 200 × 101| 106 944               | 1671    | 2.91e+03                 | 31      | 5.73e+03            | 8.441e-08                |

Table 9. Example 6: exterior Helmholtz problem solved on the domain in Figure 8 using accelerated scheme. Each ellipsoid is 5 wavelength in diameter.

| $N$     | $n$     | $T_{\text{init}}$ | $I$     | $T_{\text{solve}}$ | $E_{\infty}^\text{rel}$ |
|---------|---------|-------------------|---------|---------------------|--------------------------|
| 80 000  | 50 × 25 | 4.41e-01          | 28      | 3.60e+03            | 7.009e-03                |
| 160 000 | 100 × 25| 8.44e-02          | 28      | 5.69e+03            | 5.755e-03                |
| 163 200 | 50 × 51 | 8.22e-01          | 28      | 5.78e+03            | 1.239e-04                |
| 326 400 | 100 × 51| 1.65e+00          | 29      | 8.75e+03            | 4.806e-05                |
| 652 800 | 200 × 51| 3.36e+00          | 29      | 1.54e+04            | 5.552e-05                |
| 323 200 | 50 × 101| 1.58e+00          | 29      | 8.64e+03            | 8.232e-06                |
| 646 400 | 100 × 101| 3.24e+00         | 29      | 1.69e+04            | 1.354e-07                |
| 1 292 800| 200 × 101| 6.67e+00         | 29      | 3.01e+04            | 2.823e-08                |

Table 10. Example 6: exterior Helmholtz problem solved on the domain in Figure 8 without using accelerated scheme. Each ellipsoid is 5 wavelength in diameter.

6.3.3. **Example 7.** The accelerated scheme is applied to solve Helmholtz equation on domain in Figure 6. Each scatterer is two wavelength in diameter. Results are presented in Table 11 and Table 12 and confirm our claim regarding the efficiency of the acceleration scheme. Note that in Table 12, due to limitation of the memory, only estimations of the run time are reported when four million discretization nodes were used.

| $N$     | $n$     | $N_{\text{compressed}}$ | $k$     | $T_{\text{compressed}}$ | $I$     | $T_{\text{solve}}$ | $E_{\infty}^\text{rel}$ |
|---------|---------|--------------------------|---------|--------------------------|---------|---------------------|--------------------------|
| 252 500 | 50 × 101| 53 390                   | (775,1254,1211) | 2.26e+02                 | 52      | 2.48e+03            | 4.941e-03                |
| 505 000 | 100 × 101| 57 934                  | (823,1358,1337) | 5.17e+02                 | 53      | 2.72e+03            | 2.026e-03                |
| 1 010 000| 200 × 101| 60 512                  | (856,1420,1399) | 1.14e+03                 | 54      | 2.89e+03            | 4.865e-04                |
| 502 500 | 50 × 201| 54 538                   | (789,1283,1238) | 4.89e+02                 | 53      | 2.63e+03            | 9.276e-03                |
| 1 005 000| 100 × 201| 59 036                  | (838,1384,1363) | 1.10e+02                 | 54      | 2.90e+03            | 4.392e-03                |
| 2 010 000| 200 × 201| 61 488                  | (872,1443,1419) | 2.70e+03                 | 56      | 3.10e+03            | 7.709e-06                |
| 4 020 000| 400 × 201| 61 664                  | (888,1428,1427) | 1.50e+04                 | 57      | 3.31e+03            | 1.856e-06                |
| 2 005 000| 100 × 401| 60 106                  | (853,1409,1388) | 2.58e+03                 | 56      | 3.04e+03            | 9.632e-04                |
| 4 010 000| 200 × 401| 61 818                  | (885,1441,1427) | 1.54e+04                 | 57      | 3.32e+03            | 2.452e-07                |

Table 11. Example 7: exterior Helmholtz problem solved on the domain in Figure 6 using accelerated scheme. Each scatterer is 2 wavelength in diameter.
Table 12. Example 7: exterior Helmholtz problem solved on the domain in Figure 6 without using accelerated scheme. Each scatterer is 2 wavelength in diameter.

7. Conclusions and Future work

We have presented a highly accurate numerical scheme for solving acoustic scattering problems on domains involving multiple scatterers in three dimensions, under the assumption that each scatterer is axisymmetric. The algorithm relies on a boundary integral equation formulation of the scattering problem, combined with a highly accurate Nyström discretization technique. For each scatterer, a scattering matrix is constructed via an explicit inversion scheme. Then these individual scattering matrices are used as a block-diagonal pre-conditioner to GMRES to solve the very large system of linear equations. The Fast Multiple Method is used to accelerate the evaluation of all inter-body interactions. Numerical experiments show that while the block-diagonal pre-conditioner does not make almost any different for “zero-frequency” scattering problems (governed by Laplace’s equation), it dramatically improves the convergence speed at intermediate frequencies.

Furthermore, for problems where the scatterers are well-separated, we present an accelerated scheme capable of solving even very large scale problems to high accuracy on a basic personal workstation. In one numerical examples in Section 6, the numbers of degrees of freedom required to solve the Laplace equation to eight digits of accuracy on a complex geometry could be reduced by a factor of 57 resulting in a reduction of the total computation time from 35 minutes to 10 minutes (9 minutes for compression and 42 seconds for solving the linear system). For a Helmholtz problem the reduction of computation time is even more significant: the numbers of degrees of freedom to reach seven digits of accuracy was in one example reduced by a factor of 65; consequently the overall computation time is reduced from 48 hours to 5 hours (4 hours for compression and 1 hour for solving the linear system).

The scheme presented assumes that each scatterer is rotationally symmetric; this property is used both to achieve higher accuracy in the discretization, and to accelerate all computations (by using the FFT in the azimuthal direction). It appears conceptually straight-forward to use the techniques of [11,14] to generalize the method presented to handle scatterers with edges (generated by “corners” in the generating curve). The idea is to use local refinement to resolve the singular behavior of solutions near the corner, and then eliminate the added “superfluous” degrees of freedom added by the refinement via a local compression technique, see [6].

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