ALTERNATIVE INTEGRAL EQUATIONS FOR THE ITERATIVE SOLUTION OF ACOUSTIC SCATTERING PROBLEMS

by X. ANTOINE[†]

(*Mathématiques pour l'Industrie et la Physique, MIP UMR*-5640, *UFR MIG, Université Paul Sabatier*, 118 *route de Narbonne*, 31062 *Toulouse cedex, France*)

and M. DARBAS[‡]

(*Département de Génie Mathématique, INSA, MIP UMR*-5640, *Complexe Scientifique de Rangueil*, 31077, *Toulouse cedex* 4, *France*)

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Summary

This paper addresses the first step of the derivation of well-conditioned integral formulations for the iterative solution of exterior acoustic boundary-value problems. These new formulations are designed to be implemented in a fast multipole method coupled to a Krylov subspace iterative algorithm. Their construction is based on the on-surface radiation condition formalism. Both theoretical developments and numerical aspects are examined in detail. This approach can be viewed as a generalization of the usual Burton–Miller integral equations.

1. Introduction

A very popular method for solving the acoustic scattering problem of a time-harmonic wave in an unbounded domain is provided by the integral equation method (**1** to **3**). Even if other efficient approaches may be employed (**4** to **7**), this technique has the advantage of being accurate. Indeed, the method is based on a formulation equivalent to the initial-boundary-value problem. The resulting equation is set on the finite surface of the scatterer and consequently allows a gain of one dimension of space. However, the price to pay is that the equation is defined by a non-local pseudodifferential operator. From a discrete point of view, the associated linear system is complex, non-hermitian and dense. When the size n of this system (corresponding to the number of degrees of freedom of the discretization) becomes large (which it does for high-frequency problems), its solution by using a Krylov subspace iterative method (**8**, **9**) is usually preferred to the use of a direct solver. The computational cost is then of the order $\mathcal{O}(n^{\text{iter}}n^2)$, where n^{iter} denotes the number of iterations needed to get a satisfactory approximate solution. Actually, the cost $\mathcal{O}(n^2)$ arising from the matrix-vector products arising in the iterative algorithm can be reduced to $\mathcal{O}(n \log n)$ using, for example, the fast multipole method (**2**, **10**). The number of iterations n^{iter} is essentially linked to the conditioning of both the integral equation and the linear system which are solved. Integral equations

[†] ⟨antoine@mip.ups-tlse.fr⟩

[‡] ⟨darbas@gmm.insa-tlse.fr⟩

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can be ill-conditioned. Thus, their efficient solution might require the use of a preconditioner to improve the convergence rate. Several methods exist. Without being exhaustive, let us cite for instance the methods based on the splitting of operators (**11** to **13**) or the sparse pattern approximate inverse and their variants (**13** to **16**). These are directly applied to the linear system. Recently, another approach has been initiated by Steinbach and Wendland (**17**) who build some analytic preconditioners based on the Calderón relations. In the particular case of acoustic scattering, these methods have been extended by Christiansen and Nédélec (**18**, **19**).

In this paper, we propose to rather directly construct some well-conditioned alternative integral formulations. To the best of the authors' knowledge, the first tentative steps in stating such a formalism were taken by Levadoux (**20**) who designs a generalization of the combined field integral equation (CFIE) by using a combination of the single- and double-layer potentials and by regularizing one of them with the aid of a pseudodifferential operator. Unlike Levadoux, we choose here to derive a differential local pseudoinverse operator of the underlying integral operator and not to use a non-local pseudodifferential operator. In fact, these operators exactly correspond to high-frequency approximations of the DN or ND pseudodifferential operators. In this sense, they can be included in the general background of the on surface radiation condition (OSRC) techniques introduced in the middle of the eighties by Kriegsmann *et al.* (**21** to **23**). Moreover, the most elementary formulations (that is, using the lowest-order OSRCs) correspond to the well-known equations of Burton and Miller (**24**) or of Brakhage–Werner type (**25**) useful in acoustic scattering. This theoretical framework provides an interpretation in terms of operators of these classical formulations and proposes their systematic improvement. As a consequence, this justifies the previous numerical studies (**8**, **11**, **26** to **29**) which succeeded in quantifying the almost-optimal coupling parameter arising in these methods and whose aim is to minimize the conditioning of the integral equation.

The plan of the paper is the following. We briefly introduce in section 2 the scattering problem of a wave incident on a sound-soft or a sound-hard body and much useful notation. Furthermore, some results concerning essentially potential theory and integral representations associated with the Helmholtz equation are succinctly reviewed. This allows us to introduce the new alternative integral formulations for the sound-soft and the sound-hard scattering problems. This approach requires the use of some high-frequency approximations of the DN and ND pseudodifferential operators for both the Dirichlet and the Neumann problems. For this reason, section 3 is devoted to recalling some results concerning these operators, referring to (**23**) for further details. In section 4, we develop the spectral analysis of the new integral operators in the case of the unit sphere. We construct some second-order implicit alternative integral operators which have a condition number independent of the density of discretization points per wavelength and almost independent of the wave number. Moreover, they are characterized by a behaviour close to a second-kind Fredholm operator and have some interesting eigenvalue clustering properties. These two characteristics are essential to exhibit a faster convergence of a Krylov subspace iterative solver. In addition, this study shows that the new integral equations have a better convergence rate than the usual Burton–Miller (**24**) or Brakhage–Werner types (**25**) integral equations. A fifth section outlines the developments required for the numerical treatment of two-dimensional scattering problems by a general surface. These new formulations are tested in the case of the generalized minimum residual (GMRES) subspace Krylov iterative solver. The numerical experiments show that the convergence rate is independent of the mesh refinement and almost independent of the frequency. Finally, we draw a conclusion and outline some future perspectives in section 6.

2. Alternative integral equation representations for acoustic scattering problems

2.1 *The acoustic scattering problem and integral representations*

Let Ω^- be a smooth bounded domain of $\mathbb{R}^d$, for $d = 2, 3$. For the sake of simplicity, we assume that the boundary $\Gamma = \partial\Omega^-$ of Ω^- has a $\mathcal{C}^\infty$ regularity. We designate by $\Omega^+ = \mathbb{R}^d/\overline{\Omega^-}$ the associated exterior domain of propagation. Let us consider an incident time-harmonic acoustic field u^{inc} defined by the wave number $k = 2\pi/\lambda$, where λ is the wavelength of the signal. Then, the boundary-value problem under study is given as: find $u \in H^1_{\text{loc}}(\overline{\Omega^+})$ solution to

$$\left.\begin{array}{l} \Delta u + k^2 u = 0 \quad \text{in } \mathcal{D}'(\Omega^+), \\ u = g \ \text{ in } H^{1/2}(\Gamma) \quad \text{or } \ \partial_{\mathbf{n}} u = g \quad \text{in } H^{-1/2}(\Gamma), \\ \lim\limits_{|x|\to+\infty} |x|^{(d-1)/2} \left(\nabla u \cdot [x/|x|] - iku\right) = 0, \end{array}\right\} \tag{2.1}$$

where $H^1_{\text{loc}}(\overline{\Omega^+})$ is the Fréchet space of solutions of finite energy on any compact set

$$H^1_{\text{loc}}(\overline{\Omega^+}) := \left\{ v \in \mathcal{D}'(\Omega^+) | \psi v \in H^1(\Omega^+), \forall \psi \in \mathcal{D}(\mathbb{R}^d) \right\}.$$

Equation $(2.1)_1$ is the Helmholtz equation. The boundary conditions are either of Dirichlet (with $g = -u^{\text{inc}}$) or Neumann type (with $g = -\partial_{\mathbf{n}} u^{\text{inc}}$). These respectively correspond to the scattering problem by a sound-soft or a sound-hard obstacle. The vector $\mathbf{n}$ stands for the outward unit normal to Ω^-. Finally, the condition at infinity is the Sommerfeld radiation condition which leads to the uniqueness of the solution to the boundary-value problem. This condition selects the physical outgoing wave. We do not define the fundamental functional and Sobolev spaces and refer to (**30**) for further details.

The numerical solution to (2.1) can be obtained by using integral formulations (**1** to **3**). To this end, we recall some basic results (**1**, **3**) concerning the potential theory and the integral representations used later. Let L, M, N and D be the integral operators defined for two densities p and ϕ by the relations

$$\left.\begin{array}{l} Lp(x) = \displaystyle\int_\Gamma G(x,y)\, p(y)\, d\Gamma(y), \quad \forall x \in \Omega^- \cup \Gamma \cup \Omega^+, \\ M\phi(x) = -\displaystyle\int_\Gamma \partial_{\mathbf{n}(y)} G(x,y)\, \phi(y)\, d\Gamma(y), \quad \forall x \in \Omega^- \cup \Gamma \cup \Omega^+, \\ Np(x) = \partial_{\mathbf{n}(x)} \displaystyle\int_\Gamma G(x,y)\, p(y)\, d\Gamma(y) = -M^t p(x), \quad \forall x \in \Gamma, \\ D\phi(x) = -\partial_{\mathbf{n}(x)} \displaystyle\int_\Gamma \partial_{\mathbf{n}(y)} G(x,y)\, \phi(y)\, d\Gamma(y), \quad \forall x \in \Gamma. \end{array}\right\} \tag{2.2}$$

The function G is the Green kernel associated with the Helmholtz operator $\Delta + k^2$ and given in the d-dimensional case by the relation

$$G(x,y) = \frac{i}{4} \left(\frac{k}{2\pi\,|x-y|} \right)^{(d-2)/2} H^{(1)}_{(d-2)/2}(k\,|x-y|), \quad x \neq y, \tag{2.3}$$

where $H^{(1)}_t$ is the Hankel function of the first kind and of order t. The integral operators L, M and N map $H^{-1/2+s}(\Gamma)$ onto $H^{1/2+s}(\Gamma)$ for any real s if Γ is $\mathcal{C}^\infty$. This is not the case for the first-order

pseudodifferential operator D which acts from $H^{1/2+s}(\Gamma)$ onto $H^{-1/2+s}(\Gamma)$ (**30**). Its symmetrical weak variational formulation is generally used for numerical purposes; see, for example, (**8**, **24**).

With the notation, we have the Helmholtz integral representation formula for the exterior field u, the solution to the boundary-value problem (2.1), as a linear combination of the single-layer potential L and the double-layer potential M applied to the normal trace and trace of u,

$$u = -Mu - L(\partial_{\mathbf{n}} u). \tag{2.4}$$

Since our goal consists in writing an integral equation on Γ, it is necessary to express the first two exterior traces of the single- and double-layer potentials L and M. We have the following classical result (**1**, **3**).

THEOREM 2.1. *Using the above notation, we have the representation of the first two exterior traces of the solution u by the direct elementary formulations*

$$u = (\tfrac{1}{2} I - M)u - L(\partial_{\mathbf{n}} u) \quad \textit{on } \Gamma \tag{2.5}$$

and

$$\partial_{\mathbf{n}} u = (\tfrac{1}{2} I - N)\partial_{\mathbf{n}} u - Du \quad \textit{on } \Gamma, \tag{2.6}$$

where I designates the identity operator.

2.2 *Alternative integral formulations for the Dirichlet problem*

Let us begin to consider the case of a Dirichlet datum. We use (2.5) as elementary integral representation

$$(\tfrac{1}{2} I - M)u - L(\partial_{\mathbf{n}} u) = g \quad \text{on } \Gamma. \tag{2.7}$$

A well-known fact is that this equation is not uniquely solvable if we directly replace u by g and solve the resulting equation according to the normal derivative trace (**3**, **24**, **28**). To overcome this problem, indirect integral formulations as for instance for the Burton–Miller (**24**) or Brakhage–Werner type (**25**) formulations are often preferred. It can be proved that these formulations are uniquely solvable at any frequency; see for instance (**3**). In fact, these two well-known and widely used formulations can be embedded in a unified setting as proposed below.

Let us consider the computation of the scattered field u as a combined layer potential

$$u = -M\psi - L\varphi, \tag{2.8}$$

where the densities φ and ψ are related by an operator $\mathcal{N}$, $\varphi = \mathcal{N}\psi$. In the case of the Brakhage–Werner formulation for the Dirichlet problem, the operator $\mathcal{N}$ is taken as ik as proposed by Kress (**26**). However, a wider class of operators can be *a priori* chosen. Now, if u is represented as (2.8), then it satisfies automatically the Helmholtz equation and the radiation condition. Moreover, from the jump relations for the single- and double-layer potentials, the Dirichlet boundary condition is satisfied if one has

$$\mathcal{A}_{\mathcal{N}}\psi = g \quad \text{on } \Gamma, \tag{2.9}$$

where $\mathcal{A}_{\mathcal{N}} = (\frac{1}{2}I - M) - L\mathcal{N}$. Then, solving (2.9) gives the scattered field.

Now, all the difficulty consists in choosing a suitable operator for $\mathcal{N}$. One possible solution would be to consider the DN operator $\mathcal{N}$ (**23**) defined by

$$\mathcal{N} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma), \quad u_{|\Gamma} \mapsto \partial_{\mathbf{n}} u_{|\Gamma} = \mathcal{N} u_{|\Gamma}. \tag{2.10}$$

Hence, the solution of the integral equation (2.7) would be straightforward by giving $\partial_{\mathbf{n}} u_{|\Gamma}$ from $u_{|\Gamma}$. Unfortunately, a calculation of this operator cannot be carried out for a general regular surface Γ and in fact leads to the solution of an integral equation. An alternative choice is rather to choose a local differential approximation of $\mathcal{N}$ in the high-frequency regime. More precisely, we consider, for each $\ell \in \mathbb{N}$, a differential operator $\mathcal{N}_\ell$ of order ℓ approximating the exact DN operator $\mathcal{N}$ for a certain set of spatial frequencies. These operators yield an approximate boundary condition usually called an on-surface radiation condition (OSRC and referred to here as DN-type OSRC of order ℓ) (**21** to **23**) and generate a differential relation of the form

$$\varphi = \mathcal{N}_\ell \psi \quad \text{on } \Gamma, \tag{2.11}$$

where (φ, ψ) designates an approximation of the Cauchy data $(\partial_{\mathbf{n}} u_{|\Gamma}, u_{|\Gamma})$. Therefore, following the proposed strategy, we solve the following alternative integral equation: find the fictitious density ψ such that

$$\mathcal{A}_{\mathcal{N}_\ell} \psi = g \quad \text{on } \Gamma, \tag{2.12}$$

where

$$\mathcal{A}_{\mathcal{N}_\ell} = (\tfrac{1}{2}I - M) - L\mathcal{N}_\ell. \tag{2.13}$$

A suitable choice of the operator $\mathcal{N}_\ell$ should yield a well-conditioned integral equation with behaviour similar to a Fredholm integral equation of the second kind. One important property of the operators $\mathcal{N}_\ell$ is that they are local. As a consequence, they give rise from a discrete point of view to sparse linear systems and to some explicit matrix-vector evaluations with a linear cost with the dimension of the approximation space. The implementation of the OSRC in an iterative solver requires a matrix-vector product at each step of the algorithm. For this reason, the integral formulation (2.12), (2.13) will be referred to as the alternative *explicit* integral equation of order ℓ. One interesting point of this approach is that, if we consider the DN-type OSRC of order $\frac{1}{2}$ given by the operator $\mathcal{N}_{1/2} = ik$ (Sommerfeld surface radiation condition), we find again the well-known Burton–Miller (**24**) or Brakhage–Werner operator (**26**)

$$\mathcal{A}_{\mathcal{N}_{1/2}} = (\tfrac{1}{2}I - M) - ikL. \tag{2.14}$$

Hence, the approach can be seen as a generalization of the Burton–Miller integral formulation with the almost-optimal coupling parameter of Kress (**26**).

Now, let us define the Neumann–Dirichlet (ND) operator $\mathcal{D}$ by

$$\mathcal{D} : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma), \quad \partial_{\mathbf{n}} u_{|\Gamma} \mapsto u_{|\Gamma} = \mathcal{D} \partial_{\mathbf{n}} u_{|\Gamma}. \tag{2.15}$$

To follow a similar approach to the one developed for the DN operator, we assume that we have designed a family of local operators $\mathcal{D}_\ell$ (called ND-type OSRCs) of order ℓ approximating $\mathcal{D}$ in the

limit of high-frequencies: $\psi = \mathcal{D}_\ell \varphi$, on Γ. Then, we can always represent the exterior field by (2.8) solving now the alternative integral formulation

$$\mathcal{A}_{\mathcal{D}_\ell} \psi = g \quad \text{on } \Gamma, \tag{2.16}$$

where

$$\mathcal{A}_{\mathcal{D}_\ell} = (\tfrac{1}{2} I - M) - L(\mathcal{D}_\ell)^{-1}. \tag{2.17}$$

Choosing a suitable operator $\mathcal{D}_\ell$ should yield well-conditioned integral formulations. One difference from the previous explicit formulations is that we have a differential operator to invert. For this reason, formulation (2.16), (2.17) is called an alternative *implicit* integral formulation of order ℓ. From a discrete point of view, the inversion of $\mathcal{D}_\ell$ requires the solution of a sparse linear system which can be handled by a direct or an iterative procedure.

2.3 *Alternative integral formulations for the Neumann problem*

In the case of the Neumann boundary condition, we consider the direct differentiated Helmholtz integral formulation given by

$$\partial_{\mathbf{n}} u = (\tfrac{1}{2} I - N)\partial_{\mathbf{n}} u - Du \quad \text{on } \Gamma. \tag{2.18}$$

Similarly to the Dirichlet case, this equation is ill-posed for certain characteristic frequencies if we replace the normal derivative trace by g and solve the equation according to the trace. As above, we choose to represent the solution u as combined layer potentials (2.8). If we consider the jump relations given by (2.6) for the two densities (φ, ψ), we get the following alternative integral equation for the ND-OSRC of order ℓ:

$$\mathcal{B}_{\mathcal{D}_\ell} \varphi = g \quad \text{on } \Gamma, \tag{2.19}$$

with

$$\mathcal{B}_{\mathcal{D}_\ell} = (\tfrac{1}{2} I - N) - D\mathcal{D}_\ell. \tag{2.20}$$

The equation is referred to as alternative *explicit* integral equation of order ℓ. Another possibility consists in choosing the operator $\mathcal{N}_\ell$ in the representation. We designate by $\mathcal{B}_{\mathcal{N}_\ell}$ the operator defining the integral equation,

$$\mathcal{B}_{\mathcal{N}_\ell} = (\tfrac{1}{2} I - N) - D(\mathcal{N}_\ell)^{-1}. \tag{2.21}$$

We are now led to solve the alternative *implicit* integral equation of order ℓ:

$$\mathcal{B}_{\mathcal{N}_\ell} \varphi = g \quad \text{on } \Gamma. \tag{2.22}$$

Once again, if we consider the OSRC of order $\frac{1}{2}$ given by $\psi = \varphi / ik$, we find the Burton–Miller operator for the Neumann problem (**26**).

Note that, in this paper, we do not tackle the problem of the existence and uniqueness of the solution of the integral equations proposed here. The case of the half-order condition is treated in (**24**). However, we give some numerical results in section 5 to illustrate the fact that the integral equations seem to be uniquely solvable at any frequency.

3. Local approximations of the operators $\mathcal{N}$ and $\mathcal{D}$

This section first outlines results concerning the construction of local approximations of the DN operator (**23**). We next give results for the local approximations of the ND operator.

3.1 *Local approximations of the DN operator*

We do not detail here the complete construction of the local approximations of the DN operator described in (**23**) which would require too extensive a development. Essentially, the approach consists in first rewriting the Helmholtz equation in a generalized coordinates system associated with the surface Γ. Next, using the Nirenberg factorization theorem (**31**, Chapter II), we can compute recursively the asymptotic expansion in homogeneous symbols of the total symbol of the DN operator. Retaining the first 2ℓ symbols and using their second-order Taylor approximation with respect to the small parameter $1/k$ (high frequency approximation), we get (**23**) the following first- and second-order OSRCs which are some local approximations of the DN operator.

THEOREM 3.1. *The ℓth order DN-type OSRC is given by*

$$\varphi = \mathcal{N}_\ell \psi \quad \text{on } \Gamma, \tag{3.1}$$

where the different surface operators $\mathcal{N}_\ell$ are defined by $\mathcal{N}_1 = ik - \mathcal{H}$ and

$$\mathcal{N}_2 = -div_\Gamma \left(\frac{1}{2ik} \left(\mathbb{I} - \frac{i\mathcal{R}}{k} \right) \nabla_\Gamma \cdot \right) + ik - \mathcal{H} - \frac{i}{2k} \left(1 - \frac{2i\mathcal{H}}{k} \right) (\mathcal{K} - \mathcal{H}^2) + \frac{\Delta_\Gamma \mathcal{H}}{4k^2}. \tag{3.2}$$

Let us make the notation precise. The local construction of the OSRCs is developed in the principal basis of the tangent plane at a point of the surface Γ. Consider a coordinate patch $(\mathcal{V}, \Psi)$ of Γ, where $\Psi : \mathcal{V} \subset \mathbb{R}^2 \to \Gamma$. If we consider a point p of $\Psi(\mathcal{V}) \subset \Gamma$, then $p = \Psi(s)$ and the normal vector to Γ is given by the following construction. The coordinate patch leads to a basis $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ of the tangent plane $T_p(\Gamma)$ which is defined by $\boldsymbol{\tau}_j = \partial_{s_j} \Psi$, for $j = 1, 2$, denoting by s_j the coordinates of s. Furthermore, we assume that this coordinate patch is compatible with the orientation of the outward unit normal vector $\mathbf{n}$ to Γ

$$\mathbf{n} = \frac{\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2}{|\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2|}, \tag{3.3}$$

where $\times$ stands for the usual vector product. The derivatives $\partial_{s_j} \mathbf{n} = \mathcal{R}\boldsymbol{\tau}_j$, for $j = 1, 2$, lead to the definition of the curvature tensor at $p = \Psi(s)$. This operator is a self-adjoint operator of the tangent plane and gives the curvatures of Γ. If we consider $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ as the principal basis of $T_p(\Gamma)$, then $(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2)$ are the eigenvectors of $\mathcal{R}$ and are better known as the principal curvature directions of Γ. They satisfy $\mathcal{R}\tau_j = \kappa_j \boldsymbol{\tau}_j$, κ_j being the principal curvatures of Γ. We define the Gauss and mean curvatures respectively by $\mathcal{K} = \kappa_1 \kappa_2$ and $\mathcal{H} = (\kappa_1 + \kappa_2)/2$. The operator $\mathbb{I}$ is the identity operator of the tangent plane. The operators div_Γ and ∇_Γ denote respectively the surface divergence of a distribution surface vector field and the surface gradient of a surface field. The Laplace–Beltrami operator is $\Delta_\Gamma = \mathrm{div}_\Gamma \nabla_\Gamma$. In the two-dimensional case, the following simplifications hold: $\mathcal{H} = \kappa/2$ and $\mathcal{K} = 0$, where κ is the scalar curvature of the scatterer. Moreover, the differential operators are given by $\mathrm{div}_\Gamma = \nabla_\Gamma = \partial_s$ and $\Delta_\Gamma = \partial_s^2$, where s designates the anticlockwise directed curvilinear abscissa along Γ.

3.2 *Local approximations of the ND operator*

The construction of the local approximations of the ND operator is quite similar to the one developed in (**23**) for the DN operator. Therefore, we only sketch the proof and refer to (**32**) for further details. Since $\mathcal{DN} = \mathbb{I}$, we deduce the relation $\sigma(\mathcal{DN}) = 1$ at the symbol level, where $\sigma(A)$ denotes the symbol of a pseudodifferential operator A (**33**). Using the symbolic formula of the composition rule of two pseudodifferential operators (**33**) and the asymptotic expansion of the DN operator in homogeneous symbols in the principal basis (**23**), we can recursively compute the asymptotic expansion of the ND operator. A few calculations and the same high-frequency criterion as for the computation of the local approximation of the DN operator lead to the following theorem.

THEOREM 3.2. *The operators $\mathcal{D}_\ell$ are given, for $\ell = 1, 2$, by the relations*

$$\mathcal{D}_1 = \frac{1}{ik} - \frac{\mathcal{H}}{k^2}$$

and

$$\mathcal{D}_2 = -\frac{1}{2ik^3} div_\Gamma \left(\left(\left[1 + \frac{2\mathcal{H}}{ik} \right] \mathbb{I} + \frac{\mathcal{R}}{ik} \right) \nabla_\Gamma \cdot \right) + \left(\frac{1}{ik} - \frac{\mathcal{H}}{k^2} + \frac{1}{2ik^3}(\mathcal{K} - 3\mathcal{H}^2) + \frac{\mathcal{H}(3\mathcal{H}^2 - 2\mathcal{K})}{k^4} + \frac{3\Delta_\Gamma \mathcal{H}}{4k^4} \right).$$

4. Spectral analysis of the integral operators $\mathcal{A}_{\mathcal{N}_\ell,\mathcal{D}_\ell}$ and $\mathcal{B}_{\mathcal{N}_\ell,\mathcal{D}_\ell}$ for the spherical scatterer

Since our goal is to apply an iterative solver to the proposed integral equations, a better understanding of their spectra is required. To this end, we propose an analysis in the case of the sphere of radius R. Essentially, we analyse the eigenvalue clustering of these operators, which provides a good measure of the convergence rate for a given iterative solver. Moreover, we estimate the condition number of these operators to have a simpler quantification of the iterative algorithm behaviour.

4.1 *Basic results*

Let S_R be the sphere of radius R centred at the origin and let $L^2([0,\pi] \times [0, 2\pi])$ be the space of square integrable functions endowed with the following scalar product:

$$(v, u)_0 = \int_0^\pi \int_0^{2\pi} v(\theta_1, \theta_2)\overline{u}(\theta_1, \theta_2) R^2 \sin(\theta_1) d\theta_1 d\theta_2, \quad \forall u, v \in L^2([0,\pi] \times [0, 2\pi]). \tag{4.1}$$

Let us now introduce Y_m^n as the spherical harmonics of order m (**3**), for $n = -m, \ldots, m$, with $m \in \mathbb{N}$. The functions Y_m^n form a complete orthonormal system of $L^2([0,\pi] \times [0, 2\pi])$. In the case of the sphere of radius R, they constitute a basis of eigenvectors for the four integral operators L, M, N and D. This property allows an exact calculation of the associated eigenvalues (see (**8**, **26**)).

THEOREM 4.1. *For $m = 0, 1, \ldots, n = -m, \ldots, m$, Y_m^n is an eigenfunction of the operators L, M, N and D. The corresponding eigenvalues L_m, M_m, N_m and D_m are, respectively,*

$$\begin{aligned} L_m &= \{ikR^2 j_m(kR) h_m^{(1)}(kR)\}, \\ M_m &= \{\tfrac{1}{2} - i(kR)^2 j_m'(kR) h_m^{(1)}(kR)\}, \quad N_m = -M_m, \\ D_m &= \{-ik^3 R^2 j_m'(kR) h_m^{(1)'}(kR)\}, \end{aligned} \tag{4.2}$$

where j_m ($h_m^{(1)}$) denotes the spherical Bessel (Hankel) function of order m.

4.2 *Sound-soft sphere*

Since there exist $2m+1$ linearly independent spherical harmonics Y_m^n of order m, there are $2m+1$ linearly independent eigenfunctions Y_m^n corresponding to each eigenvalue Z_m ($Z = L$, M, N or D). For an index m, we denote by $\mathcal{A}_{\mathcal{N}_\ell,m}$ the eigenvalue of the operator $\mathcal{A}_{\mathcal{N}_\ell}$. We recall that the boundary operator $\mathcal{N}_\ell$ is a second-order partial differential operator which is given by $\mathcal{N}_\ell = -\alpha\Delta_\Gamma + \beta$, for $\ell = 1, 2$. The two complex constants α and β are given for $\ell = 1$ by

$$\alpha = 0 \text{ and } \beta = ik - R^{-1},$$

and for $\ell = 2$ by

$$\alpha = \frac{1}{2ik}\left(1 - \frac{i}{kR}\right) \text{ and } \beta = ik - \frac{1}{R}.$$

The particular simple form of this operator leads after a few calculations to the exact computation of the eigenvalues of $\mathcal{A}_{\mathcal{N}_\ell}$:

$$\mathcal{A}_{\mathcal{N}_\ell,m} = L_m\left[k\frac{j_m'(kR)}{j_m(kR)} - \beta - \frac{\alpha}{R^2}m(m+1)\right]. \tag{4.3}$$

Similarly, the eigenvalues $\mathcal{A}_{\mathcal{D}_\ell,m}$ of the implicit integral operators are given by

$$\mathcal{A}_{\mathcal{D}_\ell,m} = L_m\left[k\frac{j_m'(kR)}{j_m(kR)} - \frac{1}{\beta + \alpha m(m+1)R^{-2}}\right] \tag{4.4}$$

for $\mathcal{D}_\ell = -\alpha\Delta_\Gamma + \beta$, $\ell = 1, 2$, setting (see Theorem 3.2) for $\ell = 1$

$$\alpha = 0 \text{ and } \beta = (ik)^{-1} - (k^2R)^{-1},$$

and for $\ell = 2$

$$\alpha = \frac{1}{2ik^3}\left(1 + \frac{3}{ikR}\right) \text{ and } \beta = \frac{1}{ik} - \frac{1}{k^2R} - \frac{1}{ik^3R^2} + \frac{1}{k^4R^3}.$$

To analyse the behaviour of the eigenvalues of the new integral operators, we fix the size kR of the scatterer and separate their asymptotic analysis into three zones: the elliptic zone E where the indexes m are such that $m \gg kR$ (evanescent modes), the hyperbolic region H of indexes m satisfying $m \ll kR$ (propagating modes) and finally the zone of physical surface modes satisfying $m \simeq kR$. Let us start with the asymptotic study of the eigenvalues $\mathcal{A}_{\mathcal{N}_\ell,m}$ of the explicit operators $\mathcal{A}_{\mathcal{N}_\ell}$, $\ell = 1, 2$, in the elliptic region E. To this end, we come back to the definition of the spherical Bessel and Hankel functions

$$j_m(kR) = \sqrt{\frac{\pi}{2kR}}J_{m+1/2}(kR), \quad h_m^{(1)}(kR) = \sqrt{\frac{\pi}{2kR}}H_{m+1/2}^{(1)}(kR), \tag{4.5}$$

where $J_{m+1/2}$ and $H_{m+1/2}^{(1)}$ are the fractional Bessel and Hankel functions of order $m + \frac{1}{2}$. Let us

recall the following asymptotic expansions of the Bessel and Neumann functions for large orders (see for instance (**34**, p. 365, Section 9.3))

$$J_\nu(z) \underset{\nu\to\infty}{\simeq} \frac{1}{\sqrt{2\pi\nu}}\left(\frac{ez}{2\nu}\right)^\nu \quad \text{and} \quad Y_\nu(z) \underset{\nu\to\infty}{\simeq} -\sqrt{\frac{2}{2\pi\nu}}\left(\frac{ez}{2\nu}\right)^{-\nu} \tag{4.6}$$

for z fixed. In our analysis, we fix the high-frequency parameter $z = kR$ and consider that we are in the elliptic zone setting $\nu = m + \frac{1}{2} \gg kR$. Then, we can derive the following estimates for the eigenvalues of the operators given in Theorem 4.1 and consequently for the proposed integral operators:

$$L_m = \frac{R}{2m+1} + \mathcal{O}(m^{-3}), \quad N_m = \mathcal{O}(m^{-3}), \quad M_m = \mathcal{O}(m^{-3}), \quad D_m = \frac{m+1/2}{2R} + \mathcal{O}(m^{-3}).$$

Moreover, the eigenvalues of the integral operators $\mathcal{A}_{\mathcal{N}_\ell}$, $\ell = 1, 2$, satisfy

$$\mathcal{A}_{\mathcal{N}_1,m} = \frac{m+1}{2m+1} + \mathcal{O}(m^{-1}), \quad \mathcal{A}_{\mathcal{N}_2,m} = \frac{(ikR+1)m^2}{2(kR)^2(2m+1)} + \mathcal{O}(1). \tag{4.7}$$

As shown by this last result, we observe the clustering of the eigenvalues of the explicit operator $\mathcal{A}_{\mathcal{N}_1}$ at the accumulation point $\frac{1}{2}$ (this also arises for the Burton–Miller operator (**32**)). This is not the case of the operator $\mathcal{A}_{\mathcal{N}_2}$ for which the eigenvalues behave like $im/(4kR)$. This is related to the fact that $\mathcal{A}_{\mathcal{N}_1}$ is a pseudodifferential operator of order 0 whereas $\mathcal{A}_{\mathcal{N}_2}$ is of order 1 in the elliptic zone (because the composition of L by $\mathcal{N}_2$ gives a first-order pseudodifferential operator). This property finally throws discredit on this operator since there is no clustering of its eigenvalues. Therefore, we cannot expect good behaviour from an iterative solver applied to this integral equation compared with the usual Burton–Miller equation. This is the reason why, from now on, we will not give the results relating to $\mathcal{A}_{\mathcal{N}_2}$.

Proceeding as above, we obtain the clustering around $\frac{1}{2}$ of the eigenvalues $\mathcal{A}_{\mathcal{D}_2,m}$ of the operator $\mathcal{A}_{\mathcal{D}_2}$ in the elliptic region since $L(\mathcal{D}^2)^{-1}$ is an elliptic operator of order -3. This implies that the associated integral operator has behaviour close to a Fredholm operator of the second kind in the elliptic part.

Now, we examine the behaviour of the spectrum of the integral operators in the hyperbolic zone H. We use here the following asymptotic expansion of the Hankel functions for large arguments z (see (**34**, p. 364, section 9.2))

$$H_\nu^{(1)}(z) \underset{|z|\to\infty}{\simeq} \sqrt{\frac{2}{\pi z}} e^{i\left(z-\frac{1}{2}\nu\pi-\frac{1}{4}\pi\right)} \quad (-\pi < \arg z < 2\pi). \tag{4.8}$$

Applying this estimate, we can prove the following behaviour of the eigenvalues of the integral operators $\mathcal{A}_{\mathcal{N}_1}$ and $\mathcal{A}_{\mathcal{D}_2}$ if $m \ll kR$ (hyperbolic zone):

$$\mathcal{A}_{\mathcal{N}_1,m} \approx 1 + \mathcal{O}\left((kR)^{-1}\right), \quad \mathcal{A}_{\mathcal{D}_2,m} \approx 1 + \mathcal{O}\left((kR)^{-2}\right). \tag{4.9}$$

Both formulations have a clustering of the eigenvalues around 1 for the propagating modes with a better localization for $\mathcal{A}_{\mathcal{D}_2}$. It seems from this first analysis that $\mathcal{A}_{\mathcal{D}_2}$ should yield the best convergence rate. Concerning the Burton–Miller equation, we obtain the same results as for $\mathcal{A}_{\mathcal{N}_1}$.

To have a better understanding of which parameters degrade the conditioning of the different operators, we propose an estimate of the condition number using some suitable asymptotic expansions of the Hankel functions following the analysis introduced by Chew *et al.* (**2**). Let us recall that, since the elementary integral operators are normal (**2**), the singular values of these matrices are equal to the magnitudes of the eigenvalues. Therefore, we can obtain the condition number $K(\mathcal{P})$ of an operator $\mathcal{P}$ from the extremal values

$$K(\mathcal{P}) = \lambda_{\max}/\lambda_{\min}, \tag{4.10}$$

where $\lambda_{\max} = \sup_m |\lambda_m|$, $\lambda_{\min} = \inf_m |\lambda_m|$ and $\mathcal{P}Y_m^n = \lambda_m Y_m^n$.

Let us begin to consider the operator $\mathcal{A}_{\mathcal{N}_1}$. Similar arguments as on (**2**, p. 264) show that the modulus $|\mathcal{A}_{\mathcal{N}_1,m}|$ attains its maximal value at $m \simeq kR$. This mode physically corresponds to a surface mode and accounts for the non-local effects of the coupling between the propagating and the evanescent modes. Using some adequate asymptotic expansions of the functions $J_\nu(\nu)$ and $H_\nu^{(1)}(\nu)$ and of their associated derivatives (see (**34**, Section 9.3 pp. 368–369)) when the argument ν tends toward infinity, we deduce an approximate calculation of the maximal eigenvalue $\mathcal{A}_{\mathcal{N}_1,\max}$ of the operator $\mathcal{A}_{\mathcal{N}_1}$:

$$\mathcal{A}_{\mathcal{N}_1,\max} = \frac{2\pi(1-i\sqrt{3})}{6^{4/3}\Gamma_g(2/3)^2}(kR)^{1/3} + \frac{i\pi(1-i\sqrt{3})}{3\Gamma_g(2/3)\Gamma_g(1/3)} + \frac{i\pi(1-i\sqrt{3})}{6^{4/3}\Gamma_g(2/3)^2(kR)^{2/3}} + \mathcal{O}\left(\frac{1}{kR}\right),$$

where Γ_g is the Gamma function.

Now, let us assume that we want to qualitatively measure the effect of a finite-dimensional approximation of the integral operator on the conditioning of the associated matrix. To this end, we denote by $u^{(N)}$ the truncated series for the first $N+1$ harmonics:

$$u^{(N)}(\theta_1,\theta_2) = \sum_{m=0}^{N}\sum_{n=-m}^{m} a_{mn} Y_m^n(\theta_1,\theta_2). \tag{4.11}$$

Ideally, all the indices m are present in the exact solution of the integral equation. However, if we make a finite-dimensional approximation, then the spectrum shows a cutoff near a maximal spatial frequency N representable in the finite-dimensional basis of spherical harmonics (**2**). If we consider the simpler case of the two-dimensional scattering problem by a circular cylinder, then we can see that the quantity $\Theta_N = (2N+1)/kR$ corresponds to a density of harmonics per wavelength. Concretely, a higher density Θ_N of harmonics leads to an improvement of the accuracy of the computed solution. Now if we rather consider a linear Galerkin finite element approximation, then the density Θ_N is qualitatively replaced by the density of discretization points per wavelength $n_\lambda = \lambda/h$ arising in a regular discretization of the disk for an average element size h.

An analysis of $|\mathcal{A}_{\mathcal{N}_1,m}|$ shows (**32**) that the minimal value is given in the elliptic part for the higher representable spatial mode of index N and can be estimated (see (4.7)) by $\mathcal{A}_{\mathcal{N}_1,\min} \simeq \frac{1}{2}$. After several simplifications (**32**), an estimate of the condition number $K(\mathcal{A}_{\mathcal{N}_1})$ of the operator $\mathcal{A}_{\mathcal{N}_1}$ may be given as

$$K(\mathcal{A}_{\mathcal{N}_1}) \approx 1{\cdot}2\left((kR)^{1/3} + 1 + \tfrac{1}{2}(kR)^{-2/3}\right) + \mathcal{O}((kR)^{-1}). \tag{4.12}$$

It can be proved that the same estimates hold for the Burton–Miller integral operator.

A similar study (**32**) shows that the maximal modulus of the eigenvalues of the implicit integral operator $\mathcal{A}_{\mathcal{D}_2}$ is obtained for $m \simeq kR$ (grazing modes) while the minimal value is reached for the maximal evanescent mode of index N. We get the estimates

$$\mathcal{A}_{\mathcal{D}_2,\max} \approx 0{\cdot}6\left(\tfrac{2}{3}(kR)^{1/3} + 1 + \tfrac{1}{2}(kR)^{-2/3}\right) + \mathcal{O}((kR)^{-1}). \tag{4.13}$$

Since the smallest eigenvalue is $\mathcal{A}_{\mathcal{D}_2,\min} \simeq \frac{1}{2}$ (in the elliptic zone), the condition number can be estimated by

$$K(\mathcal{A}_{\mathcal{D}_2}) \approx 1{\cdot}2\left(\tfrac{2}{3}(kR)^{1/3} + 1 + \tfrac{1}{2}(kR)^{-2/3}\right) + \mathcal{O}((kR)^{-1}). \tag{4.14}$$

It follows that this operator has a slightly smaller condition number and a better clustering of its eigenvalues compared to the usual Burton–Miller operator. These interesting spectral properties should yield a satisfactory convergence rate of a Krylov-type iterative solver. However, one must keep in mind that the solution of a sparse system is needed at each step of the iterative algorithm. These aspects will be analysed when dealing with the numerical simulations.

4.3 *Sound-hard sphere*

Let us denote by $\mathcal{B}_{\mathcal{D}_\ell,m}$ the eigenvalues of the integro-differential operator $\mathcal{B}_{\mathcal{D}_\ell}$ associated with a mode of index m and given by

$$\mathcal{B}_{\mathcal{D}_\ell,m} = i(kR)^2 h_m^{(1)'}(kR)\left[kj_m'(kR)(\beta + \alpha R^{-2}m(m+1)) - j_m(kR)\right], \tag{4.15}$$

where the complex constants α and β are defined by the various OSRCs of ND-type (see Theorem 3.2). If we consider instead $\mathcal{N}_\ell$, the eigenvalues of the associated operator $\mathcal{B}_{\mathcal{N}_\ell}$ can be expressed as

$$\mathcal{B}_{\mathcal{N}_\ell,m} = i(kR)^2 h_m^{(1)'}(kR)\left[\frac{kj_m'(kR)}{(\beta + \alpha m(m+1)R^{-2})} - j_m(kR)\right], \tag{4.16}$$

with the complex constants α and β defined in Theorem 3.1.

Let us begin to examine the spectrum of the explicit operator $\mathcal{B}_{\mathcal{D}_2}$. Using the asymptotic expansions given in Theorem 4.1, we get (**32**) the following behaviour of the eigenvalues in the elliptic zone E

$$\mathcal{B}_{\mathcal{D}_2,m} \approx \tfrac{1}{4}m^3(kR)^{-3} + \mathcal{O}(m^2). \tag{4.17}$$

Therefore, the modulus of the eigenvalues tends to grow as $m^3/(kR)^3$. This penalizes the conditioning of the operator and more particularly when a mesh refinement is employed (thus increasing the higher spatial mode of index N to represent). Moreover, the dispersion of the eigenvalues in the elliptic region of the operator is a drawback from using a Krylov iterative solver. For these reasons, this operator is disqualified from now on and we focus our study on the implicit integral formulations. We can prove (**32**) that, if $m \gg kR$ (elliptic zone), the behaviour of the eigenvalues of the integral operators $\mathcal{B}_{\mathcal{N}_\ell}$, $\ell = 1, 2$, is given by

$$\mathcal{B}_{\mathcal{N}_1,m} \approx \frac{-m}{2(ikR-1)} + \mathcal{O}(1), \quad \mathcal{B}_{\mathcal{N}_2,m} \approx \tfrac{1}{2} + \mathcal{O}(m^{-1}). \tag{4.18}$$

We observe a dispersion of the eigenvalues of the first-order operator (as in the case of the Burton–Miller formulation for a Neumann problem). This drawback is avoided with the second-order implicit formulation: the evanescent eigenvalues cluster at $\frac{1}{2}$.

Let us now analyse the operators in the hyperbolic zone. As for the Dirichlet problem, we observe a clustering of the eigenvalues relative to the propagating modes at 1 for the implicit operators

$$\mathcal{B}_{\mathcal{N}_1,m} \approx 1 + \mathcal{O}\left((kR)^{-1}\right), \quad \mathcal{B}_{\mathcal{N}_2,m} \approx 1 + \mathcal{O}\left((kR)^{-2}\right). \tag{4.19}$$

Once again, the clusterings of the two eigenvalues characterize the spectrum of the second-order implicit operator: one at 1 (propagating modes) and the other one at point $\frac{1}{2}$ (evanescent modes). A few eigenvalues corresponding to the grazing modes are not localized and tend to increase the conditioning of the operator through an eigenvalue of maximal modulus (much larger than in the Dirichlet case). However, this maximal value slightly diminishes when the order of the OSRC increases.

Let us now derive some estimates of the condition numbers for the implicit operators. A study (**32**) of the modulus of the eigenvalues $\mathcal{B}_{\mathcal{N}_1,m}$ according to m shows that the maximal value is attained at N (elliptic zone) and the minimal value at $m \simeq kR$ (grazing zone). To estimate the largest modulus of the eigenvalues, we use the approximation: $|\mathcal{B}_{\mathcal{N}_1,\max}| \approx N/(2kR) + \mathcal{O}(1)$. Using the expansions of the Hankel functions in terms of Airy functions (see (**34**, section 9.3, pp. 368–369)), we obtain the following estimate of the minimal eigenvalue: $\mathcal{B}_{\mathcal{N}_1,\min} = 0{\cdot}6 + \mathcal{O}((kR)^{-1/3})$. Hence, we deduce the approximation of the condition number

$$K(\mathcal{B}_{\mathcal{N}_1}) \approx N/(1{\cdot}2kR) + \mathcal{O}(N(kR)^{-4/3}). \tag{4.20}$$

This last relation highlights the linear dependence of the condition number with respect to the ratio of the index of the higher-order spatial mode by kR (that is, of the density of discretization points per wavelength). Moreover, it makes precise its behaviour with respect to the high-frequency parameter kR. The same estimates hold for the Burton–Miller operator.

Following a similar study (**32**), it can be proved that $|\mathcal{B}_{\mathcal{N}_2,m}|$ is minimal at N and maximal for $m \simeq 7kR/5$. The following approximations can be derived: $\mathcal{B}_{\mathcal{N}_2,\max} \approx kR/3 + \mathcal{O}(1)$ and $\mathcal{B}_{\mathcal{N}_2,\min} \approx \frac{1}{2} + \mathcal{O}(1/N)$. Therefore, an estimate of the condition number is given by

$$K(\mathcal{B}_{\mathcal{N}_2}) \approx \tfrac{2}{3}kR + \mathcal{O}(kR/N), \tag{4.21}$$

and essentially depends on the high-frequency parameter kR.

4.4 *A second-order damped and implicit alternative integral equation*

The involvement of the $\mathcal{N}_2$ operator in the alternative implicit integral formulation avoids the condition number dependence according to the density of discretization points per wavelength. However, the price to pay is that a linear dependence with respect to kR appears, unlike in the Burton–Miller formulation. We propose now a modification of $\mathcal{N}_2$ which leads to a condition number almost independent of the value of the parameter kR.

As proved above, the maximal eigenvalue is localized in the zone of creeping rays. Let us recall that the initial classical asymptotic expansion of the symbol of the DN operator is not uniform for any frequency (k, ξ) (**35**), where ξ denotes the covariable of s by Fourier transform (**23**). Indeed, the expansion breaks down for frequencies satisfying $|\xi| \simeq k$ (grazing zone). A possible way to

locally attenuate the discrepancy linked to these modes is to introduce a damping coefficient in the approximation process of the principal symbol. Let $\lambda_1 = ik\sqrt{1+X}$ be the classical principal symbol of the DN operator (**23**), where $X = -|\xi|^2/k^2$. We consider the complex approximation of the square root operator developed by Lu (**36**), $\sqrt{1+X} \simeq 1 + X/(2+i\gamma)$, where γ is a real positive parameter fixed later. This approximation has been introduced in (**36**) for the numerical approximation of evanescent modes in the beam propagation method (BPM) for optical waveguides. This is a generalization of the Padé approximants taking a real positive parameter γ as initial value in the iterative construction procedure of the usual Padé approximants. This gives a satisfactory interpolation for the complex values of the square root $\sqrt{1+X}$ for purely real values of X slightly smaller than -1 (this is obviously not the case for the classical Taylor expansions for $\gamma = 0$). This modification leads to a damped OSRC using the approximation

$$\lambda_1 \simeq ik\left(1 - \frac{|\xi|^2}{(2+i\gamma)k^2}\right). \tag{4.22}$$

As a consequence, the new damped operator is given by

$$\begin{aligned}\mathcal{N}_2^\gamma = &-\mathrm{div}_\Gamma\left(\frac{1}{(2+i\gamma)ik}\left(\mathbb{I} - \frac{(2+i\gamma)i\mathcal{R}}{2k}\right)\nabla_\Gamma\right)\\ &+ik - \mathcal{H} - \frac{i}{2k}\left(1 - \frac{2i\mathcal{H}}{k}\right)(\mathcal{K} - \mathcal{H}^2) + \frac{\Delta_\Gamma \mathcal{H}}{4k^2}.\end{aligned} \tag{4.23}$$

Until now, γ is a free parameter. In fact, an adequate choice can be determined to minimize the condition number of the resulting indirect formulation based on $\mathcal{N}_2^\gamma$. Some similar approximations as for $\gamma = 0$ yield the following estimate of the condition number:

$$K(\mathcal{B}_{\mathcal{N}_2^\gamma}) \approx g(\gamma) = \frac{(7 + 3\sqrt{\gamma/2})k}{5|f(\gamma)|} + \mathcal{O}(kR/N), \tag{4.24}$$

with $f(\gamma) = |\alpha(\gamma)[(7+3\sqrt{\gamma/2})kR/5]^2 + \beta|$, $\beta = ik - 1/R$ and

$$\alpha(\gamma) = [(2+ik)ik]^{-1}[1 - (2+i\gamma)/(2kR)].$$

To minimize the condition number of the damped operator, we have to choose the parameter γ that minimizes the first term of the function $\gamma \mapsto g(\gamma)$. A straightforward study shows that the optimal parameter is given by $\gamma = 2$ ($|f(2)| = (kR+3)/R$) yielding

$$K(\mathcal{B}_{\mathcal{N}_2^2}) \approx \frac{2kR}{kR+3} + \mathcal{O}(kR/N). \tag{4.25}$$

The resulting integral equation has a condition number that is now both independent of the index N of the higher-order spatial mode (and incidentally also of the density of discretization points n_λ) and almost independent of the high-frequency parameter kR. Moreover, the evanescent modes are correctly approximated and the modulus of the corresponding maximal eigenvalue is efficiently diminished. As a conclusion, the resulting integral equation has better behaviour than the usual Burton–Miller and $\mathcal{N}_2$-based formulations.

5. Numerical experiments for two-dimensional scattering problems

5.1 *Implementation for a linear Galerkin boundary element method*

Let us consider the alternative implicit integral equation of order ℓ for the Dirichlet problem

$$\mathcal{A}_{\mathcal{D}_\ell}\psi = g \quad \text{on } \Gamma, \qquad \text{with} \quad \mathcal{A}_{\mathcal{D}_\ell} = (\tfrac{1}{2}I - M) - L(\mathcal{D}_\ell)^{-1}. \tag{5.1}$$

If Z represents a continuous operator, then $[Z]$ designates its discrete representation after interpolation of the exact boundary Γ by a polygonal curve $\Gamma_h = \bigcup_{T\in\mathcal{T}_h} T$ involving a regular triangulation $\mathcal{T}_h$ and discretization by a $\mathbb{P}_1$ Galerkin boundary element method. Let us introduce n as the total number of degrees of freedom of the boundary element method and n_λ as the average density of discretization points per wavelength defined by $n_\lambda = \lambda/h_{\max}$, where $h_{\max} = \max_{T\in\mathcal{T}_h}|T|$ is the maximal length of the finite elements T. We do not describe the classical numerical approximation of the integral equations by linear boundary elements. Concerning the finite element approximation of the OSRC formulations, see (**22**) where extended developments are available. The discretization of (5.1) is hence

$$[\mathcal{A}_{\mathcal{D}_\ell}]\psi_h = \mathbf{g}_h, \tag{5.2}$$

where we have set

$$[\mathcal{A}_{\mathcal{D}_\ell}] = (\tfrac{1}{2}[I] - [M]) - [L][\mathcal{D}_\ell]^{-1}. \tag{5.3}$$

The n-dimensional complex-valued vectors ψ_h and $\mathbf{g}_h$ designate respectively the discrete unknown and second member. The GMRES algorithm without restart is chosen as Krylov iterative solver for computing the solution to (5.2). The tolerance on the residue is arbitrarily fixed to 10^{-8}. At each step of the iterative algorithm, a matrix-vector product $\mathbf{z} = [\mathcal{A}_{\mathcal{D}_\ell}]\mathbf{y}$ has to be computed. The implementation is made by first solving the sparse linear system *via* a direct Gauss elimination solver with a cost of order $\mathcal{O}(n)$

$$[\mathcal{D}_\ell]\mathbf{x} = \mathbf{y}, \tag{5.4}$$

and then computing the two matrix-vector products in a parallel way

$$\mathbf{z} = (\tfrac{1}{2}[I] - [M])\mathbf{y} - [L]\mathbf{x}. \tag{5.5}$$

The solution to (5.4) can be also computed by a GMRES solver preconditioned by an incomplete LU factorization with a threshold equal to 10^{-3}. Approximately two or three iterations are needed to get a residue of 10^{-8}. The cost is therefore still linear with respect to n.

One suitable parameter to observe the convergence rate of an iterative solver of Krylov-type applied to a linear system issued from the discretization of an integral equation is the total number of dense matrix-vector products needed to get a satisfactory residue. Let us mention that one matrix-vector product can be performed in $\mathcal{O}(n^2)$ operations if the system is dense or $\mathcal{O}(n\log n)$ if the system is sparse using, for example, a fast multipole algorithm (**2**, **10**). We do not report the convergence rates for other iterative solvers (CGS and BiCGSTAB) which are always larger than for the GMRES. The same strategy is developed for solving the alternative implicit integral formulations for the Neumann problem.

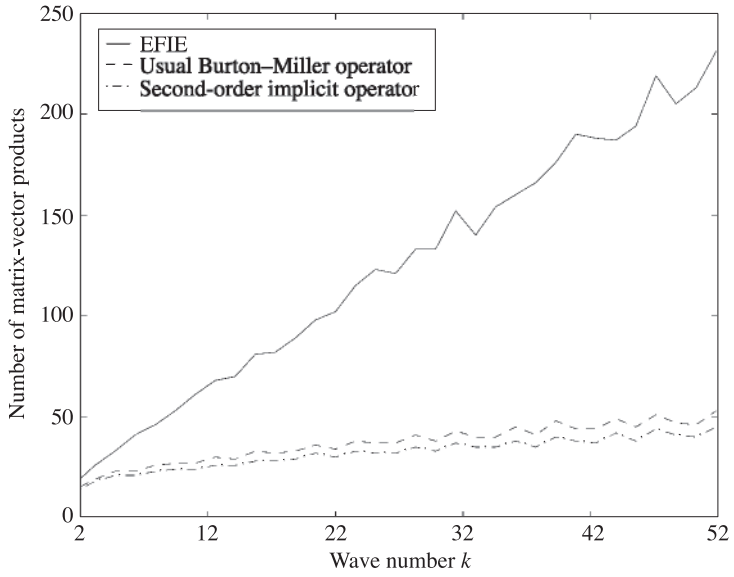

Fig. 1 Sound-soft square cylinder with cavity. Evolution of the number of matrix-vector products involved in the GMRES iterative solver as a function of the wave number k ($n_\lambda = 10$ and incidence of 30 degrees) for the various integral formulations

5.2 *Sound-soft scattering problem*

We consider an incident plane wave $u^{\text{inc}}(x) = \exp\{-ik(x_1 \cos\theta^{\text{inc}} + x_2 \sin\theta^{\text{inc}})\}$, where θ^{inc} is the angle of incidence in the $\mathbb{R}^2$-plane. Cartesian coordinates are denoted by $x = (x_1, x_2)$. Following similar calculations as in the three-dimensional case, one gets the following estimates of the condition numbers for the circular cylinder of radius R:

$$K(\mathcal{A}_{\text{BM},\mathcal{N}_1}) \approx 1{\cdot}2(1 + (kR)^{1/3}) + \mathcal{O}((kR)^{-2/3}) \tag{5.6}$$

and

$$K(\mathcal{A}_{\mathcal{D}_2}) \approx 1{\cdot}2\left(1 + \tfrac{2}{3}(kR)^{1/3}\right) + \mathcal{O}((kR)^{-2/3}). \tag{5.7}$$

We recall that the theoretical spectral study has been developed on the continuous operators and not the discrete ones. However, since consistent numerical schemes have been used for the numerical approximation of the integral equations, all the conclusions should remain the same at the discrete level. A more precise and rigorous analysis would require some developments similar to the ones introduced by Chew and Warnick (**2**).

From formulae (5.6) and (5.7), we can expect a slight improvement of the convergence rate of the GMRES by increasing the frequency but not by remeshing since the Burton–Miller (BM) formulation involves a Fredholm integral operator of the second kind. To complete the comparisons, we also report the results for the electric field integral equation (EFIE) given for the Dirichlet problem by $-Vp = g$ on Γ, where p is an unknown density. This first-kind integral equation is well

known for admitting internal resonances and being unstable for closed bodies (**2**). This problem is overcome by the BM formulation (**3**, **24**) and quite reasonably also by the formulation involving the operator $\mathcal{A}_{\mathcal{D}_2}$ as can be observed in Fig. 1 (no peak in the convergence curves due to small eigenvalues). The scatterer is a square cylinder with a reentrant cavity. This non-convex scatterer is composed of the square cylinder with a side length equal to 2 and an inner cavity of vertices $(-1, 0{\cdot}4)$, $(0, 0{\cdot}4)$, $(0, -0{\cdot}4)$ and $(-1, -0{\cdot}4)$. We do not really observe a significant improvement coming from the alternative implicit integral formulation compared to the BM equation since the gain of a few iterations can be practically lost in the solution of system (5.4).

5.3 *Sound-hard obstacle*

Let us now analyse the results concerning the Neumann problem. The estimates of the condition numbers are given by

$$K(\mathcal{B}_{BM,\mathcal{N}_1}) \approx \frac{n_\lambda}{2{\cdot}4 + 2(kR)^{-1/3}} + \mathcal{O}(n_\lambda (kR)^{-4/3}), \tag{5.8}$$

$$K(\mathcal{B}_{\mathcal{N}_2}) \approx \frac{4kR}{5} + \mathcal{O}(kR/n_\lambda) \quad \text{and} \quad K(\mathcal{B}_{\mathcal{N}_2^2}) \approx \frac{4kR}{2kR+5} + \mathcal{O}(kR/n_\lambda). \tag{5.9}$$

Figure 2 shows how the number of matrix-vector products of the integral formulations varies with the wave number (a) and the density of discretization points (b) for the elliptical cylinder centred at the origin with a semi-axis $a = 1{\cdot}8$ (respectively $b = 0{\cdot}3$) along the direction x_1 (respectively x_2). We also present the results for the EFIE (**2**) given for a Neumann problem by the integral equation $-Dp = g$ on Γ. The peaks observable in Fig. 1 show the instability of this integral equation. This characteristic does not seem present for the other formulations. We remark that the number of matrix-vector products arising in the BM and $\mathcal{A}_{\mathcal{N}_2^2}$-based formulations is almost independent of k, unlike the formulation involving $\mathcal{A}_{\mathcal{N}_2}$. These results confirm qualitatively the estimates of (5.8) and (5.9) derived for the circular cylinder. Moreover, the second-order implicit alternative damped integral equation requires approximately 60 per cent fewer iterations to be solved than the BM formulation for high-frequencies. Unlike the second-order alternative implicit integral equations (second-kind integral equations), we observe that the number of matrix-vector products increases with n_λ for the BM equation (first-kind integral equation). From these results, we conclude that the $\mathcal{A}_{\mathcal{N}_2^2}$-based formulation leads to a significant gain concerning the number of matrix-vector products in the iterative algorithm. To complete the computations, we show in Fig. 3 some results for the square cylinder with cavity. Once again, the same conclusions hold even though we are dealing with a non-convex scatterer. Finally, error computations on the surface fields have been performed and show that similar relative errors occur in the different formulations.

6. Conclusion and perspectives

We have developed some well-conditioned alternative integral equations for the iterative solution of three-dimensional acoustic scattering problems. Their construction is based on the introduction of some suitable differential on-surface radiation conditions into the integral representations. Second-order (eventually damped) implicit alternative integral equations provide the best convergence rates. These equations behave like second-kind integral equations. The most interesting improvements are obtained for the sound-hard scattering problem. The convergence rate is independent of the

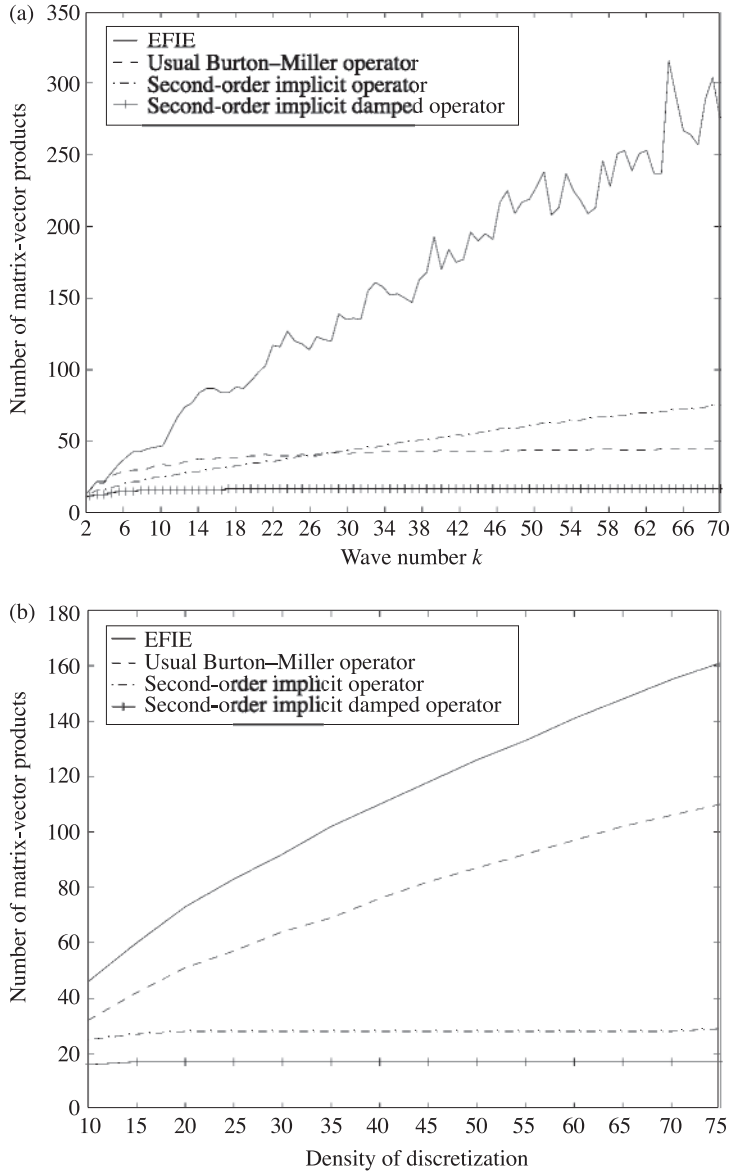

Fig. 2 Sound-hard elliptical cylinder. Evolution of the number of matrix-vector products involved in the GMRES iterative solver as a function of the wave number k ((a): $n_\lambda = 10$ and null incidence) and the density of discretization points n_λ ((b): $k = 10$ and null incidence) for the various integral formulations

density of discretization points per wavelength and almost independent of the wave number. Two-dimensional numerical results confirm the theoretical analysis. Finally, the proposed approach

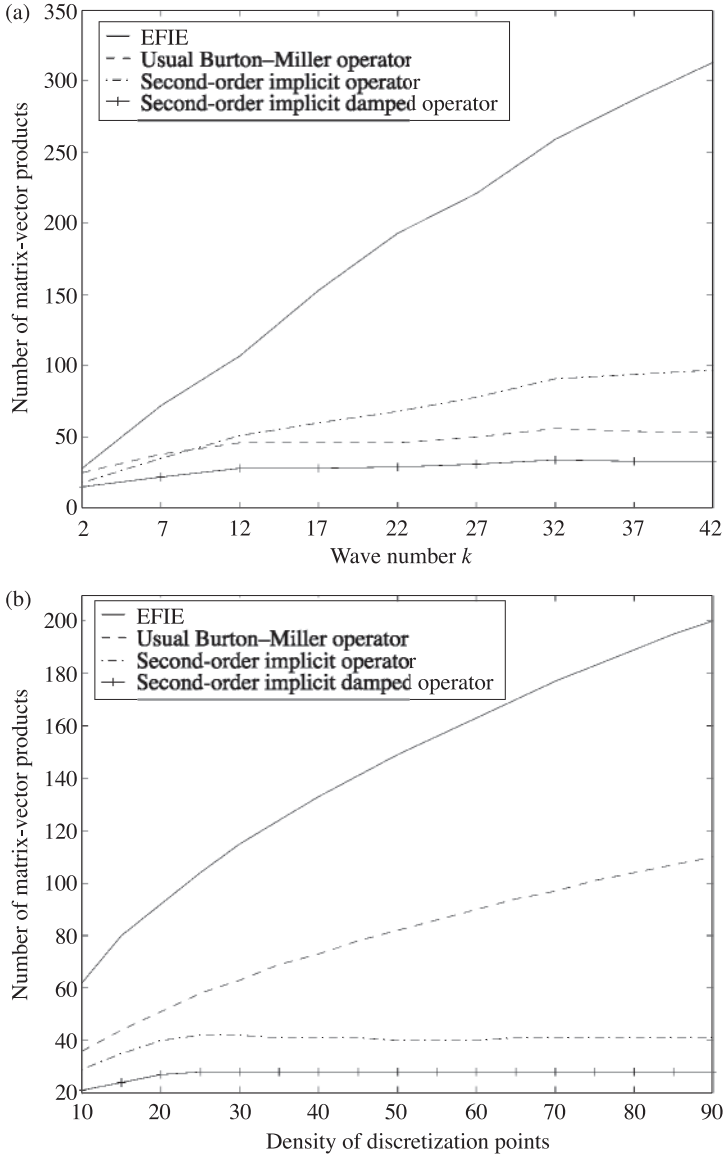

Fig. 3 Sound-hard square cylinder with cavity. Evolution of the number of matrix-vector products involved in the GMRES iterative solver as a function of the wave number k ((a): $n_\lambda = 10$ and incidence of 30 degrees) and the density of discretization points n_λ ((b): $k = 5$ and incidence of 30 degrees) for the various integral formulations

provides a suitable generalization and justification of the usual Burton–Miller and Brakhage–Werner integral equations widely used in acoustic scattering.

Concerning the perspectives and improvements of the method, the analysis of the construction of the OSRCs by the pseudodifferential calculus (**23**) provides several directions for future work. A first development in progress concerns the numerical extension of the method to the three-dimensional case and to complex scatterers with different shapes (**22**). It may be also interesting to investigate how to increase the accuracy of the OSRCs by a paraxialization (**37**) of the truncated symbolic asymptotic expansions of the DN and ND operators. The extension to the three-dimensional full Maxwell equations is actually developed (**38**) as well as the possibility of extension to a Fourier–Robin or mixed boundary condition. Other problems can be studied, such as the problem of increasing the order of the finite element method or the discretization by a collocation method. Finally, other interesting investigations would be the development of the spectral and error analysis of the discrete formulations using for instance the recent works of Chew *et al.* (**2**).

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