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Numerical Analysis

An alternative to Dirichlet-to-Neumann maps for waveguides

Une alternative aux opérateurs de Dirichlet–Neumann pour les guides d'ondes

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ABSTRACT

We are interested by the treatment of the radiation condition at infinity for the numerical solution of a problem set in an unbounded waveguide. We propose an alternative to the classical approach involving a modal expression of Dirichlet-to-Neumann (DtN) operators. This method is particularly easy to implement since it only requires the solution of boundary value problems with local boundary conditions. The corresponding approximate solution is comparable in accuracy to the one obtained by truncating the infinite series in the DtN maps.

RÉSUMÉ

Nous nous intéressons au traitement de la condition de rayonnement à l'infini pour la résolution numérique d'un problème posé dans un guide d'ondes non borné. Nous proposons une alternative à l'approche classique reposant sur une expression modale d'opérateurs de type Dirichlet–Neumann (DtN). Cette méthode est particulièrement simple à mettre en œuvre puisqu'elle ne requiert que la résolution de problèmes aux limites dont les conditions aux limites sont locales. La solution approchée correspondante est d'une précision comparable à celle obtenue en tronquant la série infinie dans les opérateurs DtN.

Version française abrégée

Nous considérons un problème de diffraction acoustique dans un guide d'onde semi-infini pouvant être localement perturbé. Plus précisément, nous nous intéressons à la résolution numérique du problème aux limites (1) complété d'une condition de rayonnement à l'infini. Cette condition, qui impose que la solution soit « sortante » à l'infini, peut être explicitée au moyen d'un développement en série sur les modes du guide. Une approche numérique classique consiste à discrétiser par une méthode d'éléments finis une formulation équivalente du problème, posée dans un domaine borné Ω_ℓ, obtenue en écrivant sur une frontière artificielle S_ℓ une condition aux limites non locale de type Dirichlet–Neumann (DtN), faisant intervenir la série modale tronquée, le rang de troncature pouvant être choisi d'autant plus petit (mais toujours supérieur au nombre de modes propagatifs) que la frontière S_ℓ est éloignée du sous-domaine Ω_0 contenant les perturbations (voir la Fig. 1). Un inconvénient de ce procédé est que la non-localité de la condition transparente fait en partie perdre sa structure creuse au système linéaire associé au problème discrétisé et complique par ailleurs l'implémentation de la méthode.

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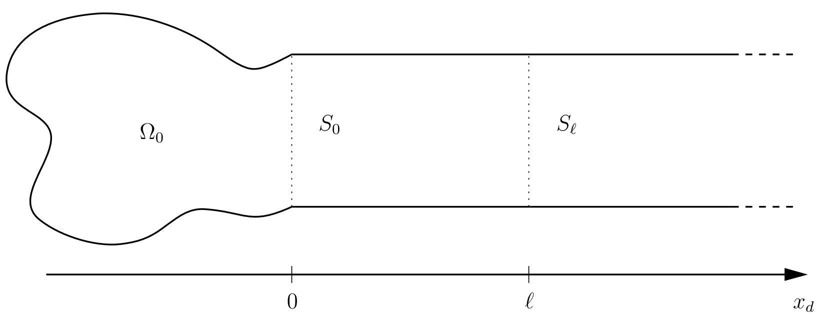

Fig. 1. A realization of the domain Ω.

Fig. 1. Une réalisation du domaine Ω.

Dans cette Note, nous proposons une méthode qui s'appuie sur la résolution de problèmes ne faisant intervenir que des conditions aux limites *locales*. Pour ce faire, nous introduisons le problème (4), dans lequel la condition non locale a été remplacée par une condition de Robin, et considérons l'écart entre la solution u_r de ce problème et la solution u recherchée. Nous montrons tout d'abord, en utilisant l'analyse modale, que le champ u_r satisfait un problème équivalent, posé sur Ω_0 et faisant intervenir une condition aux limites artificielle non locale. On observe alors que la différence entre cette condition approchée et la condition « exacte » est la somme de deux contributions, définies par (7), dont l'une fait apparaître un opérateur de rang fini et l'autre peut être rendue négligeable. On montre ainsi que la différence $u - u_r$ est solution (à des termes négligeables près) d'un problème dont la donnée appartient à un espace de dimension finie. Nous en déduisons un procédé de construction d'une « correction » du champ u_r de la forme (11), requérant la détermination de champs auxiliaires, solutions de la famille finie de problèmes bien posés (13), et d'autant de coefficients scalaires, obtenus par résolution d'un système linéaire dont nous prouvons qu'il admet une unique solution.

Il est important de noter que les matrices (creuses) des systèmes algébriques résultant de la discrétisation des problèmes auxiliaires sont toutes identiques à celle issue de la discrétisation du problème (4). Ainsi, une fois cette matrice factorisée, l'obtention d'une approximation discrète de chacun des champs en question se ramène simplement à l'assemblage d'un vecteur second membre suivi de la résolution de deux systèmes triangulaires, ce travail pouvant être effectué en parallèle.

Nous concluons en mentionnant et commentant diverses extensions et utilisations possibles de cette approche.

1. The diffraction problem in a semi-infinite waveguide

In this Note, we deal with, for the sake of simplicity, an acoustic scattering problem set in a possibly locally perturbed semi-infinite waveguide. More precisely, we consider a connected unbounded domain $\Omega \subset \mathbb{R}^d$ with $d \geqslant 2$, such that $\Omega \cap \{\boldsymbol{x} = (\boldsymbol{x}_S, x_d) \mid x_d > 0\} = \{\boldsymbol{x} = (\boldsymbol{x}_S, x_d) \mid \boldsymbol{x}_S \in S,\ x_d > 0\}$, where S is a bounded subset of $\mathbb{R}^{d-1}$, and $\Omega \cap \{\boldsymbol{x} = (\boldsymbol{x}_S, x_d) \mid x_d < 0\} = \Omega_0$ is a bounded domain (see Fig. 1), and are interested in numerically solving the following boundary value problem:

$$-\Delta u - k^2 u = f \quad \text{in } \Omega, \qquad \partial_{\boldsymbol{n}} u = 0 \quad \text{on } \partial\Omega, \tag{1}$$

supplemented by a *radiation condition* at infinity. It is assumed that the source term f belongs to $L^2(\Omega)$ and is compactly supported in Ω_0, and that the wave number k is real. The vector $\boldsymbol{n}$ denotes the outward unit normal on $\partial\Omega$.

The prescribed radiation condition states that the solution is "outgoing" at infinity. It can be written down by introducing the so-called *modes* of the guide, which are functions with separated variables of the form $\varphi_n(\boldsymbol{x}_S)\, e^{\pm i\beta_n x_d}$, $n \in \mathbb{N}$, the complex numbers β_n being such that $\beta_n = \sqrt{k^2 - \lambda_n}$ for $k^2 \geqslant \lambda_n$ and $\beta_n = i\sqrt{\lambda_n - k^2}$ for $k^2 \leqslant \lambda_n$. Here, the real positive scalar λ_n denotes the nth eigenvalue of the negative Laplace operator acting in $L^2(S)$ and associated with the homogeneous Neumann boundary condition on ∂S, and the orthonormal real-valued functions φ_n are the corresponding eigenfunctions. A mode is said to be *propagative* if $\beta_n \in \mathbb{R}$, and *evanescent* if $\beta_n \in i\mathbb{R}$ (note that there is a finite number N_{prop} of propagative modes). If $k^2 \neq \lambda_n$, $\forall n \in \mathbb{N}$, saying the solution is outgoing simply means that, for any $\boldsymbol{x}$ in Ω such that $x_d > \ell \geqslant 0$, the field $u(\boldsymbol{x})$ is given by a convergent series of *rightgoing* modes $\varphi_n(\boldsymbol{x}_S)\, e^{i\beta_n x_d}$, $n \in \mathbb{N}$, that is

$$u(\boldsymbol{x}) = \sum_{n=0}^{+\infty} A_n^+(\ell, u)\, \varphi_n(\boldsymbol{x}_S)\, e^{i\beta_n (x_d - \ell)}, \quad \forall \boldsymbol{x}_S \in S,\ \forall x_d > \ell \geqslant 0.$$

In other words, the amplitudes $A_n^-(\ell, u)$, $n \in \mathbb{N}$, of the solution u on the *leftgoing* modes $\varphi_n(\boldsymbol{x}_S)\, e^{-i\beta_n (x_d - \ell)}$ must vanish. Notice that it follows from the orthonormality of the functions φ_n, $n \in \mathbb{N}$, that $A_n^+(\ell, u) = (u(\cdot, \ell), \varphi_n)_S$, where $u(\cdot, x_d)$ denotes the function u viewed as a function of the variable $\boldsymbol{x}_S$ and $(\cdot\,,\cdot)_S$ denotes the scalar product on $L^2(S)$.

For both theoretical and numerical purposes, it is convenient to replace problem (1) by an equivalent problem set on a bounded domain $\Omega_\ell = \Omega \cap \{\boldsymbol{x} = (\boldsymbol{x}_S, x_d) \mid \boldsymbol{x}_S \in S,\ x_d < \ell\}$, with $\ell \geqslant 0$. This is achieved by incorporating, using a Dirichlet-to-Neumann (DtN) map, the radiation condition into an exact nonlocal boundary condition on the artificial boundary $S_\ell = S \times \{\ell\}$, that is

$$\partial_{\boldsymbol{n}} u = T_\ell(u) = \mathrm{i}\sum_{n=0}^{+\infty} \beta_n \big(u(\cdot,\ell),\varphi_n\big)_S \varphi_n \quad \text{on } S_\ell. \tag{2}$$

Classical arguments allow to prove that the boundary value problem

$$-\Delta u - k^2 u = f \quad \text{in } \Omega_\ell, \qquad \partial_{\boldsymbol{n}} u = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_\ell, \qquad \partial_{\boldsymbol{n}} u - T_\ell(u) = 0 \quad \text{on } S_\ell, \tag{3}$$

is of Fredholm type. In what follows, we assume that uniqueness holds so that the problem is well-posed for every $\ell \geqslant 0$. Now, to compute an approximate solution to problem (3), one can discretize its natural variational formulation by a finite element method and truncate the infinite series in T_ℓ (see [3,4]). It can be seen that the rank of truncation, which is always greater or equal to N_{prop}, can be chosen smaller by increasing the length ℓ. A drawback of this approach is the nonlocality of the boundary condition, which makes both the implementation of this method more difficult and the numerical solution of the associated algebraic system more expensive, the resulting matrix not being fully sparse. Here, we propose an alternative approach, which relies solely on the solution of problems with *local* boundary conditions, and thus workable into any standard finite element code.

2. The effect of replacing the transparent condition by a Robin condition

Let us consider the following boundary value problem:

$$-\Delta u_r - k^2 u_r = f \quad \text{in } \Omega_\ell, \qquad \partial_{\boldsymbol{n}} u_r = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_\ell, \qquad \partial_{\boldsymbol{n}} u_r - \mathrm{i}\alpha u_r = 0 \quad \text{on } S_\ell, \tag{4}$$

where $\alpha \in \mathbb{R}\backslash\{0\}$ is a given parameter. Note that such a problem is well-posed; indeed, it satisfies the Fredholm alternative and the uniqueness of its solution is a consequence of Holmgren's theorem.

To compare u_r with the solution u to (1), we proceed as in [2] and derive an equivalent problem satisfied by u_r in the subdomain Ω_0 (we emphasize that this problem, which involves a nonlocal boundary condition, is a theoretical tool never to be used numerically). Knowing that the solution to (4) can be expanded on the guided modes as follows

$$u_r(\boldsymbol{x}) = \sum_{n=0}^{+\infty} \big(A_n^+(0,u_r)\, e^{\mathrm{i}\beta_n x_d} + A_n^-(0,u_r)\, e^{-\mathrm{i}\beta_n x_d}\big)\varphi_n(\boldsymbol{x}_S), \quad \forall \boldsymbol{x} \in S \times [0,\ell], \tag{5}$$

and using the boundary condition on S_ℓ, one has

$$\mathrm{i}\beta_n\big(A_n^+(0,u_r)\, e^{\mathrm{i}\beta_n\ell} - A_n^-(0,u_r)\, e^{-\mathrm{i}\beta_n\ell}\big) = \mathrm{i}\alpha\big(A_n^+(0,u_r)\, e^{\mathrm{i}\beta_n\ell} + A_n^-(0,u_r)\, e^{-\mathrm{i}\beta_n\ell}\big), \quad \forall n \in \mathbb{N}.$$

Setting

$$\frac{A_n^-(0,u_r)}{A_n^+(0,u_r)} = \frac{\beta_n - \alpha}{\beta_n + \alpha}\, e^{2\mathrm{i}\beta_n\ell} = R_n(\ell), \quad \forall n \in \mathbb{N},$$

we finally obtain that u_r satisfies the condition:

$$\partial_{\boldsymbol{n}} u_r - \mathrm{i}\sum_{n=0}^{+\infty} \beta_n \frac{1 - R_n(\ell)}{1 + R_n(\ell)} \big(u_r(\cdot,0),\varphi_n\big)_S \varphi_n = 0 \quad \text{on } S_0 = S \times \{0\}.$$

The coefficient $R_n(\ell)$ gives a measure of the reflection on the nth mode caused by the truncation of the domain and the use of a Robin boundary condition at $x_d = \ell$. It vanishes if $\alpha = \beta_n$ and is otherwise nonzero, but it can be made arbitrarily small by choosing ℓ sufficiently large when the nth mode is evanescent. Owing to this remark, the problem satisfied by u_r in Ω_0 can be rewritten as follows

$$-\Delta u_r - k^2 u_r = f \quad \text{in } \Omega_0, \qquad \partial_{\boldsymbol{n}} u_r = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_0, \qquad \partial_{\boldsymbol{n}} u_r - T_0(u_r) = L_\ell^N(u_r) + S_\ell^N(u_r) \quad \text{on } S_0. \tag{6}$$

In the above problem, the difference between the "exact" boundary condition, which involves the DtN operator T_0 (consider (3) with $\ell = 0$), and the approximate one has been split into two contributions respectively defined by

$$L_\ell^N(u) = \mathrm{i}\sum_{n=0}^{N-1} \frac{2\beta_n R_n(\ell)}{1 + R_n(\ell)} \big(u(\cdot,0),\varphi_n\big)_S \varphi_n \quad \text{and} \quad S_\ell^N(u) = \mathrm{i}\sum_{n=N}^{+\infty} \frac{2\beta_n R_n(\ell)}{1 + R_n(\ell)} \big(u(\cdot,0),\varphi_n\big)_S \varphi_n, \tag{7}$$

where N is an integer such that

$$\big\| S_\ell^N \big\|_{\mathcal{L}(H^{1/2}(S),H^{-1/2}(S))} \leqslant C \max_{n \geqslant N} \left| \frac{R_n(\ell)}{1 + R_n(\ell)} \right| \sim C\, e^{-2\,\mathrm{Im}(\beta_N \ell)} \leqslant \varepsilon, \tag{8}$$

with $\varepsilon > 0$ a prescribed tolerance. Observe that we must have $N \geqslant N_{prop}$ for the last inequality in (8) to be satisfied, as we use the fact that $|R_n(\ell)|$ decreases exponentially as $|\beta_n \ell|$ increases if the nth mode is evanescent.

3. The auxiliary fields and the recomposed approximate solution

Since the operator S_ℓ^N can be rendered negligible, the discrepancy between the approximate solution u_r and the actual solution u is mainly due to the operator L_ℓ^N. Our idea is to use both the fact that L_ℓ^N is of finite rank N and the linearity of the problem to construct a new approximate solution $\tilde{u}$ verifying

$$-\Delta\tilde{u} - k^2\tilde{u} = f \quad \text{in } \Omega_0, \qquad \partial_{\boldsymbol{n}}\tilde{u} = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_0, \qquad \partial_{\boldsymbol{n}}\tilde{u} - T_0(\tilde{u}) = S_\ell^N(\tilde{u}) \quad \text{on } S_0. \tag{9}$$

One can show, taking inspiration from [2], that, for ε small enough (that is, for ℓ and/or N large enough), problem (9) is well-posed and that we have the estimate $\|u - \tilde{u}\|_{H^1(\Omega_0)} \leqslant C\varepsilon$, where C is a constant independent of both ℓ and N.

To effectively build the approximation $\tilde{u}$, we set $\tilde{u} = u_r + u_c$, the corrective field u_c being, by linearity, solution to

$$-\Delta u_c - k^2 u_c = 0 \quad \text{in } \Omega_0, \qquad \partial_{\boldsymbol{n}} u_c = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_0, \qquad \partial_{\boldsymbol{n}} u_c - T_0(u_c) - S_\ell^N(u_c) = -L_\ell^N(u_r) \quad \text{on } S_0.$$

Since the range of L_ℓ^N is included in the N-dimensional vector space $V_N = \operatorname{span}\{\varphi_0, \ldots, \varphi_{N-1}\}$, this correction may be written down as a linear combination of N functions $u^{(j)}$, $j = 0, \ldots, N-1$, satisfying $-\Delta u^{(j)} - k^2 u^{(j)} = 0$ in Ω_0, $\partial_{\boldsymbol{n}} u^{(j)} = 0$ on $\partial\Omega \cap \partial\Omega_0$, and such that the family $\{g^{(j)}\}_{j=0,\ldots,N-1}$ of functions defined by

$$g^{(j)} = \partial_{\boldsymbol{n}} u^{(j)}{}_{|S_0} - T_0\big(u^{(j)}\big) - S_\ell^N\big(u^{(j)}\big), \quad j = 0, \ldots, N-1, \tag{10}$$

form a basis of V_N. Assuming for a moment the existence of such functions $u^{(j)}$, $j = 0, \ldots, N-1$, (a particular choice is proposed below), we then have

$$\tilde{u} = u_r + \sum_{j=0}^{N-1} \mu^{(j)} u^{(j)}, \tag{11}$$

where the coefficients $\mu^{(j)}$, $j = 0, \ldots, N-1$, are such that

$$\sum_{j=0}^{N-1} \mu^{(j)} g^{(j)} = -L_\ell^N(u_r). \tag{12}$$

In practice, the fields $u^{(j)}$, $j = 0, \ldots, N-1$, can be conveniently obtained as the solutions to

$$-\Delta u^{(j)} - k^2 u^{(j)} = 0 \quad \text{in } \Omega_\ell, \qquad \partial_{\boldsymbol{n}} u^{(j)} = 0 \quad \text{on } \partial\Omega \cap \partial\Omega_\ell, \qquad \partial_{\boldsymbol{n}} u^{(j)} - \mathrm{i}\alpha u^{(j)} = \varphi_j \quad \text{on } S_\ell, \tag{13}$$

as this choice leads to a family of linearly independent functions $g^{(j)}$, $j = 0, \ldots, N-1$, defined by (10). Indeed, suppose that $\sum_{j=0}^{N-1} \mu^{(j)} g^{(j)} = 0$. Setting $u^* = \sum_{j=0}^{N-1} \mu^{(j)} u^{(j)}$ and using (10), we see that u^* satisfies problem (9) with $f = 0$. This problem being well-posed, one has $u^* \equiv 0$. In view of the definition (13) of the auxiliary fields $u^{(j)}$, $j = 1, \ldots, N-1$, it follows that $0 = \partial_{\boldsymbol{n}} u^* - \mathrm{i}\alpha u^* = \sum_{j=0}^{N-1} \mu^{(j)} \varphi_j$ on S_ℓ, which implies that $\mu^{(j)} = 0$, $j = 1, \ldots, N-1$.

4. Implementation

To sum up, the solution method we propose consists of computing successively, using finite element approximations (other discretization techniques are, of course, possible), the field u_r, which is solution to problem (4), the auxiliary fields $u^{(j)}$, $j = 0, \ldots, N-1$, which solve the family of problems (13), and the coefficients $\mu^{(j)}$, $j = 0, \ldots, N-1$, the approximate solution $\tilde{u}$ being finally recomposed according to (11). We stress that these various computations do not require to build and solve $N+1$ algebraic systems associated with the finite element discretization, since these systems only differ by their respective right-hand sides. Hence, once the (sparse) matrix of the systems has been factorized, the solutions (which can moreover be performed in parallel) merely amount to forward and backward substitutions.

As it is impractical to compute the scalars $\mu^{(j)}$, $j = 0, \ldots, N-1$ from system (12), we need to derive another linear system satisfied by these coefficients. To do so, notice that the second boundary condition in (9) imposes that the field $\partial_{\boldsymbol{n}}\tilde{u}_{|S_0} - T_0(\tilde{u})$ is orthogonal to V_N, which means that no reflection occurs on the N first guided modes. In particular, we have $A_j^-(0, \tilde{u}) = 0$, $j = 0, \ldots, N-1$, or, equivalently, $A_j^-(\ell, \tilde{u}) = A_j^-(0, \tilde{u})\, e^{-\mathrm{i}\beta_m \ell} = 0$, $j = 0, \ldots, N-1$. Therefore, using (11), we find that the scalars $\mu^{(j)}$ are the unique solution to the following linear system:

$$\sum_{i=0}^{N-1} \mu^{(i)} A_j^-\big(\ell, u^{(i)}\big) = -A_j^-(\ell, u_r), \quad j = 0, \ldots, N-1. \tag{14}$$

An advantage of the above system is that the computation of its $N(N+1)$ coefficients $A_j^-(\ell, u_r)$ and $A_j^-(\ell, u^{(i)})$, $i, j = 0, \ldots, N-1$, is inexpensive. Indeed, using (and differentiating) equality (5) and the boundary condition satisfied by u_r on S_ℓ, it follows that

$$A_j^{\pm}(\ell, u_r) = \frac{1}{2}\left(\left(u_r(\cdot,\ell),\varphi_j\right)_S \pm \frac{1}{\mathrm{i}\beta_j}\left(\partial_{x_d} u_r(\cdot,\ell),\varphi_j\right)_S\right) = \frac{1}{2}\left(1 \pm \frac{\alpha}{\beta_j}\right)\left(u_r(\cdot,\ell),\varphi_j\right)_S, \quad j = 0,\dots,N-1.$$

A similar approach may be used to evaluate the coefficients $A_j^{\pm}(\ell, u^{(i)})$, $i, j = 0,\dots,N-1$.

Finally, one obviously sees that taking $\alpha = \beta_m$ for a given index m in $\{0,\dots,N-1\}$ reduces by one unit the rank of the operator L_ℓ^N, and therefore only $N-1$ auxiliary functions and $N-1$ associated coefficients need to be computed in that case. A natural choice is then $\alpha = \beta_0 = k$.

5. Additional comments and possible extensions

The present method is applicable to the case of an infinite guide, at the expense of introducing twice as many auxiliary fields and associated coefficients. It can also be used to solve diffraction problems by bounded scatterers in $\mathbb{R}^d$ by substituting spherical harmonics for modes. It is not restricted to acoustic or scalar waves; gravity, electromagnetic or elastic waves could have also been considered. However, in the later cases, the difficulty is that the transverse modes are generally not orthogonal. One may circumvent this problem by resorting to a biorthogonality framework (see [1] in an elastic waveguide setting for instance).

The Robin boundary condition (used in problems (4) and (13)) can be replaced by any other convenient homogeneous local boundary condition, as long as it leads to a well-posed problem for the field u_r. Still, if a Dirichlet boundary condition is employed, the computation of the traces of normal derivatives on S_ℓ, which are needed to obtain the coefficients of the algebraic system (14), is not a trivial issue anymore and requires some post-processing based on Green's formula.

Finally, the number of auxiliary fields to be computed, which has to be greater than the number of propagative guided modes, can be significantly reduced by combining the proposed approach with the perfectly matched layer (PML) technique. Actually, this solution method was initially devised to overcome the disastrous effects that the so-called backward waves have on the PMLs (see [5] for an example). These aspects, as well as numerical results, will be presented in a future publication.

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