A Posteriori Error Estimation for Acoustic Wave Propagation Problems

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Abstract. The main purpose of this paper is to review a posteriori error estimators for the simulation of acoustic wave propagation problems by computational methods. Residual-type (explicit and implicit) and recovery-type estimators are presented in detail in the case of the Helmholtz problem. Recent work on goal-oriented error estimation techniques with respect to so-called quantities of interest or output functionals are also accounted for. Fundamental results from a priori error estimation are presented and issues dealing with pollution error at large wave numbers are extensively discussed.

Contents

1 INTRODUCTION

1.1 Introductory remarks on a posteriori error estimation

We begin with a quote from [5]: "The combination of powerful modern computers with effective numerical procedures, particularly finite element methods, has transformed what were once purely qualitative theories of mechanics and physics into effective bases for simulation of physical phenomena in countless engineering applications and scientific predictions. A major problem with such simulations is this: No matter how sophisticated and appropriate the mathematical models of an event, all computational results obtained using them involve numerical error. Discretization error can be large, pervasive, unpredictable by classical heuristic means, and can invalidate numerical predictions. For these reasons, a mathematical theory for estimating and quantifying discretization error is of paramount importance to the computational sciences. Equally important, knowledge of such errors, their magnitude, and their distribution provides a basis for adaptive control of the numerical process, the meshing, the choice of algorithms, and, therefore, the efficiency and even the feasibility of the computation. Understandably, a theory of *a posteriori* error estimation has become an important area of research and has found application in an increasing number of commercial software products and scientific programs."

The use of heuristic measures of error to control time steps in the numerical solution of ordinary differential equations probably represents the first use of *a posteriori* estimates to control discretization error in numerical solutions of initial- or boundary-value problems. These types of estimates date back to the 1960's and possibly earlier. To the authors knowledge, the first use of error estimates for adaptive meshing strategies in significant engineering problems was given in the work of Guerra [51] in 1977; the paper of Babuška and Rheinboldt [16] published in 1978 is often cited as the first work aimed at developing rigorous global error bounds for finite element approximations of linear elliptic two-point boundary-value problems. In the period spanning over two decades since these works, significant advances, have been made. A brief history of the subject is given in the book of Ainsworth and Oden [5]; see also the books and survey articles of Verfürth [95], Babuška and Strouboulis [18], Oden and Demkowicz [69]. It can be argued that until quite recently, the vast majority of the published work on *a posteriori* error estimation dealt with global estimates of errors in finite element approximations of linear elliptic problems, these estimates generally being in energy-type norms. In the late 1990's, techniques for computing local estimates and estimates of errors in "quantities of interest" began to appear, where, mathematically speaking, such quantities

manifest themselves as functionals on the solutions of boundary- and initial-value problems. These estimates provide the basis of so-called "goal-oriented adaptivity" wherein adaptive meshing procedures are devised to control error in quantities such as point values of the solution, averaged fluxes over a subdomain, or averaged gradients. The key to the estimation of error in such quantities of interest is to use so-called duality arguments in which an adjoint or dual problem is defined with data characterizing the quantity of interest. Such techniques were actually proposed for one-dimensional elliptic problems by Gartland [48] as early as 1984, but the development of a more general setting with applications in two and three dimensions came much later, for example in the papers of Becker and Rannacher [29], Oden and Prudhomme [84,72], Paraschivoiu, Patera, and Peraire [78,76,81,80], and Babuška and Strouboulis [91]. A general account of such duality methods, with applications to both linear and nonlinear problems was contributed by Becker and Rannacher [30]; applications to three-dimensional problems in solid and fluid mechanics were reported by Prudhomme et al. [74,85,86], Süli and Houston [93], and Hoffman and Johnson [55]. We make no attempt here to give a complete account of the rapidly growing body of literature of so-called duality methods or goal-oriented methods of error estimation; the references cited can be consulted for additional contributions to this subject.

Our view of the current status of *a posteriori* error estimation is that while a general theoretical framework exists for developing error estimates, the details of implementation, the specific forms and structures these estimates take, and the quality of results remain problem dependent; that is, different problem types may require different approaches within the general framework of the theory. Challenging areas of research are time-dependent problems, nonlinear problems, stochastic PDE's, although some work in each of these areas can already be found in the literature. Also, in very recent times, extensions of the theory to cover *a posteriori* estimation of modeling errors as opposed to discretization error have been made (see, e.g., Oden and Prudhomme [73]), and this area could develop into one of active research.

In this review, we attempt to report on the state-of-the-art in a posteriori error estimation for numerical approximations of acoustic wave phenomena. In particular, we concentrate on time-harmonic waves in interior regions, modeled by the Helmholtz equation and approximated by the finite element method. We will discuss other problems and/or other methods of discretization we judge to bring new insights or complementary results useful to the reader. The wave and Helmholtz equations for linear acoustics are presented in the following subsection, while objectives and scope of the present review are discussed at the end of this section.

1.2 Model problems in acoustics

Although wave propagation phenomena manifest themselves in a broad range of applications, we will confine ourselves in the present review to coupled fluid-structure problems, and more particularly, to acoustic wave propagation problems in fluids.

1.2.1 The wave and Helmholtz equations for linear acoustics

Propagation of sound in fluids corresponds to infinitesimal variations of the density and pressure fields. The equations of linear acoustics are derived from the equations governing isentropic compressible flows with the assumption that the fluid motions are very small. Let (u, p, ρ) denote the velocity, pressure, and density of the background flow (in the absence of fluctuations) with $u \approx 0$. Let $(\tilde{u}, \tilde{p}, \tilde{\rho})$ represent infinitesimal variations of velocity, pressure,

Symbols	Parameters	Relationships
c	speed of sound	
ω	angular frequency	
f	frequency	$f = \dfrac{\omega}{2\pi}$
τ	time period	$\tau = f^{-1} = \dfrac{2\pi}{\omega}$
k	wave number	$k = \dfrac{\omega}{c}$
λ	wavelength	$\lambda = c\,\tau = 2\pi\dfrac{c}{\omega} = \dfrac{2\pi}{k}$

Table 1. Definitions of parameters for acoustic problems.

and density, respectively, superposed to the background flow. We assume that no external forces act on the flow and that the fluid is inviscid and barotropic (i.e. the pressure depends only on the density, e.g. $p = g(\rho)$). The pressure variations $\tilde{p}$ are then governed by the wave equation:

$$\frac{\partial^2 \tilde{p}}{\partial t^2} - c^2 \Delta \tilde{p} = 0 \tag{1}$$

where c denotes the speed of sound in the acoustic medium, i.e. $c^2 = dp/d\rho$, and Δ denotes the Laplacian operator.

Upon considering time-harmonic acoustic (steady-state) waves, i.e. $\tilde{p}(x,t) = \phi(x)e^{-i\omega t}$, the wave equation reduces to the Helmholtz equation:

$$\Delta\phi + k^2\phi = 0 \tag{2}$$

where $k = \omega/c$ is the wave number and ω the angular frequency. Definitions of parameters encountered in wave propagation phenomena are recorded in Table 1.

We now introduce several types of problems which frequently occur in practical applications. Problems of wave propagation phenomena are usually classified as interior or exterior, depending on whether one is interested in the sound field in bounded or unbounded regions in space. The reader familiar with the subject can skip the remainder of this subsection. Derivations of the classical interior and exterior problems for acoustics are given below for future reference.

1.2.2 Interior problems

Interior problems (cavity or room acoustics problems) deal with acoustic phenomena in enclosed regions of space. Let Ω be a bounded open domain of $\mathbb{R}^d$, $d = 1$, 2, or 3, with boundary $\partial\Omega$. In the following, normal derivatives $\partial\phi/\partial n = n \cdot \nabla\phi$ in the direction of the outward normal vector n to $\partial\Omega$ will simply be denoted by $\phi_{,n}$.

In the absence of vibrating walls in the cavity, the most general form of a local boundary condition is expressed by the homogeneous Robin condition

$$\phi_{,n} - i\rho ckG\phi = 0 \tag{3}$$

where G denotes the field admittance in the normal direction. The quantity $Z = 1/G$ is called the impedance and is defined as the ratio of the force generated by a change in the pressure by the velocity in the normal direction. The value of G depends on the nature of the

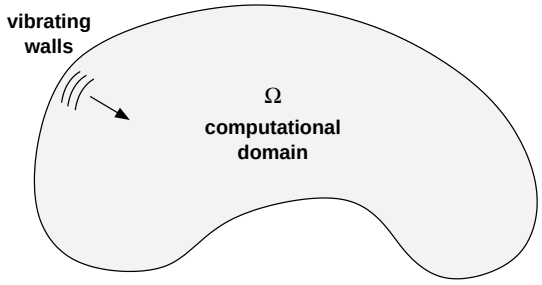

Fig. 1. Vibro-acoustic problems in interior region Ω.

enclosure. If $G = 0$, we are in the presence of a rigid wall for which the Neumann condition $\phi_{,n} = 0$ is prescribed; in the limit case as $G \to \infty$, the wall is said to be acoustically soft and one recovers the homogeneous Dirichlet boundary condition $\phi = 0$. For $0 < G < \infty$, the wall acts as an absorbing surface, and the Robin condition (3) is usually referred to as an *absorbing boundary condition*. The Helmholtz equation together with homogeneous boundary conditions of the type (3), $0 \leq G \leq \infty$, represents an eigenvalue problem for the determination of eigenfrequencies and eigenmodes of the enclosed fluid.

Vibro-acoustic problems deal with forced acoustic fields produced from vibrational parts of the enclosing walls (see Figure 1). If the wall is rigid and vibrates with normal velocity v_n, the Neumann boundary condition[1] $\phi_{,n} = i\rho ckv_n$ is prescribed. A pressure release condition is given in the form of the Dirichlet boundary condition $\phi = \phi_0$. The most general form of boundary condition is embodied in the Robin condition

$$\phi_{,n} - i\rho ckG\phi = g \tag{4}$$

where g is a prescribed complex-valued function.

Vibro-acoustic boundary value problems consist in finding the spatial component of the acoustic pressure field $\phi : \bar{\Omega} \to \mathbb{C}$ such that:

$$\begin{cases} \Delta\phi + k^2\phi = 0, & \text{in } \Omega \\ \phi = \phi_0, & \text{on } \Gamma_D \\ \phi_{,n} = i\rho ckv_n, & \text{on } \Gamma_N \\ \phi_{,n} - i\rho ckG\phi = g, & \text{on } \Gamma_R \end{cases} \tag{5}$$

where $\overline{\Gamma_D \cup \Gamma_N \cup \Gamma_R} = \partial\Omega$, and $\Gamma_D \cap \Gamma_N = \Gamma_D \cap \Gamma_R = \Gamma_N \cap \Gamma_R = \varnothing$. Note that in the case v_n, ϕ_0, and g are all equal to zero, Problem (5) reduces to an eigenvalue problem, as mentioned earlier.

1.2.3 Exterior problems (radiation, scattering, transmission problems)

Exterior problems are concerned with the characterization of the acoustic field in the surrounding space of a given structure. The main difficulty in dealing with this class of problems is that the computational domain is unbounded in space.

We first start with the radiation problem. Let $D \subset \mathbb{R}^d$, $d = 1$, 2, or 3 be the region occupied by a body embedded in a homogeneous isotropic medium at rest. The domain D is a bounded

[1] This condition is derived from the equation $\rho\partial\tilde{u}/\partial t + \nabla\tilde{p} = 0$, governing the variations of fluid motions, and by considering time-harmonic waves $\tilde{u}(x,t) = v(x)e^{-i\omega t}$ and $\tilde{p}(x,t) = \phi(x)e^{-i\omega t}$. This rigid condition becomes $\phi_{,n} = -i\rho ckv_n$ when $\tilde{u}(x,t) = v(x)e^{i\omega t}$ and $\tilde{p}(x,t) = \phi(x)e^{i\omega t}$.

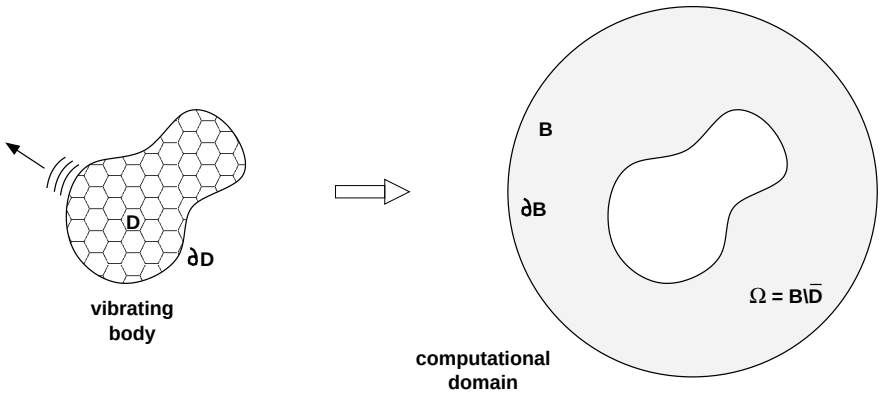

Fig. 2. Radiation problem for a vibrating body D and computational domain Ω.

simply connected domain with smooth boundary ∂D (see Figure 2). Suppose that the walls of the body vibrate with normal velocity v_n and that the radiated waves propagate in free space. The physical requirement that all radiated waves cannot be reflected at infinity leads to the Sommerfeld radiation condition (see [56])

$$\lim_{r\to\infty} r^{\frac{d-1}{2}}\phi = 0, \qquad \lim_{r\to\infty} r^{\frac{d-1}{2}}\left(\frac{\partial\phi}{\partial r} - ik\phi\right) = 0$$

where $r = |x|$ and $\partial/\partial r$ denotes the derivative in the radial direction. Imposing the Sommerfeld radiation condition requires that we solve the Helmholtz equation on an infinite domain and prevents the immediate use of traditional computational methods designed for bounded domains, such as finite element or finite difference methods. To overcome this difficulty, one introduces a sufficiently large ball $B \subset \mathbb{R}^d$, with boundary ∂B, which contains D, and using the Dirichlet-to-Neumann map (DtN) technique (see [56, Chapt. 3] for details), one can approximate the Sommerfeld condition at infinity by the Robin-type (non-reflecting) boundary condition on ∂B,

$$\frac{\partial\phi}{\partial n} - ik\phi = q, \qquad \text{on } \partial B \tag{6}$$

where n denotes the unit normal on ∂B. Making use of this boundary condition, the computational domain reduces to the region $\Omega \in \mathbb{R}^d$, $\Omega = B\backslash\bar{D}$, with boundary $\partial\Omega = \partial B \cup \partial D$ (see Figure 2). The radiation problem for a vibrating body consists then in finding the spatial component of the radiated acoustic pressure field $\phi : \bar{\Omega} \to \mathbb{C}$ such that:

$$\begin{cases} \Delta\phi + k^2\phi = 0, & \text{in } \Omega \\ \phi_{,n} = i\rho ckv_n, & \text{on } \partial D \\ \phi_{,n} - ik\phi = q, & \text{on } \partial B \end{cases} \tag{7}$$

Note that the pressure-release condition $p = p_0$ and the absorbing condition $\phi_{,n} - i\rho ckG\phi = g$ may also be prescribed on parts of the boundary ∂D.

We now consider the scattering problem in which an incident plane wave $\phi^i(x) = e^{ik\alpha\cdot x}$ is scattered by an obstacle D (see Figure 3). Here $\alpha \in \mathbb{R}^d$ denotes the unit vector defining the direction of the wave. The acoustic field scattered by the obstacle D is given by ϕ^s and the total acoustic field by:

$$\phi(x) = \phi^s(x) + \phi^i(x) \tag{8}$$

The total acoustic field ϕ, the incoming plane wave ϕ^i and, thus, the scattered field ϕ^s, all satisfy the Helmholtz equation in $\mathbb{R}^d\backslash D$. Similarly to the radiation problem, the infinite outer

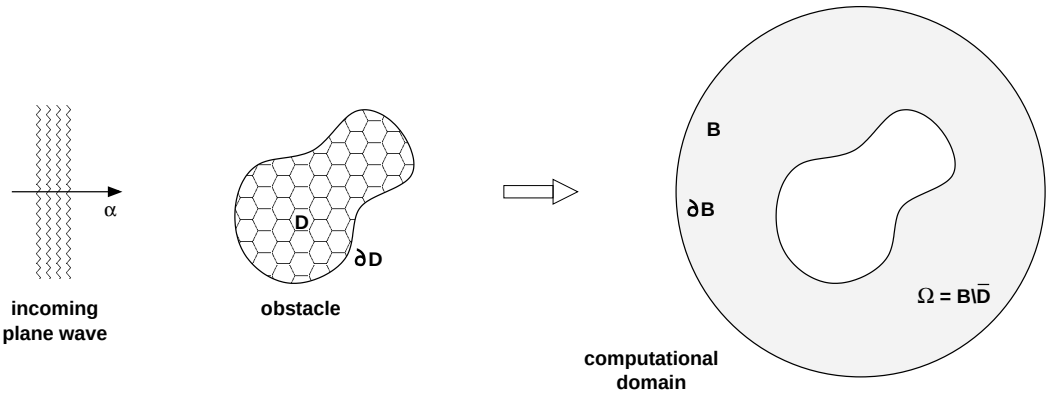

Fig. 3. Scattering and transmission problems: obstacle D hit by plane wave and computational domain Ω.

region will be restricted to a ball B with boundary ∂B on which the scattered field ϕ^s satisfies the absorbing boundary condition (6). A perfectly sound-soft obstacle leads to the Dirichlet condition $\phi = 0$, or $\phi^s = -\phi^i$. For an acoustically rigid scatterer, acoustic waves satisfy the Neumann boundary condition $\phi_{,n} = 0$, or $\phi^s_{,n} = -\phi^i_{,n}$. Finally, obstacles characterized by an acoustic admittance G will satisfy the Robin boundary condition $\phi_{,n} - i\rho ckG\phi = 0$. Naturally, the obstacle can be such that Dirichlet, Neumann and Robin boundary conditions are prescribed on parts of the boundary ∂D, namely on Γ_D, Γ_N, and Γ_R, respectively, where $\overline{\Gamma_D \cup \Gamma_N \cup \Gamma_R} = \partial D$, and $\Gamma_D \cap \Gamma_N = \Gamma_D \cap \Gamma_R = \Gamma_N \cap \Gamma_R = \varnothing$. Hence the general formulation of the scattering problem consists in finding the spatial component of the scattered acoustic pressure field $\phi^s : \bar{\Omega} \to \mathbb{C}$ such that:

$$\begin{cases} \Delta\phi^s + k^2\phi^s = 0, & \text{in } \Omega \\ \phi^s = -\phi^i, & \text{on } \Gamma_D \\ \phi^s_{,n} = -\phi^i_{,n}, & \text{on } \Gamma_N \\ \phi^s_{,n} - i\rho ckG\phi^s = -\phi^i_{,n} + i\rho ckG\phi^i, & \text{on } \Gamma_R \\ \phi^s_{,n} - ik\phi^s = q, & \text{on } \partial B \end{cases} \tag{9}$$

The transmission problem is different from the scattering problem in the sense that the incident sound is allowed to penetrate the obstacle. If the obstacle D is made of another fluid with different sound speed and density, the transmission problem leads to a coupled problem in which the total pressure $\phi = \phi^s + \phi^i$ outside of D and the interior pressure ϕ^b in D both satisfy the Helmholtz equation. On the boundary of the obstacle, the pressure and normal velocities are assumed continuous, so that the transmission conditions are given by $\phi = \phi^b$ or $v_n = v^b_n$ on ∂D. If the obstacle is an elastic solid, the acoustic waves from the surrounding medium cause forced elastic vibrations inside the obstacle and the transmission problem consists of a general coupled system of equations for fluid-solid interactions involving the acoustic and elastodynamics equations along with transmission conditions. This problem, also referred to as the elastic scattering problem, is described in e.g. [56].

1.3 Objectives and scope of review

The main objective of this paper is to report on existing techniques for a posteriori error estimation which have been developed and applied to acoustic wave problems over approx-

imatively the last ten years. Our main concern will be to provide a homogeneous description of the various methods, not necessarily in the format chosen by the authors, in order to facilitate comparisons and put in evidence their respective advantages or disadvantages. However, we will not review the many possible numerical methods available for the wave and Helmholtz equations. We will concentrate on results obtained using finite element methods and pinpoint only significant results for other methods when they shed light on particular results. Moreover, little will be said on the topic of mesh adaptation.

We found it useful to briefly review a priori error estimates for these types of problems, as they characterize the convergence rates of error in finite element approximations of the Helmholtz equation. We will present a fundamental result which allows us to identify and distinguish discretization error and pollution error. We will see that pollution effects usually degrade the quality of a posteriori error estimators for large wave numbers.

Most work on a posteriori error estimation for acoustic wave propagation problems deal with the Helmholtz equation. The a posteriori error estimators usually considered are those based on residual and recovery methods which were originally developed for static elliptic problems. These techniques provide error estimates measured with respect to global norms, the so-called energy norms. We will show that these estimators have the natural tendency to underestimate the true error as the wave number k increases.

Some contributions on goal-oriented error estimation for the Helmholtz equation have been recently published. This class of estimators allows one to estimate the error in so-called quantities of interest defined as functionals of the pressure field. We provide the general foundations for such types of error estimators and discuss difficulties, shortcomings and possible directions for further research.

The paper is organized as follows: following this introduction, we present in Section 2 two model problems of the Helmholtz equation and show how to approximate them by the finite element method. We briefly recall in Section 3 some a priori error estimates for finite element solutions of acoustic problems and introduce the notion of pollution error and the rule of thumb. We then devote Section 4 and Section 5 to global norm a posteriori error estimation and to goal-oriented error estimation, respectively. A brief analysis for the *hp* finite element method and a short review of a posteriori error estimation for the boundary element method are presented in Section 6 and in Section 7. Concluding remarks are finally reported in Section 8.

2 NUMERICAL METHODS FOR HELMHOLTZ EQUATION

2.1 Model problems

To simplify the presentation, and without loss of generality, we will consider vibro-acoustic problems in one space dimension approximated by the finite element method. For simplicity, the data c and ρ, which depend on the nature of the fluid, will be chosen such that $\rho c = 1$. We believe that these problems are simple enough to provide a clear exposition of concepts, yet complex enough to touch upon most technical issues pertaining to the numerical simulation of acoustic phenomena.

We define the interior domain as $\Omega = (0, 1)$. In the first model problem, we consider the reduced wave equation with Dirichlet boundary condition at one end and absorbing boundary condition at the other, setting $G = \rho c = 1$. The model problem consists in finding the

spatial component of the acoustic pressure field $\phi : \bar{\Omega} \to \mathbb{C}$ such that

$$\text{(Model Problem 1)} \qquad \begin{cases} \phi'' + k^2\phi = 0, & \text{in } \Omega \\ \phi = 1, & \text{at } x = 0 \\ \phi' - ik\phi = 0, & \text{at } x = 1 \end{cases} \tag{10}$$

Problem 1 models the uniaxial propagation of the plane wave:

$$\phi(x) = e^{ikx} = \cos kx + i \sin kx.$$

Remark 1. Using the principle of superposition, the above model problem can be recast as the general problem of finding the scalar field $\phi : \bar{\Omega} \to \mathbb{C}$ such that

$$\begin{cases} -\phi'' - k^2\phi = f, & \text{in } \Omega \\ \phi = 0, & \text{at } x = 0 \\ \phi' - ik\phi = 0, & \text{at } x = 1 \end{cases} \tag{11}$$

Model problem 1 was considered in this form by Ihlenburg and Babuška in [57]. In this case, the right-hand side of Helmholtz equation is given by $f = \phi_p'' + k^2\phi_p$ where ϕ_p is a smooth function satisfying $\phi_p(0) = 1$ and $\phi_p(1) = \phi_p'(1) = 0$. One can choose for example $\phi_p(x) = (1-x)^2$. For an arbitrary function f, the exact solution of this problem is given by:

$$u(x) = \int_0^1 G(x,s) f(s)\, ds$$

where G is the Green's function:

$$G(x,s) = \frac{1}{k} \begin{cases} \sin(kx)\, e^{iks}, & 0 \le x \le s \\ \sin(ks)\, e^{ikx}, & s \le x \le 1 \end{cases}$$

Hereafter, Problem (11) will be referred to Model Problem 1.

We will also consider a second model problem for which the boundary at $x = 1$ is vibrating with velocity v_n. The acoustic field $\phi : \bar{\Omega} \to \mathbb{C}$ satisfies in this case:

$$\text{(Model Problem 2)} \qquad \begin{cases} \phi'' + k^2\phi = 0, & \text{in } \Omega \\ \phi = 0, & \text{at } x = 0 \\ \phi' = ikv_n, & \text{at } x = 1 \end{cases} \tag{12}$$

The exact solution of this model problem is given by:

$$\phi(x) = i\frac{v_n}{\cos k} \sin kx$$

whenever $\cos k \neq 0$. The values $k = \pi(m - 1/2)$, $m \in \mathbb{N}$, correspond to the eigenvalues of the homogeneous problem, i.e. $v_n = 0$, with associated eigenmodes given by $\sin \pi(m - 1/2)x$, $m \in \mathbb{N}$. Model Problem 2 is thus singular whenever the wave number k equals one of the eigenvalues.

2.2 Notation and weak formulation

For any complex number $z \in \mathbb{C}$, let $\bar{z}$ be the complex conjugate of z. We denote by $L^2(\Omega)$ the space of square-integrable complex-valued functions $v : \Omega \to \mathbb{C}$ with inner-product:

$$(u, v) = \int_\Omega u(x)\bar{v}(x)\, dx$$

and norm

$$\|v\|_0 = \sqrt{(v, v)}$$

By $H^s(\Omega)$, s an integer, we denote the usual Sobolev spaces:

$$H^s(\Omega) = \{v : \Omega \to \mathbb{C}; v \in L^2(\Omega), D^m v \in L^2(\Omega), 1 \leq m \leq s\}$$

where $D^m v$ is the m^{th}-derivative of v in the distributional sense. We denote the seminorm and norm of a function v in $H^s(\Omega)$ by $|v|_s = \|D^s v\|_0$ and $\|v\|_s = (\sum_{0 \leq m \leq s} |v|_m^2)^{1/2}$, respectively.

We proceed by introducing the weak formulation of Model Problem 1 in the form (11). Let $v : \bar{\Omega} \to \mathbb{C}$ be a sufficiently smooth function such that $v = 0$ at $x = 0$. Upon integrating the Helmholtz equation against a test function $\bar{v}$, the complex conjugate of v, integrating by parts and applying the boundary conditions $v(0) = 0$ and $\phi'(1) = ik\phi(1)$, we obtain:

$$\int_\Omega \phi' \bar{v}'\, dx - k^2 \int_\Omega \phi \bar{v}\, dx - ik\phi(1)\bar{v}(1) = \int_\Omega f \bar{v}\, dx \tag{13}$$

For convenience, we introduce the sesquilinear form $B_1(\cdot, \cdot)$ and antilinear form $F_1(\cdot)$:

$$\begin{aligned} B_1(\phi, v) &= \int_\Omega \phi' \bar{v}'\, dx - k^2 \int_\Omega \phi \bar{v}\, dx - ik\phi(1)\bar{v}(1) \\ F_1(v) &= \int_\Omega f \bar{v}\, dx \end{aligned} \tag{14}$$

and the space of functions V:

$$V = \{v \in H^1(\Omega); v(0) = 0\} \tag{15}$$

The weak formulation of Model Problem 1 reads:

$$\text{Find } \phi \in V \text{ such that} \qquad B_1(\phi, v) = F_1(v), \quad \forall v \in V \tag{16}$$

In a similar manner, the weak formulation of Model Problem 2 is given by:

$$\text{Find } \phi \in V \text{ such that} \qquad B_2(\phi, v) = F_2(v), \quad \forall v \in V \tag{17}$$

where

$$\begin{aligned} B_2(\phi, v) &= \int_\Omega \phi' \bar{v}'\, dx - k^2 \int_\Omega \phi \bar{v}\, dx \\ F_2(v) &= ikv_n \bar{v}(1) \end{aligned} \tag{18}$$

2.3 Galerkin finite element method

Given a domain Ω, we use the usual notation $\mathcal{P}_h$ to denote a finite element partition of Ω into elements K:

$$\overline{\Omega} = \bigcup_{K \in \mathcal{P}_h} K \qquad \text{with } K \cap L = \varnothing,\ \forall K \neq L. \tag{19}$$

For convenience, summation over all elements K of a partition $\mathcal{P}_h$ of Ω will be written $\sum_K$ rather than $\sum_{K \in \mathcal{P}_h}$. We denote by h_K the size of elements and define $h = \max_{K \in \mathcal{P}_h} h_K$. The partitions of Ω will be assumed quasi-uniform. Finite element spaces associated with the partitions $\mathcal{P}_h$ are denoted by V^h.

By the Galerkin finite element method, one solves, instead of the weak formulations (16) and (17), the finite dimensional problems:

$$\text{Find } \phi_h \in V^h \text{ such that} \qquad B_1(\phi_h, v) = F_1(v), \qquad \forall v \in V^h \tag{20}$$

$$\text{Find } \phi_h \in V^h \text{ such that} \qquad B_2(\phi_h, v) = F_2(v), \qquad \forall v \in V^h \tag{21}$$

respectively.

In either case, we will denote by e the error in the finite element approximation ϕ_h, i.e. $e = \phi - \phi_h$. Note that $e \in V$. Since the problems are linear, it is not difficult to show that the errors satisfy the following error equations:

$$B_1(e, v) = F_1(v) - B_1(\phi_h, v) = \mathcal{R}_1(v), \qquad \forall v \in V \tag{22}$$

$$B_2(e, v) = F_2(v) - B_2(\phi_h, v) = \mathcal{R}_2(v), \qquad \forall v \in V \tag{23}$$

where the functionals $\mathcal{R}_1$ and $\mathcal{R}_2$ are generally referred to as the residuals. We note that the errors and the residuals satisfy the so-called *Galerkin orthogonality property*:

$$\mathcal{R}_1(v) = B_1(e, v) = 0, \qquad \forall v \in V^h \tag{24}$$

$$\mathcal{R}_2(v) = B_2(e, v) = 0, \qquad \forall v \in V^h \tag{25}$$

This property is important in the derivation of a priori and a posteriori error estimates.

2.4 Least-Squares finite element method

Galerkin least-squares finite element formulations of the Helmholtz problem have been considered to provide phase accuracy with fewer mesh points than the classical Galerkin approach for propagating solutions (see [53,54] for a detailed derivation). They consist in adding a stabilizing terms to the weak formulations (16) and (17). Introducing the Helmholtz operator $\mathcal{L}\phi = \Delta\phi + k^2\phi$, the Galerkin least-squares forms of the continuous problems read:

$$\begin{aligned} &\text{Find } \phi_h \in V^h \text{ s.t.} \quad B_1(\phi_h, v) + \tau(\mathcal{L}\phi_h, \mathcal{L}v) = F_1(v) - \tau(f, \mathcal{L}v), \qquad \forall v \in V^h \\ &\text{Find } \phi_h \in V^h \text{ s.t.} \quad B_2(\phi_h, v) + \tau(\mathcal{L}\phi_h, \mathcal{L}v) = F_2(v), \qquad \forall v \in V^h \end{aligned} \tag{26}$$

where the parameter τ has the dimension of length-squared and can be found in [90]. Note that the terms $(\mathcal{L}\phi_h, \mathcal{L}v)$ and $(f, \mathcal{L}v)$ are actually defined as sums of element-wise L^2 inner products.

3 PRELIMINARY ERROR ANALYSIS

In this section, we first recall the abstract analysis of a priori error estimation for the finite element method. We then apply the error analysis to the acoustic problems and present fundamental results which highlight the behavior of the numerical error in approximations of the Helmholtz equation. In particular, the notion of pollution error and the rule of thumb are introduced.

3.1 Abstract analysis

Let us consider the abstract problem:

$$\text{Find } u \in V \text{ such that} \qquad \mathcal{B}(u,v) = \mathcal{F}(v), \qquad \forall v \in V \tag{27}$$

where V is a Hilbert space with norm $\|\cdot\|$ and where $\mathcal{B}(\cdot,\cdot)$ and $\mathcal{F}(\cdot)$ are, respectively, a sesquilinear and antilinear form defined on space V. We suppose that $\mathcal{B}(\cdot,\cdot)$ and $\mathcal{F}(\cdot)$ are continuous, i.e. there exist $M > 0$ and $C > 0$ such that:

$$\begin{aligned} |\mathcal{B}(u,v)| &\leq M\|u\|\,\|v\| \quad \forall u,v \in V \\ |\mathcal{F}(v)| &\leq C\|v\| \qquad\quad \forall v \in V \end{aligned} \tag{28}$$

Moreover we assume that the sesquilinear form satisfies the inf-sup condition, i.e. there exists $\alpha > 0$ such that for all $u \in V$:

$$\sup_{v \in V\setminus\{0\}} \frac{|\mathcal{B}(u,v)|}{\|v\|} \geq \alpha\|u\| \tag{29}$$

and the condition

$$\forall v \in V\setminus\{0\}, \qquad \sup_{u\in V} |\mathcal{B}(u,v)| > 0.$$

Then it is inferred from the generalized Lax-Milgram theorem that there exists a unique solution $u \in V$ to Problem (27). Note that α and M are usually referred to as the inf-sup and continuity constants, respectively.

With the finite element method, we then solve the discrete problem:

$$\text{Find } u_h \in V^h \text{ such that} \qquad \mathcal{B}(u_h,v) = \mathcal{F}(v), \qquad \forall v \in V^h$$

where V^h denotes a conforming finite element subspace of V. In order to ensure existence and unicity of u_h, we also assume that a discrete inf-sup condition holds: namely, there exists $\alpha_h > 0$ such that for all $u_h \in V^h$

$$\sup_{v_h \in V^h\setminus\{0\}} \frac{|\mathcal{B}(u_h,v_h)|}{\|v_h\|} \geq \alpha_h\|u_h\|. \tag{30}$$

Following a standard proof generalizing Céa's lemma (see e.g. [75] or [47, page 90]), we know that a bound on the numerical error $e = u - u_h$ is given by

$$\|e\| \leq \|u - w_h\| + \|u_h - w_h\| \leq \|u - w_h\| + \frac{M}{\alpha_h}\|u - w_h\| \tag{31}$$

w_h being an arbitrary function of V^h. Thus

$$\|e\| \leq \left(1 + \frac{M}{\alpha_h}\right) \inf_{v_h \in V^h} \|u - v_h\|. \tag{32}$$

This result is fundamental for an understanding of the nature of the approximation error. For a smooth function u, we can choose w_h as the interpolant $I_h u$ of u in V^h. The error $\|e\|$ is then composed of two contributions, a discretization error $u - I_h u$ and a so-called "pollution error" $u_h - I_h u$. We observe that the latter is bounded by $(M/\alpha_h)\|u - I_h u\|$. The pollution error is closely related to the stability properties of $\mathcal{B}(\cdot, \cdot)$ through the constants M and α_h; large values of the ratio M/α_h usually means a loss of stability of the discrete approximation of the sesquilinear form.

3.2 Application to Model Problem 1

In the remainder of this section, $\mathcal{P}_h$ is a finite element partition of $\Omega = (0, 1)$ of N elements K of uniform size $h_K = h = 1/N$. The elements are the segments $[x_{l-1}, x_l]$, $l = 1, \ldots, N$, where $x_l = lh$, $l = 0, 1, \ldots, N$ are the node coordinates. We further consider the finite element subspace $V^h \subset V$ of continuous piecewise linear functions satisfying the homogeneous Dirichlet condition at $x = 0$.

The results presented in the previous subsection are now applied to Model Problem 1 as defined in (11). This problem was extensively studied by Ihlenburg and Babuška in [57]. The weak form of this problem is given in (20) and the definition of the sesquilinear and antilinear forms in (14). The space V is equipped here with the norm $|v|_1$ since, from the Poincaré inequality, the norm $\|v\|_1$ and seminorm $|v|_1$ are actually equivalent.

The authors show in [57] that there exists a unique solution to (20). In particular, they show that the sesquilinear form $B_1(\cdot, \cdot)$ is continuous and satisfies continuous and discrete inf-sup conditions. The major results are summarized as follows:

Continuity of sesquilinear form: Applying the Poincaré inequality, we can show that there exists a constant M, dependent on k, such that

$$|B_1(\phi, v)| \leq M|\phi|_1|v|_1$$

For $k \geq 1$, the continuity constant can be chosen as $M = C_0 k^2$ where $C_0 \leq 3$.

Inf-sup stability condition [57, Theorem 1]: Let $B_1 : V \times V \to \mathbb{C}$ be the sesquilinear form defined in (14). There exists a positive constant α, dependent on k, such that for all $\phi \in V$

$$\sup_{v \in V \setminus \{0\}} \frac{|\mathcal{B}_1(\phi, v)|}{|v|_1} \geq \alpha |\phi|_1 \tag{33}$$

More precisely, the stability constant α is of order k^{-1}; that is, there exist C_1 and C_2, independent of k, such that

$$\frac{C_1}{k} \leq \alpha \leq \frac{C_2}{k} \tag{34}$$

provided that $k \geq 1$.

Discrete inf-sup stability condition [57, Theorem 4]: Let $B_1 : V^h \times V^h \to \mathbb{C}$ be the sesquilinear form defined in (14). Then, provided that $hk < 1$ and $k \geq 1$, there exists a

positive constant α_h, dependent on k, such that for all $\phi_h \in V$

$$\sup_{v_h \in V^h \setminus \{0\}} \frac{|\mathcal{B}_1(\phi_h, v_h)|}{|v_h|_1} \geq \alpha |\phi_h|_1 \tag{35}$$

More precisely, the stability constant α_h is of order k^{-1}; that is, there exist C_1 and C_2, independent of k and h, such that

$$\frac{C_1}{k} \leq \alpha_h \leq \frac{C_2}{k}. \tag{36}$$

By simple analogy with (31), the approximation error $e = \phi - \phi_h$ for Model Problem 1 therefore satisfies:

$$|e|_1 \leq |\phi - \phi_I|_1 + |\phi_h - \phi_I|_1 \leq (1 + Ck^3) \, |\phi - \phi_I|_1 \tag{37}$$

where ϕ_I is the interpolant of ϕ on V^h. Using classical approximation properties for $\phi \in H^2(\Omega)$, i.e. $|\phi - \pi_h \phi|_1 \leq Ch|\phi|_2$, we arrive at the error estimate:

$$|e|_1 \leq (C_1 h + C_2 k^3 h) \, |\phi|_2 \tag{38}$$

This estimate shows that the error may increase for large values of the wave number k. However, a sharper bound can be obtained, as shown in the next subsection.

3.3 A fundamental result

We now recall a fundamental result proved by Ihlenburg and Babuška [57, Theorem 5]. It provides for a sharp bound on the error in the H^1-seminorm. Beforehand, we state without proof the following lemma [57, Lemma 3]:

Lemma 1. *Let $u_h \in V^h$ be the finite element to the variational problem (20) for given data $f \in L^2(\Omega)$, $\Omega = (0,1)$. Then, if h is small such that $hk \leq 1$, there exists a constant C not depending on h and k such that*

$$|u_h|_1 \leq C \|f\|_0. \tag{39}$$

Theorem 1. *Let $\phi \in V \cap H^2(\Omega)$ be the solution of the variational problem (11) and $\phi_h \in V^h$ the finite element approximation of ϕ. Then, if $hk < 1$, and $k \geq 1$, there exist constants C_1 and C_2, independent of h and k, such that*

$$|\phi - \phi_h|_1 \leq (C_1 h + C_2 h^2 k^2) |\phi|_2 \tag{40}$$

Moreover, since the solution is a sinusoidal wave with wave number k, then constants C_1' and C_2' exist such that

$$\frac{|\phi - \phi_h|_1}{|\phi|_1} \leq C_1' hk + C_2' h^2 k^3. \tag{41}$$

Proof. We will present the main steps of the proof.
1) The proof starts as usual with the triangle inequality, as in (37). However, the main issue here is to show that the difference between the interpolant $\phi_I \in V^h$ of ϕ and the finite element approximation $\phi_h \in V^h$ can be bounded by:

$$|\phi_h - \phi_I|_1 \leq Ck^2 \|\phi - \phi_I\|_0.$$

For an arbitrary $v \in V^h$, introducing $z_h = \phi_h - \phi_I$ and using the orthogonal property (24), we have:

$$B_1(\phi - \phi_I, v) = B_1(e, v) + B_1(z_h, v) = B_1(z_h, v)$$

so that

$$B_1(z_h, v) = B_1(\phi - \phi_I, v), \qquad \forall v \in V^h.$$

From the definition of the sesquilinear form $B_1(\cdot, \cdot)$,

$$B_1(\phi - \phi_I, v) = \int_\Omega (\phi - \phi_I)' \bar{v}' \, dx - k^2 \int_\Omega (\phi - \phi_I) \bar{v} \, dx - ik(\phi - \phi_I)(1)\bar{v}(1)$$

The first integral on the right-hand side can be simplified to:

$$\int_\Omega (\phi - \phi_I)' \bar{v}' \, dx = \sum_K \int_K (\phi - \phi_I)' \bar{v}' \, dx = -\sum_K \int_K (\phi - \phi_I) \bar{v}'' \, dx + \sum_K (\phi - \phi_I) \bar{v}' \Big|_{x_l}^{x_{l+1}}$$

Since $v \in V^h$, v is linear on each element K, $v'' = 0$. Moreover, since ϕ_I is the interpolant of ϕ, $\phi - \phi_I$ vanishes at all nodes x_l. It follows that

$$\int_\Omega (\phi - \phi_I)' \bar{v}' \, dx = 0, \qquad \text{and} \quad (\phi - \phi_I)(1)\bar{v}(1) = 0$$

which leads to:

$$B_1(\phi - \phi_I, v) = -k^2 \int_\Omega (\phi - \phi_I) \bar{v} \, dx;$$

that is

$$B_1(z_h, v) = -k^2(\phi - \phi_I, v), \qquad \forall v \in V^h.$$

Applying Lemma 1 with $f = -k^2(\phi - \phi_I)$, there exists a constant C independent of h and k, such that:

$$|z_h|_1 \leq Ck^2 \|\phi - \phi_I\|_0$$

where h is assumed to be small, i.e. $hk \leq 1$.
2) Incorporating the above bound into the triangle inequality, we have:

$$|e|_1 \leq |\phi - \phi_I|_1 + |\phi_h - \phi_I|_1 \leq |\phi - \phi_I|_1 + Ck^2 \|\phi - \phi_I\|_0$$

and using classical interpolation estimates yields:

$$|e|_1 \leq C_1 h |\phi|_2 + C_2 h^2 k^2 |\phi|_2$$

which is simply the estimate (40).
3) Finally, the exact solution of Model Problem 1 being a sinusoidal wave $\phi = A \sin kx + B \cos kx$, $k \geq 1$, we can show that there exists a constant C such that

$$\frac{|\phi|_2}{|\phi|_1} \leq Ck \tag{42}$$

It follows that

$$\frac{|e|_1}{|\phi|_1} \leq C_1' hk + C_2' h^2 k^3$$

which is exactly the estimate (41). □

Computational experiments (see e.g. [57]) actually show that estimate (41) is sharp, meaning that the upper bound cannot be further improved. Similar a priori estimates have been derived for the *hp* finite element method [58,56,1] and are summarized in Section 6.

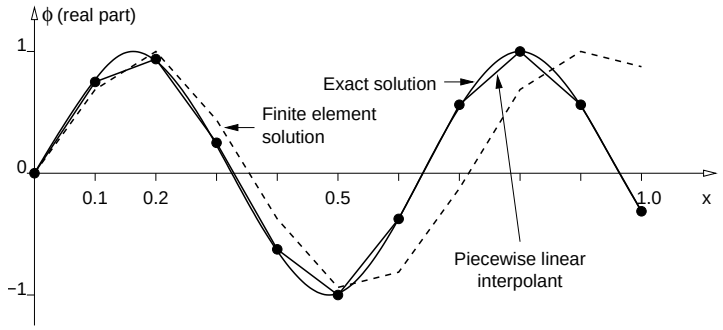

Fig. 4. Illustrative example of exact solution ϕ, interpolant ϕ_I, and FE solution ϕ_h.

3.4 Rule of thumb and pollution error

Estimate (41) indicates that the accuracy of the finite element solution is intimately dependent on the wave number k. As a matter of fact, it has long been recognized that the mesh size h had to be adjusted following the so-called rule of the thumb [53,57]:

$$hk = \text{constant} \tag{43}$$

so that the mesh resolution n_{res}, i.e. the number of elements per wavelength λ, remains fixed for any value of k:

$$n_{\text{res}} = \frac{\lambda}{h} = \frac{2\pi}{hk} \tag{44}$$

For instance, in the illustrative example of Figure 4, $h = 0.1$, $\lambda = 2\pi/10$, so that $n_{\text{res}} = 2\pi \approx 6$, $hk = 1$, and $k = 10$. The larger n_{res} is, the smaller hk is and, a fortiori, the smaller the relative error should be. This intuitive result is not surprising in view of estimate (41) since the interpolation error $\phi - \phi_I$ is controlled by a term of order hk, i.e.:

$$\frac{|\phi - \phi_I|_1}{|\phi|_1} \leq C_1' hk \tag{45}$$

In other words, using the rule of the thumb (43), and preferably taking $hk \leq 1$, ensures that the finite element space can approximate (interpolate) reasonably well plane waves. However, according to estimate (41), enforcing the rule of the thumb does not guarantee that the relative error be controlled in the finite element solution. Indeed, the second contribution to the error originates from the difference $\phi_h - \phi_I$ and is bounded by:

$$\frac{|\phi_h - \phi_I|_1}{|\phi|_1} \leq C_2'(hk)hk^2 \tag{46}$$

If hk^2 is sufficiently small, i.e. $hk^2 < 1$ or $h < 1/k^2$, the error is controlled by hk and the finite element solution is then quasioptimal, i.e. equivalent to the best approximation. Thus, the condition $h < 1/k^2$ corresponds to the asymptotic range. On the other hand, when $h > 1/k^2$, i.e., in the pre-asymptotic range, the difference between the interpolant and the finite element solution remains the dominant part of the relative error. In other words, one would observe large errors for k large even if hk is restricted (see Table 2).

The difference between the finite element solution ϕ_h and the interpolant ϕ_I, i.e. $\epsilon = \phi_h - \phi_I$ has been referred to as *the pollution error*. The pollution effect is related to the loss of stability of the Helmholtz operator at large wave numbers. The pollution error is actually

Range of h	$h \leq 1/k^2$	$1/k^2 \leq h \leq 1/k$	$1/k \leq h$
Error estimate	$e_r \leq Chk$	$e_r \leq Ch^2k^3$	–
Regime	asymptotic range of convergence	pre-asymptotic range of convergence	rule of thumb not respected

Table 2. A priori error estimates for the relative error $e_r = |e|_1/|\phi|_1$ for $k > 1$.

related to the phase lag between ϕ_I and ϕ_h as seen in Figure 4, in other words, to the dispersive character of the waves. The phase lag has a global effect that builds up over the whole computational domain. The pollution effect has been studied in more detail in [45,50]. A consequence of the pollution effect is that the finite element method may be prohibitive for very large values of k; which lead Babuška and Sauter to ask the legitimate question "Is the pollution effect of the FEM avoidable for the Helmholtz equation considering high wave numbers?" as the title of the articles [24,25]. In these contributions, it is shown that a version of the generalized finite element method (GFEM) [7,10,15,46,71] in one dimension yields pollution-free solutions with respect to the wave number. However, it is also proved that GFEM cannot completely eliminate the pollution effects in two or more space dimensions.

Remark 2. The pollution error has also been defined as the difference between the exact solution ϕ and a shifted function $\tilde{\phi}$ (see [8] and Section 4.3.3). The shifted function is in phase with the finite element solution ϕ_h and is constructed from ϕ_h.

3.5 Application to Model Problem 2

From the preceding discussion, we have seen that the pollution error may become significant for increasing values of the wave number. This fact prompted Bouillard and Ihlenburg [33] to introduce the concept of *k-singularity* "... defined by the error between the interpolant wave and the finite element wave. Its influence grows with the nondimensional wave number k and is not controlled by the traditional rule of thumb $hk =$ constant."

In the case of the undamped interior Model Problem 2, the resulting system exhibits eigensolutions in the form of standing waves. Bouillard and Ihlenburg [33] talked in this case of *λ-singularity* "... defined by the singularity of the discretized Helmholtz system of equations at the natural frequencies."

The main issue with Model Problem 2 is that the sesquilinear form

$$B_2(\phi, v) = \int_\Omega \phi' \bar{v}' \, dx - k^2 \int_\Omega \phi \bar{v} \, dx$$

is not necessarily positive definite. In others words, there exist values of k, corresponding to natural frequencies, for which the kernel of $B_2(\cdot, \cdot)$, i.e.

$$\text{Ker } B_2 = \{\phi \in V;\ B_2(\phi, v) = 0,\ \forall v \in V\}$$

is a non-empty set. It immediately follows that there exists $\phi \in V$ such that

$$\sup_{v \in V \setminus \{0\}} \frac{|B_2(\phi, v)|}{|v|_1} = 0$$

implying that the inf-sup constant is zero. Similarly, the discrete inf-sup constant may also be zero for certain values of k, which may be different from those in the continuous case. It follows that the continuous problem (17) and discrete problem (21) are singular at those continuous and discrete natural frequencies and reliable error estimators cannot be constructed whenever the wave number corresponds to one of these.

4 A POSTERIORI ERROR ANALYSIS: Global Norm Estimators

One distinctive characteristic of a priori error estimation is that the error $e = \phi - \phi_h$ is estimated without employing the discrete solution ϕ_h. Indeed, the primary objective is to derive rates of convergence with respect to the discretization parameters h and p in order to evaluate the performance of a given numerical method. It follows that a priori error estimates generally involve unknown constants (independent of h and p) that prevent them to provide useful information about the quantitative error of a particular solution ϕ_h.

In contrast, a posteriori error estimation aims at developing quantitative methods in which the error $e = \phi - \phi_h$ is estimated in post-processing procedures using the solution ϕ_h as data for the error estimates. A posteriori error estimates become useful in two ways: one to assess the accuracy of a given instance ϕ_h, the other as a basis for an adaptive strategy.

In this section, we are concerned with a posteriori error estimation techniques in which the error is measured in terms of global (integral) norms computed over the whole solution domain. Note that even if the the norms are global, the resulting estimates are always decomposable into local contributions which provide the necessary information for adaptivity. We will describe in particular explicit residual methods, implicit residual methods, and recovery-type methods.

4.1 Abstract analysis

We first return to the abstract problem (27). Since $\mathcal{B}(\cdot,\cdot)$ is a sesquilinear form, the approximation error $e = u - u_h$ is governed by the equation:

$$\mathcal{B}(e, v) = \mathcal{R}(v), \qquad \forall v \in V \tag{47}$$

where $\mathcal{R}(v) = \mathcal{F}(v) - \mathcal{B}(u_h, v)$ is the residual functional. Obviously, the residual is the source for the error given in terms of the problem data embodied in $F(v)$ and the approximate solution u_h. From the continuity and the inf-sup condition of the sesquilinear form $\mathcal{B}(\cdot,\cdot)$, it is straightfoward to show that the norm of the error is equivalent to the norm of residual, i.e.

$$\alpha\|e\| \leq \|\mathcal{R}\|_* \leq M\|e\| \tag{48}$$

or

$$\frac{1}{M}\|\mathcal{R}\|_* \leq \|e\| \leq \frac{1}{\alpha}\|\mathcal{R}\|_* \tag{49}$$

where $\|\mathcal{R}\|_*$ is defined as the dual norm:

$$\|\mathcal{R}\|_* = \sup_{v \in V\setminus\{0\}} \frac{|\mathcal{R}(v)|}{\|v\|}. \tag{50}$$

The motivation behind the so-called residual methods is to evaluate the norm of the residual rather than the norm of the error itself since the problem (47) for the error e is as complex

to solve as the original problem. However, from (49), we observe that the quality of the error estimates will essentially depend on the values of M and α, which themselves depend on the choice for the norm $\|\cdot\|$. For instance, when the sesquilinear form $\mathcal{B}$ is positive-definite and hermitian, the best choice of the error measure norm is given by $\|v\| = \sqrt{\mathcal{B}(v,v)}$, since in that case $M = 1$ and $\alpha = 1$. In other words, the norm of the residual is simply equal to the norm of the error, i.e. $\|\mathcal{R}\|_* = \|e\|$. For "unstable" problems, those for which the inf-sup constant is small ($\alpha \ll 1$), the norm of the residual may yield a poor estimate of the error in the sense that $\|\mathcal{R}\|_*$ may be small, but $\|e\|$ large. Or, in the case of large values of M ($M \gg 1$), $\|\mathcal{R}\|_*$ may be large, but $\|e\|$ small. The conclusion of this brief analysis is that residual methods can yield reliable error estimates as long as the norms are chosen such that the constants M and α remain close to unity.

Switching to acoustic wave propagation, we have seen in the previous section that M and α for Model Problem 1 were of the order k^2 and k^{-1}, respectively, when considering the H^1-seminorm on V. Without further elaboration, we can stipulate that residual methods **will not provide reliable error estimates** (in the global H^1-seminorm) unless k remains close to unity. Note however that the bounds on the error include the worst possible cases and hence are pessimistic. In numerical applications, the estimators usually yield poor results for large values of k as long as one lies outside of the asymptotic regime (i.e. when the pollution error is not controlled). We now describe some of the error estimators available in the literature.

4.2 Explicit residual methods

Residual methods are usually classified into explicit and implicit methods. Explicit methods are those which do not require solving any auxiliary problems. In constrast, implicit methods involve the solution of local or global problems, set up in such a way that the solving cost is a fraction of the computational cost of obtaining the finite element solution. We describe the approach for the one-dimensional Model Problem 1 and extend the results to the corresponding problem in two-space dimensions.

4.2.1 One-space dimension analysis

The main idea in explicit residual methods is to relate the residual functional to the residual associated with the original strong solution of the differential equation. In this section, we consider again Model Problem 1, for which the residual functional $\mathcal{R}_1(v)$ was defined in (22). Let us define the so-called interior residuals r_K on each element K as

$$r_K = f + \phi_h'' + k^2\phi_h \tag{51}$$

where f and ϕ_h in the above definition are understood as restrictions of f and ϕ_h to K.

Theorem 2. *Let $\phi_h \in V^h$ be the solution of the finite element problem (20). Then the residual $\mathcal{R}_1(v) = F_1(v) - B_1(\phi_h, v)$ satisfies*

$$\|\mathcal{R}_1\|_* \leq \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2} \tag{52}$$

where h_K is the size of element K in the mesh.

Proof. See Appendix A.1. □

Remark 3. When ϕ_h is a continuous piecewise linear function, the second derivative of ϕ_h vanishes inside each element. It follows that the interior residuals reduce to $r_K = f + k^2\phi^h$.

Since the quantities $\|r_K\|_{0,K}$ are readily computable, Theorem 2 suggests the following a posteriori error estimator of the error in the global H^1-seminorm

$$\eta_{\text{exp}} = \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2}$$

with element-wise contributions $\eta_{K,\text{exp}} = h_K\|r_K\|_{0,K}$ to the global error. In one-space dimension, the estimator η_{exp} should provide reasonable estimates of the residual $\|\mathcal{R}_1\|_*$. However, we emphasize again that η_{exp} may fail to yield an accurate estimate of the true error since, with small values of the inf-sup constant α (i.e. large values of the wave number k), we would have $|e|_1 \leq \alpha^{-1}\eta_{\text{exp}}$.

Finally, we note that the residual $\mathcal{R}_2(v)$ associated with Model Problem 2 also satisfies $\|\mathcal{R}_2\|_* \leq (\sum_K h_K^2\|r_K\|_{0,K}^2)^{1/2}$ where the interior residual is now defined as $r_K = \phi_h'' + k^2\phi_h$. The conclusions are the same as for Model Problem 1; in addition, the error estimator is expected to be inefficient when k takes values close to the eigenvalues of the Helmholtz operator.

4.2.2 Two-space dimension analysis

Let us now consider the Helmholtz Model Problem 1 on a bounded domain $\Omega \subset \mathbb{R}^2$ with Dirichlet and Robin boundary conditions prescribed on parts Γ_D and Γ_R, respectively, of the boundary $\partial\Omega$. The model problem in two-space dimension corresponding to Model Problem 1 thus reads:

$$\text{Find } \phi \in V \text{ such that} \qquad A(\phi, v) = F(v), \qquad \forall v \in V \tag{53}$$

where

$$A(\phi, v) = \int_\Omega \nabla\phi \cdot \nabla\bar{v}\, dx - k^2 \int_\Omega \phi\bar{v}\, dx - ik \int_{\Gamma_R} \phi\bar{v}\, ds$$

$$F(v) = \int_\Omega f\bar{v}\, dx$$

$$V = \{v \in H^1(\Omega);\ v = 0 \text{ on } \Gamma_D\}$$

Suppose that we have available a finite element approximation $\phi_h \in V^h$ of Problem (53) in a suitable conforming finite element subspace V^h of V. In a manner similar to the one-dimensional case, we introduce the interior residuals r_K for each element K of the partition:

$$r_K = f + \Delta\phi_h + k^2\phi_h \tag{54}$$

and boundary residuals $j_{\gamma,K}$ for each boundary edge γ of an element K:

$$j_{\gamma,K} = \begin{cases} 0, & \text{if } \gamma \subset \Gamma_D \\ \partial_n\phi_h - ik\phi_h, & \text{if } \gamma \subset \Gamma_R \\ \frac{1}{2}\left[\partial_n\phi_h\right], & \text{if } \gamma \subset \partial K \backslash \partial\Omega \end{cases} \tag{55}$$

Theorem 3. *Let $\phi_h \in V^h$ be the finite element approximation of problem (53). Then the dual norm of the residual $\mathcal{R}(v) = F(v) - A(\phi_h, v)$ defined with respect to the H^1-seminorm satisfies*

$$\|\mathcal{R}\|_* \leq C \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2} \tag{56}$$

where C is a constant independent of the discretization parameters h_K and the wave number k.

Proof. See Appendix A.2. □

The main difference with the one-dimensional case is that a constant C appears in the bound on $\|\mathcal{R}\|_*$. This constant is naturally unknown for general applications as it results from the use of interpolation estimates and Poincaré's inequality. For practical purposes, the constant is commonly set to unity and the quantity η_{exp}

$$\eta_{\text{exp}} = \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2} \tag{57}$$

is then often referred to as an "error indicator" (rather than an error estimator). In other words, we cannot be guaranteed that η_{exp} provides a reliable quantitative estimate of $\|\mathcal{R}\|_*$, even less of $|e|_1$, especially when the wave number takes on large values. The quantity η_{exp} can still be decomposed into element-wise contributions

$$\eta_K = \sqrt{h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2}.$$

Note that these contributions provide local measures of the magnitude of the residual and should yield adequate refinement indicators for adaptive strategies since the residual is viewed as the source of errors.

Hence, the principal motivation in developing implicit residual methods is to be able to compute more accurate estimates of the norm of the residual by avoiding introducing the unknown constants that are characteristics of explicit methods.

4.2.3 Numerical applications

In [59], the authors employed an explicit residual method to compute estimates of the error in approximations of Model Problem 1 and of a slightly different version of Model Problem 2. The proposed explicit error estimator is equivalent to the one presented above but the error was measured with respect to the k-dependent error norm $\|\phi - \phi_h\|_{1,k}^2 = |\phi - \phi_h|_1^2 + k^2 \|\phi - \phi_h\|_0^2$. The quality of the explicit error estimator was then assessed by the global effectivity index:

$$\lambda = \frac{\eta_{\text{exp}}}{\|\phi - \phi_h\|_{1,k}}. \tag{58}$$

The conclusions of the investigation simply corroborate our predictions and can be summarized as follows: the quality of the error estimator deteriorates as the wave number k increases. In other words, the error estimator is incapable of detecting the pollution error. However, for small values of k, basically in the range of values imposed by the rule of thumb, the effectivity index is greater than one (i.e. the estimated error is an upper bound) and converges to six in the asymptotic range, for model problem 1. Finally, the quality of the error estimator is poor for wave numbers in the vicinity of the eigenvalues of Model Problem 2.

Stewart and Hughes [90] exploited explicit residual methods for the classical and least-squares finite element methods, in a slightly different context. The objective was to estimate the error in the L^2-norm following the approach introduced in the work of Aubin [6] and Nitsche [66] and based on the use of adjoint equations and duality arguments. The error estimator was constructed as the product of explicit error estimates by a stability constant. This stability constant needs to be approximated by solving global finite element eigenvalue problems on fine meshes, which makes the method rather cost-prohibitive. Two-dimensional numerical experiments included the simulation of a radiation problem and of a rigid scattering problem. In both problems, a circular cylinder imbedded in a infinite medium played the role of the vibrating body and of the scatterer. The authors computed the error estimates for cases where the waves were resolved (no pollution error) and obtained satisfactory results. They also used the explicit residual-type estimator (without including the scaling stability and interpolation constants) in an adaptive strategy and were able to generate meshes which adequately captured the various features present in the solutions. We note that only small values of the wave number were considered in this investigation.

4.3 Implicit residual methods

There exist many types of implicit residual methods; they are conveniently classified into element, subdomain, and global residual methods depending on whether the auxiliary problems are set up on elements, on subdomains (patches of elements), or on the whole computational domain. We briefly describe below the main features of the element and subdomain residual approaches.

4.3.1 Element residual method

Recall that the motivation here is to estimate the norm of the residual $\mathcal{R}_1$ defined as:

$$\|\mathcal{R}_1\|_* = \sup_{v \in V \setminus \{0\}} \frac{|\mathcal{R}_1(v)|}{|v|_1} \tag{59}$$

Unfortunately, the dual norm (59) is not readily computable. But, using the Riesz Representation theorem, we know that there exists a unique function $\xi \in V$ such that $|\xi|_1 = \|\mathcal{R}_1\|_*$, ξ being the solution of

$$(\xi, v)_1 = \mathcal{R}_1(v), \qquad \forall v \in V \tag{60}$$

where $(\cdot,\cdot)_1$ denotes the inner product associated with norm $|\cdot|_1$. The idea is then to design efficient algorithms to solve (60) for an approximation φ and to obtain the error estimator $\eta = |\varphi|_1 \approx \|\mathcal{R}_1\|_*$.

In element residual methods (see,[2] for instance, [28,3–5,60] and references therein) the global problem (60) is simply decomposed into local auxiliary problems decomposed on each element of the mesh. We define the local spaces

$$V_K = \{v \in H^1(K)/\mathbb{R};\ v = 0 \text{ on } \Gamma_D \cap \partial K\},$$

and the *broken space* associated with the mesh partition $\mathcal{P}_h$

$$V(\mathcal{P}_h) = \{v \in L^2(\Omega);\ v_K = v|_K \in V_K,\ \forall K \in \mathcal{P}_h\} \supset V \tag{61}$$

[2] Note that estimators based on the error in the constitutive law [60] can be viewed as a subclass of the element residual methods

with associated norm

$$|v|_{1,\mathcal{P}_h} = \sqrt{\sum_K \int_K |\nabla v|^2 \, dx}. \tag{62}$$

Note that $|v|_{1,\mathcal{P}_h} = |v|_1$ when $v \in V$. We denote by $(\cdot,\cdot)_{1,K}$ and $\mathcal{R}_{1,K}(\cdot)$ the restrictions of $(\cdot,\cdot)_1$ and $\mathcal{R}_1(\cdot)$ to an element K.

Theorem 4. *For each element K in the partition, let $\varphi_K \in V_K$ denote the solution of the local problem:*

$$(\varphi_K, v)_{1,K} = \mathcal{R}_{1,K}(v) + \int_{\partial K} g_K v \; ds, \qquad \forall v \in V_K, \tag{63}$$

where the flux functions g_K satisfy

$$\sum_K \int_{\partial K} g_K v_{|_K} \; ds = 0, \qquad \forall v \in V. \tag{64}$$

Define $\varphi \in V(\mathcal{P}_h)$ such that $\varphi_{|_K} = \varphi_K$. Then, the function φ provides an upper bound on the residual:

$$\|\mathcal{R}_1\|_* \leq |\varphi|_{1,\mathcal{P}_h} = \sqrt{\sum_K (\varphi_K, \varphi_K)_{1,K}}. \tag{65}$$

Proof. See Appendix A.3. □

We remark that the functions g_K have not yet been specified. The upper bound actually holds for arbitrary g_K's as long as condition (64) is satisfied. For example, these functions could all be set to zero, but this choice would not provide optimal estimates in the sense that the norm of the residual would be overestimated. First, we observe that (64) necessarily holds if:

$$\begin{aligned} &g_K = 0, && \forall \gamma \subset \partial\Omega, \\ &g_K + g_L = 0, && \forall \gamma = \bar{K} \cap \bar{L}, \;\; K \neq L, \;\; K, L \in \mathcal{P}_h. \end{aligned}$$

The choice for the g_K's is obviously not unique and their construction determine the type of element residual method. For example, we have

1. *The flux-splitting method* (see e.g. [17,28,70]). In this approach the fluxes g_K are computed on each interface γ as:

$$g_K = \begin{cases} \frac{1}{2}(n \cdot \nabla \phi_h)_K - \frac{1}{2}(n \cdot \nabla \phi_h)_L, & \text{if } \gamma \not\subset \partial\Omega, \\ 0, & \text{if } \gamma \subset \partial\Omega. \end{cases} \tag{66}$$

2. *The equilibrated flux-splitting method* (see e.g. [4,5,60,62]). Equilibrated fluxes g_K are computed such that:

$$\mathcal{R}_{1,K}(1) + \int_{\partial K} g_K \, ds = 0.$$

which represents the compatibility condition for the auxiliary problems with respect to the constant modes.

The auxiliary problems (63) have so far been defined on the infinite dimensional spaces V_K. In applications, finite element approximations φ_K^h of φ_K are actually calculated in order to derive the computable error estimator

$$\eta_{\text{erm}} = \sqrt{\sum_K (\varphi_K^h, \varphi_K^h)_{1,K}} \tag{67}$$

and local refinement indicators can be derived by considering the quantity $(\varphi_K^h, \varphi_K^h)_{1,K}$ on each element. The quantity η_{erm} often provides for an upper bound on the norm of the residual despite the fact that the finite element approximation φ_K^h of φ_K is used (see [85] for details). Finally, it is also possible to postprocess the functions φ_K to construct a lower bound on the norm of the residual. For additional details, see [72,86,19,92].

4.3.2 Subdomain residual method

In subdomain residual methods, the local problems are set up on patches of elements rather than elements. The method was initially designed by Babuška and Rheinbolt [16], and extended to meshes with hanging nodes in [14]. We also mention the recent work of Carstensen and Funkel [38], Machiels *et al.* [64], Morin *et al.* [65], Prudhomme *et al.* [83].

The subdomain residual methods rely on so-called partitions of unity. Let $\{\phi_i\}$ be the set of Lagrangian piecewise linear (in 1D or for triangles) or piecewise bilinear (for quadrilaterals) basis functions. The support of each ϕ_i is denoted by ω_i and will be referred to as the patch of elements connected to node i in the mesh. It is well-known that the functions ϕ_i form a partition of unity:

$$\sum_{1\le i\le N} \phi_i(x) = 1, \quad \forall x \in \Omega, \tag{68}$$

where N is the total number of nodes in the partition (mesh). Note that upon inserting (68) in the error equation, we have:

$$\mathcal{R}_1(v) = \mathcal{R}_1\left(v \sum_{1\le i\le N} \phi_i\right) = \sum_{1\le i\le N} \mathcal{R}_1(v\phi_i) \tag{69}$$

We introduce on patch ω_i the weighted inner product:

$$(\xi, v)_{1,\phi_i} = \int_{\omega_i} \phi_i \nabla\xi \cdot \nabla v \, dx$$

The idea is then to formulate and solve N local problems, over each patch ω_i, for the local functions $\xi_i \in W(\omega_i)$ such that

$$(\xi_i, v)_{1,\phi_i} = \mathcal{R}_1(v\phi_i), \quad \forall v \in W(\omega_i). \tag{70}$$

The spaces $W(\omega_i)$ are defined in such a way that the above problems are well-posed. Then we can show:

Theorem 5. *With above assumptions and definitions,*

$$\|\mathcal{R}_1\|_* \le \sqrt{\sum_{i\le i\le N} (\xi_i, \xi_i)_{1,\phi_i}}. \tag{71}$$

Proof. See Appendix A.4. □

The spaces $W(\omega_i)$ are infinite dimensional. In practice, the auxiliary problems (70) are solved on adequate finite element subspaces for approximations ξ_i^h of ξ_i. A computable error estimator consists then in calculating the quantity

$$\eta_{\text{sub}} = \sqrt{\sum_{i \le i \le N} (\xi_i^h, \xi_i^h)_{1,\phi_i}}. \tag{72}$$

We refer to [83] for details. It is also possible to postprocess the functions ξ_i to construct a lower bound on the norm of the residual. One advantage of subdomain methods over element residual methods is that it is not necessary to compute fluxes at the element interfaces. One disadvantage is their higher computational costs. Finally, variations in subdomain residual methods are related to the choice of the partition of unity.

4.3.3 Numerical applications

Babuška *et al.* presented in [8,56] a one-dimensional study of an error estimator based on a variation of the element residual method for Model Problem 1. They considered Dirichlet local problems, instead of Problems (63), for the functions $\varphi_K \in V_{0,K}$ such that

$$B_{1,K}(\varphi_K, v) = \mathcal{R}_{1,K}(v), \qquad \forall v \in V_{0,K}, \tag{73}$$

where $V_{0,K}$ is the space of functions in V_K which vanish on the boundaries of element K and $B_{1,K}(\cdot,\cdot)$ is the restriction of $B_1(\cdot,\cdot)$ on K. The error estimator was then computed using a finite element approximation φ_K^h of φ_K as:

$$\eta_{\text{drm}} = \sqrt{\sum_K (\varphi_K^h, \varphi_K^h)_{1,K}}. \tag{74}$$

They showed that at high wave numbers the error estimator was actually approximating the difference between the finite element solution and the associated *shifted function* rather than the exact error. The shifted function is defined as the solution $\tilde{\phi} \in V$ of

$$(\tilde{\phi}, v)_1 = \mathcal{R}_1(v) + (\phi_h, v)_1, \qquad \forall v \in V.$$

which can be rewritten:

$$(\tilde{\phi} - \phi_h, v)_1 = \mathcal{R}_1(v), \qquad \forall v \in V.$$

Comparing the above equation with (60), we see that the shifted solution is simply equal to $\phi_h + \xi$ (note that ξ is sometimes called the Riesz representer of the residual functional $\mathcal{R}_1$ with respect to the H^1-seminorm). Recall that $|\xi|_1 = \|\mathcal{R}_1\|_*$. This observation confirms that any error estimator based on local auxiliary problems will only provide an approximation of the function ξ. We emphasize again that, in view of (49), the Riesz representer ξ does not incorporate any information about the pollution error.

Bouillard [31,32] studied an error estimator based on the equilibrated flux-splitting approach of Ladevèze [60–63] (usually referred to as error estimation in the constitutive law). The investigation is concerned with vibro-acoustic problems and is limited to low values of the wave number (non-dimensionalized) at which pollution error is known to be negligible. The various examples demonstrate that, in the case of linear or bilinear elements, such an estimator provides upper bounds on the exact error with effectivity indices of order two.

To the best knowledge of the authors, the subdomain residual method has not been used to date to calculate error estimates for the Helmholtz equation. But from the preceding discussion, one should expect to obtain similar results as the ones obtained by other implicit methods. More precisely, the fact that local problems are used will not permit one to estimate the contribution of the pollution error.

4.4 Recovery-type methods

Recovery-based error estimators were suggested by Zienkiewicz and Zhu [99] as early as 1987. Improved techniques were later proposed by the same authors [100,101]. The main motivation underlying these methods follows the simple observation that piecewise continuous finite element solutions ϕ_h generally exhibit discontinuous gradients at the interface of the elements. If the exact solution ϕ to be sought is smooth enough, such jumps in the gradients of ϕ_h are an indication that the numerical solutions are erroneous. The approach consists then in recovering piecewise continuous gradients $G(\phi_h)$ from the finite element approximation ϕ_h and in calculating the "difference" as the error measure $\mathcal{E}$, i.e.

$$\mathcal{E} \approx \eta_{\text{rec}} = \sqrt{\int_\Omega |G(\phi_h) - \nabla \phi_h|^2 \, dx}. \tag{75}$$

Various methods have been proposed in the literature to compute $G(\phi_h)$ and the reader is referred to [100,101] for an account on the Zienkiewicz-Zhu patch recovery technique. Some of the approaches rely on *superconvergence* properties of the finite element method obtained at specific points in the element (see also [5]).

We illustrate in Figure 5 a sketch of the procedure. In the first graph (top-left) we show a portion of a one-dimensional sinusoidal wave and its piecewise linear finite element approximation, representatives of solutions of Model Problem 1. In the top-right picture, we plot the first derivative (i.e. gradient) of the exact wave and of the approximated wave. We recover from the latter a continuous piecewise linear derivative $G(\phi_h)$ by simply averaging the values of the derivative at the nodes. We observe in the bottom-left corner of Figure 5 that $G(\phi_h)$ is clearly a smoother function than the original piecewise constant derivative. Finally, in the bottom-right picture, we plot the exact error $e = \phi' - \phi'_h$ and the estimated error $e_{\text{rec}} = G(\phi_h) - \phi'_h$. This example shows that e_{rec} thus obtained approximates well the exact error e near the origin but rapidly deteriorates as we move along the x-axis. As in the case with residual methods, the recovery method fails to detect the pollution (dispersion) error of the approximated wave. Another interpretation is that the recovery method provides for a smooth function (by integration of $G(\phi_h)$) in the vicinity of the finite element approximation, but this function is not necessarily "close" to the exact solution of the problem.

Bouillard and Ihlenburg [33,34] performed numerical experiments to test the quality of the recovery or smoothening technique on Model Problems 1 and 2. They show that the estimator is actually convergent for all wave numbers; i.e. the effectivity index

$$\lambda = \frac{\eta_{\text{rec}}}{|\phi - \phi_h|_1}. \tag{76}$$

converges to one as the discretization parameter tends to zero, meaning that the recovered smooth function gets closer and closer to the exact solution as the pollution error diminishes. This result however does not apply to the undamped Model Problem 2 when the wave number corresponds to a natural frequency. On the other hand, the effectivity index clearly

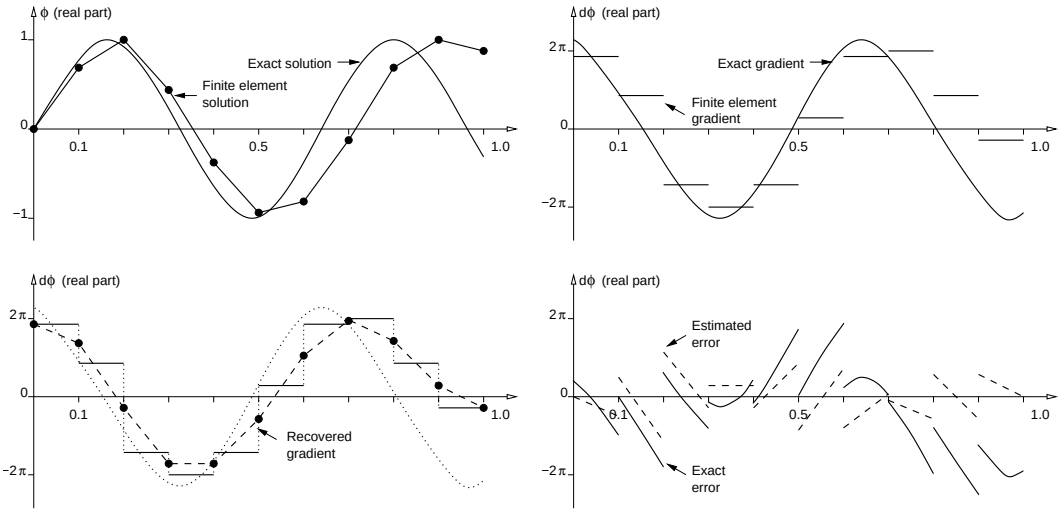

Fig. 5. Schematic description of recovery-type methods.

deteriorates when k becomes large, i.e. when dispersion becomes too significant. As an example, discretizing Model Problem 1 with a mesh size $h = 0.1$, the authors showed in Figure 7 of [33] that the effectivity index is approximatively 0.8 for $k = 10$, but only 0.4 when $k = 20$ (note also that the estimator underestimates the error). In another numerical example dealing with the vibro-acoustic simulation of the cabin of a car, the recovery-type estimator proved to be a successful basis for mesh adaptation. Recall that recovery- or residual-type error estimators by nature detect the large sources of error and thus will always be able to refine the appropriate regions in the computational domain.

4.5 Control of the pollution error

We have seen so far that the classical a posteriori error estimators, based on local computations, generally underestimate the exact error in global norms at high wave numbers. This is due to the fact that these error estimators are not capable of measuring the pollution effect in finite element solutions of the Helmholtz equation. Babuška *et al.* in [9] proposed to construct a posteriori estimates of the pollution error based on their previous work on the subject in the case of linear elasticity [20,21,23,22]. We briefly describe the approach below.

We again consider Model Problem 1. The key point in estimating the pollution error relies on the introduction of Green's function. Recall that the Green's function with respect to a point x_0 is defined as the function $G(x; x_0) \in V$ such that

$$B_1(v, G) = v(x_0), \qquad \forall v \in V. \tag{77}$$

Taking $v = e = \phi - \phi_h$, it immediately follows that

$$e(x_0) = B_1(e, G) = \mathcal{R}_1(G) = \mathcal{R}_1(G - \mathcal{I}_h G) \tag{78}$$

where we have used the orthogonality property of the residual and where $\mathcal{I}_h G$ is the interpolant of the Green's function G in V^h. Since $G - \mathcal{I}_h G$ vanishes at the endpoint of the mesh, we can rewrite the above equation as:

$$e(x_0) = \sum_K \mathcal{R}_{1,K}(G - \mathcal{I}_h G) = \sum_K B_{1,K}(\varphi_K, G - \mathcal{I}_h G) \tag{79}$$

with the function φ_K satisfying (73) on each element. Since the quantity $G - \mathcal{I}_h G$ is not computable, the authors propose to calculate the finite element approximation $G_h \in V^h$ of G and to replace $G - \mathcal{I}_h G$ in each element by the estimate $\psi_K(x_0)$ such that

$$B_{1,K}(v, \psi_K(x_0)) = v(x_0) - B_{1,K}(v, G_h), \qquad \forall v \in V_{0,K}, \tag{80}$$

so that

$$e(x_0) \approx \sum_K B_{1,K}(\varphi_K, \psi_K(x_0)) \tag{81}$$

In order to estimate the pollution error in a given element of the mesh, say element K_i, they choose one point x_i in K_i (x_i is actually chosen as the right end point of the element) and compute the quantity $E(x_i)$ such that:

$$E(x_i) = \sum_{K \neq K_i} B_{1,K}(\varphi_K, \psi_K(x_i)) \tag{82}$$

Note that the contribution from element K_i is not included in the sum as the authors argue that an estimate of the error in the interior of that element is already computed by the element residual method. Similarly, they define an estimate $E'(\bar{x}_i)$ for the first derivative $e'(\bar{x}_i)$ where $\bar{x}_i$ is chosen as the midpoint of element K_i. The derivative e' is first approximated by the finite difference

$$e'(\bar{x}_i) \approx \frac{e(x_{i+1}) - e(x_i)}{h}$$

so that

$$E'(\bar{x}_i) = \sum_{K \neq K_i} B_{1,K}\left(\varphi_K, \frac{\psi_K(x_{i+1}) - \psi_K(x_i)}{h}\right) = \sum_{K \neq K_i} B_{1,K}\left(\varphi_K, D\psi_K(\bar{x}_i)\right) \tag{83}$$

where, by definition, $D\psi_K(\bar{x}_i) = (\psi_K(x_{i+1}) - \psi_K(x_i))/h$. The authors proceed by defining the normed expression

$$E_1(\bar{x}_i) = \left(\frac{1}{h} \sum_{K \neq K_i} |B_{1,K}\left(\varphi_K, D\psi_K(\bar{x}_i)\right)|^2\right)^{1/2} \tag{84}$$

as a pollution estimator of the finite element solution ϕ_h in the H^1-norm for element K_i. Because they found numerically that the estimate E_1 exhibited large oscillations, they suggested to compute an *averaged pollution estimator* E_{pol} of the "exact averaged pollution error" e_{pol}

$$E_{\text{pol}}(K_i) = \frac{1}{N_\lambda} \sum_{m=i-n_\lambda}^{i+n_\lambda} E_1(\bar{x}_m), \qquad e_{\text{pol}}(K_i) = \frac{1}{N_\lambda} \sum_{m=i-n_\lambda}^{i+n_\lambda} |e_1(\bar{x}_m)|. \tag{85}$$

with

$$e_1(\bar{x}_i) = \left| \sum_{K \neq K_i} B_{1,K}\left(\varphi_K, (DG - \mathcal{I}_h DG)(\bar{x}_i)\right) \right|$$

In above expressions, $n_\lambda = [\lambda/4h]$, where $\lambda = 2\pi/k$ is the wavelength and the square brackets mean the largest integer not exceeding the argument. The number $N_\lambda = 2n_\lambda + 1$ is approximately the number of elements per half-wave. The quality of the averaged pollution estimator is then measured in terms of the averaged pollution effectivity index $\theta(K_i) = E_{\text{pol}}(K_i)/e_{\text{pol}}(K_i)$. They then showed on several numerical examples effectivity indices $\theta(K_i)$

ranging from one to three with wave numbers varying between 100 and 500 for solutions in the pre-asymptotic range of convergence.

A few comments about this investigation are now in order. The computed effectivity indices certainly show that the estimator is very reliable, but the averaged pollution effectivity index is defined in terms of an exact averaged pollution error (see (85)) which does not seem to correspond to the pollution error defined earlier as the difference between the exact solution ϕ of the Helmholtz equation and the shifted solution associated with the finite element approximation ϕ_h. Certain steps of the method, such as the passage from the expression for $E'(\bar{x}_i)$ in (83) to the expression for $E_1(\bar{x}_i)$ in (84), require motivation or further study. Finally, the fact that the function $G - \mathcal{I}_h G$ is replaced by the approximation ψ_K of $G - G_h$ should be analyzed in more detail. The error $G - G_h$ may be very different from the interpolation error $G - \mathcal{I}_h G$ due to pollution effects, and it is definitely not guaranteed that ψ_K provides a reliable estimate of $G - \mathcal{I}_h G$.

From (81), we observe that the quantity $\sum_K B_{1,K}(\varphi_K, \psi_K(x_0))$ actually represents an estimate of $e(x_0)$, that is, the error in ϕ_h at the given point x_0 in the mesh. It follows that the approach developed by Babuška *et al.* to measure the pollution error exhibits many features similar to goal-oriented estimates presented in the following section.

5 GOAL-ORIENTED ERROR ESTIMATION

In the previous section, we presented various types of error estimators which measure the error with respect to global norms computed over the whole computational domain. In the following, we describe a class of methods based on duality techniques (see [29,78,76,77,30,72] for example) which determine error estimates in terms of quantities of interest (the goal of a given simulation) provided by the analyst. Examples of quantities of interest are pointwise values or local averages of the solution, but could also be defined as any linear or nonlinear functionals of the solution. This new class of methods make possible significant generalizations of existing adaptive strategies and have been called *goal-oriented* adaptive methods (see [84,72]). We apply here the general theory to the Helmholtz equation. We first provide some examples of quantities of interest. We present some recent applications of the method at the end of the section.

5.1 Quantities of interest

In goal-oriented error estimation, analysts specify the goal of their calculations by identifying a quantity of interest. The quantity of interest is represented by a functional defined on the space of admissible solutions, the functional being either linear or nonlinear. Here are a few examples:

Example 1 (Averaged values). The average of the wave amplitude ϕ in an acoustic medium over a small region ω, for instance, is represented by the linear functional

$$Q(\phi) = \frac{1}{|\omega|} \int_\omega \phi \, dx. \tag{86}$$

The error in the quantity would then be defined in this case as:

$$\mathcal{E} = Q(\phi) - Q(\phi_h) = Q(e) = \frac{1}{|\omega|} \int_\omega e \, dx.$$

Example 2 (Pointwise values). Suppose that one is interested in the value of the amplitude ϕ at a specific point x_0 in the domain. The quantity of interest is then given by:

$$Q(\phi) = \phi(x_0).$$

However, when ϕ is a function of $H^1(\Omega)$, this quantity is not necessarily defined for $d \geq 2$. For that reason, we prefer to consider a local average or weighted value of the solution around the point x_0, i.e.

$$Q_\varepsilon(\phi) = \int_\Omega \phi(x)\ k_\varepsilon(x - x_0)\, dx, \tag{87}$$

where k_ε is a mollifying kernel defined as:

$$k_\varepsilon(x) = \begin{cases} C \exp\left(|x|^2/\epsilon^2 - 1\right)^{-1} & \text{if } |x| < \varepsilon \\ 0 & \text{if } |x| \geq \varepsilon \end{cases} \tag{88}$$

with C, which depends on d, ε and x_0, chosen so as to satisfy:

$$\int_\Omega k_\varepsilon(x - x_0)\, dx = 1.$$

Note that $Q_\varepsilon(\phi)$ converges to $\phi(x_0)$ as ε goes to zero when ϕ is continuous in a neighborhood of x_0.

Example 3 (L^2-norm over a subregion). If one is interested in the (square of the) L^2-norm of ϕ in a subregion ω of the computational domain, one should define the quantity of interest as:

$$\mathcal{N}(\phi) = \|\phi\|^2_{0,\omega} = \int_\omega |\phi|^2\, dx.$$

In this case, the error is determined as $\mathcal{E} = \mathcal{N}(\phi) - \mathcal{N}(\phi_h) = \|\phi\|^2_{0,\omega} - \|\phi_h\|^2_{0,\omega}$ (note that $\mathcal{E}$ is different from $\|e\|^2_{0,\omega}$). Since the functional $\mathcal{N}$ is nonlinear, we consider instead the linear functional

$$Q(v) = \mathcal{N}'(\phi_h; v) = \int_\omega 2\phi_h \bar{v}\, dx$$

where $\mathcal{N}'(\phi_h; \cdot)$ denotes the first derivative of $\mathcal{N}$ at ϕ_h. We then approximate $\mathcal{E}$ by

$$\mathcal{E} \approx \mathcal{N}'(\phi_h; e).$$

In other words, the higher-order terms in the representation of $\mathcal{N}(\phi)$ are neglected.

5.2 Methodology

We first present the methodology on the abstract problem:

$$\text{Find } u \in V \text{ such that} \qquad \mathcal{B}(u, v) = \mathcal{F}(v), \qquad \forall v \in V \tag{89}$$

for which an approximation by the finite element method is obtained by solving the discrete problem:

$$\text{Find } u_h \in V^h \text{ such that} \qquad \mathcal{B}(u_h, v) = \mathcal{F}(v), \qquad \forall v \in V^h \tag{90}$$

Let $Q(.)$ be a linear functional representing a given quantity of interest. The dual problem associated with the primal problem (91) reads:

$$\text{Find } \omega \in V \text{ such that} \qquad \mathcal{B}(v, \omega) = Q(v), \qquad \forall v \in V \tag{91}$$

The function ω is referred to as the dual solution or as the influence function. Indeed, from (89) and (91), we easily deduce that:

$$Q(u) = \mathcal{B}(u, \omega) = F(\omega)$$

and

$$Q(e) = Q(u) - Q(u_h) = \mathcal{B}(u, \omega) - \mathcal{B}(u_h, \omega) = \mathcal{B}(e, \omega) = \mathcal{R}(\omega).$$

In other words, the dual solution ω indicates how the loading $F(\cdot)$ and residual $\mathcal{R}(\cdot)$ influence the quantities $Q(u)$ and $Q(e)$, respectively. In this respect, the influence function is seen to contain all the necessary information for evaluating the pollution error with respect to the quantity of interest.

The influence function is the solution of an infinite dimensional problem and cannot in general be calculated exactly. It follows that the main objective in goal-oriented error estimation is to approximate the influence function in order to be able to compute estimates of the error $Q(e)$. If ω is approximated by a finite element function ω^h lying in the same finite element space V^h as u_h, we would have

$$\mathcal{R}(\omega_h) = 0,$$

since the residual vanishes on V^h ("orthogonality property"). This implies that $Q(e)$ would be estimated as zero. Thus, an adequate approximation of the dual solution should be in a space larger than V^h. A variety of approaches have been proposed to obtain reliable approximations of the influence function at relatively low computational costs:

1. In some rare cases, the influence function can be determined analytically, at least partially. Indeed, if one is interested in the error at a point in the domain, the influence function is actually the Green function which is known for certain classes of problems (in fact, the Green function can be given as the fundamental solution of the Laplace operator plus a harmonic function to be determined). This approach was originally used to extract accurate pointwise stresses or derivatives from finite element approximations of elasticity problems. For more details, we refer the reader to [2,11–13,37,67,68,97,98].
2. A second approach consists in computing a global finite element approximation on a finite element space larger than V^h. One method [30] is to approximate ω on the same mesh using polynomial functions of higher-degree than those used for u_h. The major drawback in this method is that the dual problem becomes much more expensive to solve than the primal problem (this method is nevertheless viable for nonlinear problems as the corresponding dual problem would still be linear).
3. Another approach takes advantage of the fact that the influence function often presents local features, especially when the quantity of interest is of local nature. The approximation of the influence function is computed on an adapted mesh based on error estimates in the energy norm. The error in the quantity of interest would then be estimated by $\eta = \mathcal{R}(\omega_H) \approx Q(e)$, where the parameter H refers to the adapted mesh for the dual problem. The main difficulty in this approach is then to handle two different meshes in the same finite element code.
4. An approximation $\omega_h \in V^h$ of ω is first calculated such that

   $$\mathcal{B}(v, \omega_h) = Q(v), \qquad \forall\ v \in V^h$$

   and a new $\tilde{\omega}^h$ is constructed from ω^h by "interpolating" polynomial functions of higher-degree than the functions in V^h [30].

5. Finally, the last approach we mention consists in estimating the error $\varepsilon = \omega - \omega_h \in V$. Since $\mathcal{R}(\omega_h) = 0$, we have:

$$Q(e) = \mathcal{R}(\omega) = \mathcal{R}(\omega) - \mathcal{R}(\omega_h) = \mathcal{R}(\omega - \omega_h) = \mathcal{R}(\varepsilon)$$

In other words, the quantity $Q(e)$ is given in terms of the residual $\mathcal{R}$, which is known, and the error ε, which can be estimated using residual- or recovery-type error estimators.

It is not the purpose of this review to describe the various approaches listed above. We will explain in more detail one of these methods in the following subsection where we apply goal-oriented error estimation to acoustic problems.

5.3 Application to acoustic problems

We now return to Model Problem 1 and suppose that the goal of the analysis is to compute the quantity of interest $Q(\phi)$. The dual problem for the influence function ω is formulated as:

$$\text{Find } \omega \in V \text{ such that} \qquad B_1(v, \omega) = Q(v), \qquad \forall v \in V \tag{92}$$

and a finite element approximation of ϕ can be computed as the solution of:

$$\text{Find } \omega_h \in V^h \text{ such that} \qquad B_1(v, \omega_h) = Q(v), \qquad \forall v \in V^h \tag{93}$$

We denote by $\mathcal{R}_1^{\phi}(\cdot)$ and by $\mathcal{R}_1^{\omega}(\cdot)$ the residuals in the primal and dual problems, respectively:

$$\mathcal{R}_1^{\phi}(v) = F_1(v) - B_1(\phi_h, v) = B_1(e, v)$$
$$\mathcal{R}_1^{\omega}(v) = Q(v) - B_1(\omega_h, v) = B_1(v, \varepsilon)$$

where $\varepsilon = \omega - \omega_h$ is the error in the influence function. It immediately follows that the error in the quantity of interest is given by:

$$Q(e) = \mathcal{R}_1^{\phi}(\varepsilon) = B_1(e, \varepsilon) = \mathcal{R}_1^{\omega}(e). \tag{94}$$

We now adapt a method proposed by Sarrate *et al.* [87] to obtain an estimate of the real part of $Q(e)$, i.e. $\Re(Q(e))$. We first introduce the Riesz representers of the residuals, i.e.

$$(\xi_{\phi}, v)_1 = \mathcal{R}_1^{\phi}(v), \qquad \forall v \in V$$
$$(\xi_{\omega}, v)_1 = \mathcal{R}_1^{\omega}(v), \qquad \forall v \in V$$

Then we have:

$$Q(e) = \mathcal{R}_1^{\omega}(e) = (\xi_{\omega}, e)_1 \tag{95}$$

and

$$B_1(e, e) = \mathcal{R}_1^{\phi}(e) = (\xi_{\phi}, e)_1. \tag{96}$$

Combining the two equations, we obtain:

$$Q(e) = (\xi_{\omega}, e)_1 + (\xi_{\phi}, e)_1 - B_1(e, e) = (\xi_{\omega} + \xi_{\phi}, e)_1 - B_1(e, e) = 2(\xi^+, e)_1 - B_1(e, e) \tag{97}$$

where we have introduced $\xi^+ = (\xi_{\phi} + \xi_{\omega})/2$. Taking the real part of $Q(e)$, i.e. $\Re(Q(e))$, we get:

$$\Re(Q(e)) = 2\Re((\xi^+, e)_1) - \Re(B_1(e, e)) = (\xi^+, e)_1 + (e, \xi^+)_1 - \Re(B_1(e, e))$$

Note that:

$$B_1(e,e) = \int_\Omega e'\bar{e}'\,dx - k^2\int_\Omega e\bar{e}\,dx - ike(1)\bar{e}(1) = (e,e)_1 - k^2(e,e) - ik|e(1)|^2$$

so

$$\Re(B_1(e,e)) = (e,e)_1 - k^2(e,e).$$

Therefore

$$\begin{aligned}\Re(Q(e)) &= (\xi^+,e)_1 + (e,\xi^+)_1 - (e,e)_1 + k^2(e,e)\\ &= (\xi^+,\xi^+)_1 - (\xi^+,\xi^+)_1 + (\xi^+,e)_1 + (e,\xi^+)_1 - (e,e)_1 + k^2(e,e)\\ &= (\xi^+,\xi^+)_1 - (e-\xi^+,e-\xi^+)_1 + k^2(e,e)\end{aligned}$$

which yields

$$|\xi^+|_1^2 = \Re(Q(e)) + |e-\xi^+|_1^2 - k^2\|e\|_0^2. \tag{98}$$

The authors argue that the term $k^2\|e\|_0^2$ is much smaller than $|e-\xi^+|_1^2$ for h small, and that $|e-\xi^+|_1^2$ should converge to zero as h tends to zero with a convergence rate of the order of $\mathcal{O}(h^2)$. We can conclude that the quantity $|\xi^+|_1^2$ approaches from above the error $\Re(Q(e))$ in the asymptotic range. We remark that $|\xi^+|_1^2$ cannot be computed exactly, but is easily estimated by one of the various explicit or implicit methods described in Section 4. A "lower" bound can be computed as well by considering $\xi^- = (\xi_\phi - \xi_\omega)/2$ instead of ξ^+. Following the same analysis, we would get:

$$-|\xi^-|_1^2 = \Re(Q(e)) - |e-\xi^-|_1^2 + k^2\|e\|_0^2. \tag{99}$$

In this case, the quantity $-|\xi^-|_1^2$ will approach $\Re(Q(e))$ from below.

Peraire and Patera [82] used a similar approach for an interior Helmholtz problem with Dirichlet boundary conditions.

5.4 Numerical examples

We now give a brief account on numerical applications from [87]. The authors considered the scattering of a plane wave by a rigid body in two dimensions. They considered as quantities of interest the normalized L^2-norm of the solution, the squared modulus over a boundary strip, and the real part of the averaged solution over the whole domain. The incident plane waves had wave numbers $k = 2\pi$, 3π, or 5π and the scatterer was a U-shaped body immersed in a unit squared domain. The authors defined the effectivity index as

$$\theta = \frac{Q(\phi_h) + \eta^Q}{Q(\phi_H)}$$

where η^Q stands for their estimates/bounds of the error $Q(\phi_H - \phi_h)$ and ϕ_H is the solution on the so-called truth mesh of mesh size H ($H \ll h$). It is assumed that the truth mesh solution "ϕ_H" provides for a very accurate approximation of ϕ. They reported effectivity indices varying between -2 and 4 and observed that the bounds were less sharp with increasing wave number, as expected (note however that θ is defined with respect to $Q(\phi_H)$ rather than $Q(e)$, as it is usually done in the literature). However, they did not mention whether the pollution error in the solutions was significant.

As another approach to goal-oriented adaptation techniques for acoustic problems, we mention [96] wherein a technique for the modeling of the external human auditory system by

the boundary element method is presented. Goal-oriented error estimation and adaptation techniques for the time-dependent wave equation (1) are studied in [26,30,27]. One technical difficulty for the formulation of wave problems in time-domain is that the influence function is the solution of a time-dependent problem to be integrated backwards in time.

6 ANALYSIS FOR THE *hp* FEM

We have seen in the previous sections that the pollution effects, or equivalently the dispersive character of waves, are responsible at large wave numbers for poor accuracy of finite element approximations of the Helmholtz equation as well as suboptimal performance of a posteriori error estimation techniques. In order to minimize the effect of numerical dispersion, one may be tempted to use higher order finite element methods, the so-called *hp* finite element methods, in which the mesh size h and the polynomial degree p are allowed to vary among the elements. Early works on the use of of high order methods have shown promising advantages [94,52]. We present in what follows the a priori estimates for the discretization and dispersion errors for *hp* methods obtained by Ihlenburg and Babuška [56] and extended by Ainsworth [1]. We then describe a viable strategy for a posteriori error estimation and mesh adaptation based on a fine/coarse grid approach and discuss the advantages and limitations of the method.

6.1 A priori error estimates

Let $p \geq 2$ and let $\phi \in V \cap H^{p+1}(\Omega)$ be the solution of Model Problem 1. We then consider the *hp* finite element approximation ϕ_{hp} of ϕ computed on a uniform mesh with mesh size h and constant polynomial degree p. Assuming that h is such that $hk \leq 1$, an estimate of the relative error [58] is given by

$$\frac{|\phi - \phi_{hp}|}{|\phi_{hp}|} \leq A(p) \left[\left(\frac{hk}{2p} \right)^p + Ck \left(\frac{hk}{2p} \right)^{2p} \right] \tag{100}$$

where C is a constant independent of h, p, and k. The quantity $A(p)$ is an approximation constant and depends only on p. See [58] for a detailed proof of this result. Note that the estimate (100) is consistent with the estimate (41) obtained for piecewise linear approximations by taking $p = 1$. As in the linear case, the first term corresponds to the approximation error and the second term represents the error due to pollution effects. We may conclude from above estimate that the pollution error is controlled whenever the mesh size is chosen sufficiently small, i.e. such that $k(kh)^p/(2p)^p \ll 1$. It is important to notice that the pollution error is actually of the same order as the phase lag or dispersion error:

$$|k - \tilde{k}| \leq \left(\frac{A(p)}{2} \right)^2 Ck \left(\frac{hk}{2p} \right)^{2p} \tag{101}$$

where $\tilde{k}$ is a discrete wave number associated with the *hp* mesh. For the definition of $\tilde{k}$, see [56]. Note that this estimate of the dispersion error holds for $p \geq 1$ and $hk < 1$.

Ainsworth improved the above result in [1] by deriving explicit expressions of the dispersion error (without generic constants). In the case of small wave numbers, i.e. $kh \ll 1$, he was able to show that:

$$\cos kh - \cos \tilde{k}h = -\frac{1}{2} \left(\frac{p!}{(2p)!} \right)^2 \frac{(kh)^{2p+2}}{2p+1} + \mathcal{O}(kh)^{2p+4} \tag{102}$$

or, if $\tilde{k}h$ is sufficiently small,

$$k - \tilde{k} = \frac{1}{2}\left(\frac{p!}{(2p)!}\right)^2 k\frac{(kh)^{2p}}{2p+1} + \mathcal{O}(kh)^{2p+3} \tag{103}$$

More interestingly, he extended this result to the case of large wave numbers, i.e. $kh \gg 1$. He showed that, for large values of kh, the error $\mathcal{E}^p = \cos kh - \cos \tilde{k}h$ passes through three distinct phases as the degree p is increased:

1. Oscillatory phase: for $2p + 1 < kh - o(kh)^{1/3}$, $\mathcal{E}^p$ oscillates, but does not decay, as p is increased.
2. Transition zone: for $kh - o(kh)^{1/3} < 2p + 1 < kh + o(kh)^{1/3}$, the error $\mathcal{E}^p$ decays algebraically at a rate $\mathcal{O}(p^{-1/3})$.
3. Super-exponential decay phase: for $2p + 1 > kh + o(kh)^{1/3}$, the error $\mathcal{E}^p$ decreases at a super-exponential rate.

The result is found useful in providing guidelines for the selection of the discretization parameters h and p. In particular, it is desirable to remain in the super-exponential regime so that p and h should be chosen such that:

$$2p + 1 > kh + \alpha(kh)^{1/3}$$

where α is a user-defined parameter.

6.2 Use of multigrid approach for a posteriori error estimation and *hp* mesh optimization

In this section, we provide a brief account on a posteriori error estimation for the *hp* finite element method. Note that a posteriori error estimation is ultimately connected with mesh adaptivity. Once a large error is detected in a part of the solution domain, the mesh in that part is refined. In the case of the h or p method, one needs only the information which elements to refine, i.e. an element error estimator or error indicator are sufficient to drive an adaptive strategy. The situation is much more difficult in the case of the *hp* method where, on top of knowing which elements to refine, a decision has to be made whether the elements should be broken or the local order of approximation increased. The problem of designing an automatic *hp* strategy has been an area of active research for the last decade and a half, with two successful techniques having emerged in context of conforming elements. The *tagging strategy* of Ainsworth is based on incorporating an a priori mathematical expertize on singularities into the *hp* FE code. The singular vertices and edges are marked and elements adjacent to them are always forced to be appropriately h-refined, if the error estimate calls for a refinement. All other elements are always p-refined. The strategy delivers optimal meshes and exponential convergence for problems with vertex and edge singularities but it does not work e.g. for problems with boundary layers or solutions with large gradients or irregularities whose location is a priori unknown, a situation typical for e.g. non linear problems.

A genuine, fully automatic *hp* strategy has been proposed in [42,44]. The strategy is built on a fundamental observation that in order to determine an optimal *hp*-refinement, one has to know the actual *error function* and not just a single number per element. This calls for solving the entire problem on a globally refined mesh. In the case of the *hp* method, the refinement has to be both in h and p, only then the fine mesh solution carries enough new

resolved "scales" to allow for a meaningful choice between the h and p refinement. The globally hp-refined *fine mesh* is typically 20-30 times larger than the original *coarse mesh* and the only practical technique to solve the fine grid problem for large coarse meshes is the multigrid. The implementation presented in [79] is based on a 2-grid solver for which the V-cycle iterations are restricted to the coarse and fine grid mesh only.

The fine grid solution drives the optimal hp refinements but it also provides an excellent a posteriori error estimate - the difference between the coarse and fine grid solutions approximates very well the actual error function - either for global error estimation, or as a basis for *goal-oriented* error estimation [89]. The fine grid solution needs not to be fully converged, it is sufficient to drive the iteration error down to a few percent of the global error estimate for the previous coarse mesh. The resulting global reflectivity indices are typically in the $0.98 - 1.02$ range, and are practically impossible to beat with other techniques.

The use of the fine grid solution for the error estimation is surprisingly effective. If N denotes the number of elements in a 3D hexahedral coarse FE mesh, and p is the average order of approximation, the cost of the fine grid solve is of order $8N \times p^9$. The exponent 9 corresponds to the cost of inversion of local patch matrices (used for the construction of a block-Jacobi smoother), and it can be further reduced if an incomplete factorization is used. Constant 8, corresponding to eight sons of a hexahedral coarse grid element, is critical here and it compares favorably with similar constants in other implicit a posteriori error estimation techniques like subdomain residual or equilibrated residual methods. At the same time, the complexity of coding is significantly smaller and the fine grid solution delivered by the 2-grid solver may always be considered to be the final (superior quality) product of mesh optimization.

An additional motivation for using the 2-grid strategy for wave propagation problems comes form the pollution (dispersion) error analysis. For Helmholtz-like equations, the Galerkin method is stable only asymptotically. The dispersion error estimates allow for a selection of minimum p for each element in the initial mesh, as a function of the element size and local wave number (material properties). If the order exceeds the maximum order supported by the code, the element has to be h-refined first. For large wave numbers, the resulting mesh delivers already such a small error that very often there is very little need for any adaptivity at all.[3] In the case of the coarse/fine grid strategy, *only the fine grid has to be in the asymptotic range*, and the error estimation and possible mesh optimization process can start very early in the preasymptotic range in terms of the coarse grid. We have several examples for which the initial mesh error is over 100 percent. There is no miracle, however. One should emphasize that, in order for the 2-grid solver to converge, *the coarse grid* must satisfy the dispersion error criterion already. In context of practical implementation this means that the fine grid problem must be initially solved using a direct solver, and only once the coarse grid satisfies the dispersion error criterion, the direct solve may be replaced with the 2-grid iterations.

In conclusion, the coarse/fine grid strategy may be an optimal approach for both error estimation and mesh optimization in context of wave propagation problems and hp methods. Moreover, compared with rather dry numbers provided by typical error estimators, having the possibility of visualizing the error function is a very helpful and intuition building experience in studying mesh optimization and quality of FE solutions.

[3] One should be perhaps more careful with this statement; there is growing evidence that the comment does not apply to solutions experiencing nearly resonant behavior, e.g. scattering from cavities, design of waveguide filters in electromagnetics or elastic scattering in acoustics.

7 SHORT REVIEW OF A POSTERIORI ERROR ESTIMATION FOR THE BOUNDARY ELEMENT METHOD

Contrary to finite elements, boundary element methods display much smaller pollution error effects with increasing wave numbers. The issue was quantitatively assessed for the problems of scattering acoustic waves on both rigid and elastic spheres in [41,39]. Consequently, estimating the Boundary Element (BE) error with a residual error is subjected to much less severe restrictions in terms of wave number range as for finite elements.

To our best knowledge, the first a posteriori error estimate for rigid scattering problems based on computing L^2-residuals was proposed in [43]. The method was implemented in context of the classical Helmholtz integral equation,

$$\frac{1}{2}\phi - K\phi = \phi^i \,,$$

with ϕ^i and ϕ denoting the incident and total pressure, respectively, and K being the double layer integral operator. Linearity of the equation leads to a simple relation between the error and residual,

$$\frac{1}{2}(\phi - \phi_h) - K(\phi - \phi_h) = r_h := \phi^i - (\frac{1}{2}\phi_h - K\phi_h) \,.$$

For smooth (Hölder continuous) boundaries Γ, the double layer potential is compact in $L^2(\Gamma)$ which implies that the second term will converge to zero faster than the first one. Consequently, we have asymptotically,

$$\|\phi - \phi_h\|_0 \approx 2\|r_h\|_0,$$

where $\|\cdot\|_0$ denotes the L^2-norm. The quality of the L^2-residual error estimator in context of large wave numbers was carefully investigated in [49]. The method remains reliable for large wave numbers and for non-smooth boundaries as well. The last fact was never explained theoretically.

Estimating the L^2-residual can be interpreted as a postprocessing error estimation technique where the exact solution is replaced with a more accurate postprocessed solution,

$$\|\phi - \phi_h\| \approx \|\phi_h^{post} - \phi_h\| \,,$$

with the Sloan's method used to construct postprocessed solution,

$$\phi_h^{post} = 2(\phi^i + K\phi_h) \,.$$

This approach was followed by Walsh and Demkowicz [96] in the context of goal-oriented error estimation for both the primal and dual solutions. The idea is similar to using Babuška's extraction formulas to postprocess FE solution for the sake of error estimation and possibly even mesh optimization, see e.g. [70]. The concept of using postprocessed solutions for error estimation remains an active area of research, see e.g. [88]. Rigorous error estimation for wave propagation problems on non-smooth manifold requires a deep analysis of the underlying functional analysis framework and remains the area of active research, especially for Maxwell equations, see [36,35]. A separate class of issues must be addressed when investigating coupled BE/FE formulations. Depending upon the formulation and order of coupled elements, either BE or FE residuals may dominate, which should be taken into account in a successful a posteriori error estimation scheme, see [40].

8 CONCLUDING REMARKS AND FUTURE WORK

We have presented a review of the state-of-the-art of a posteriori error estimation for acoustic problems. Error estimators are described and classified here according to two distinctive approaches: global norm error estimation and goal-oriented error estimation. In the first approach, the error is estimated with respect to a global norm, based on the H^1-seminorm, in the second approach, with respect to quantities of interest that are predefined by the analyst.

Techniques for global norm error estimation generally rely on residual-type and recovery-type methods. We have seen that these classes of estimators have the tendency to underestimate the true error in the pre-asymptotic range at large wave numbers. This behavior is explained by the fact that such estimators fail to detect the error component due to pollution effects. In the context of a posteriori error estimation, this pollution error is defined as the difference between the exact solution and the "shifted" solution. We have seen here that the shifted solution is nothing else but the Riesz representer of the residual. Since global norm error estimators actually provide estimates of the norm of the residual, we conclude that these methods cannot be robust unless the asymptotic regime is reached. Another way of seeing this is to recall the relationship between the error and the residual:

$$\frac{1}{M}\|\mathcal{R}\|_* \leq |e|_1 \leq \frac{1}{\lambda}\|\mathcal{R}\|_*$$

with M and λ the continuity and inf-sup constants of the bilinear form, respectively. The norm of the residual is a guaranteed upper bound on the error only if $\lambda = 1$ or a reliable estimate of the error if M and λ are both close to unity. For Model Problem 1 presented in this review, we have seen that M and λ were of order k^2 and k^{-1}, respectively, when defined with respect to the H^1-seminorm $|\cdot|_1$. In other words, the constants depart from one as k increases. Unfortunately it is doubtful that other choices of norm would provide continuity and inf-sup constants independent of the wave number; a simple analysis with the k-dependent norm $(|\phi|_1^2 + k^2\|\phi\|_0^2)^{1/2}$ reveals that M and λ are then of order k and k^{-1}. Despite these pessimistic conclusions about global norm error estimation for acoustic problems, research work on the subject should not be considered as hopeless. The 2-grid approach presented in Section 6.2 in the context of the *hp*-methods is certainly a viable approach if the computational cost associated with the fine grid solution can be reduced to a lesser extent. In addition we have seen that the pollution error is intimately related to the dispersive character of the waves. It would certainly be interesting to further investigate whether methods for estimation of the pollution error can be developed, or similarly, whether goal-oriented error estimation can be used to estimate the phase lag between the exact solution and the finite element approximation. Finally, it is noteworthy that more sophisticated PDE models for the study of acoustic problems usually involve an extra term which models the damping of waves. This "viscous" term necessarily entails a stabilizing effect, which in turn implies that the associated inf-sup constant is "bounded below" as k increases. Residual error estimators are thus expected to exhibit better results for these types of problems.

Goal-oriented error estimation is a fairly new technique for a posteriori error estimation and mesh adaptation. Unfortunately few applications have been considered to date for acoustic problems and additional theoretical and computational studies on the subject is needed to better evaluate the great promise of this technique. In particular, it would be instructive to analyze the performance of goal-oriented estimators for large wave numbers (i.e. to check whether the method is sensitive to pollution error) and for various types of quantities of

interest. It would be also interesting to experiment with goal-oriented mesh adaptivity and investigate the increase in the rate of convergence at which specific features of the solution would be attained. This aspect is of paramount importance for acoustic problems as simulations are often limited due to the restriction $k^2h \leq 1$. Work on goal-oriented $h-p$ adaptivity for electromagnetic wave problems have already shown superior performance and accuracy over traditional approaches.

Acknowledgment The support of this work by the Office of Naval Research under Contract N00014-95-0401 is greatfully acknowledged.

A APPENDIX

For completeness of the presentation, we collect here proofs of some theorems presented in the review.

A.1 Proof of Theorem 2.

Theorem 2. *Let $\phi_h \in V^h$ be the solution of the finite element problem (20). Then the residual $\mathcal{R}_1(v) = F_1(v) - B_1(\phi_h, v)$ satisfies*

$$\|\mathcal{R}_1\|_* \leq \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2} \tag{104}$$

where h_K is the size of each element K in the mesh.

Proof. From the definition of $F_1(v)$ and $B_1(\phi_h, v)$, we can write for an arbitrary $v \in V$

$$\mathcal{R}_1(v) = \int_\Omega f\bar{v}\,dx - \int_\Omega \phi_h'\bar{v}'\,dx + k^2 \int_\Omega \phi_h\bar{v}\,dx + ik\phi_h(1)\bar{v}(1)$$

Decomposing the domain integrals into element integrals, and using integration by parts:

$$\begin{aligned}
\mathcal{R}_1(v) &= \sum_K \left(\int_K f\bar{v}\,dx - \int_K \phi_h'\bar{v}'\,dx + k^2 \int_K \phi_h\bar{v}\,dx \right) + ik\phi_h(1)\bar{v}(1) \\
&= \sum_K \left(\int_K f\bar{v}\,dx + \int_K \phi_h''\bar{v}\,dx + k^2 \int_K \phi_h\bar{v}\,dx \right) - \sum_K (\phi_h'\bar{v})|_{x_1}^{x_2} + ik\phi_h(1)\bar{v}(1) \\
&= \sum_K \int_K \left(f + \phi_h'' + k^2\phi_h\right)\bar{v}\,dx \\
&\qquad + \phi_h'(0)\bar{v}(0) + \sum_{j=1}^{N-1} (\phi_h'(x_j^+) - \phi_h'(x_j^-))\bar{v}(x_j) - (\phi_h'(1) - ik\phi_h(1))\bar{v}(1)
\end{aligned}$$

Let $v_I \in V^h$ be the piecewise linear interpolant of v. From the orthogonality property, i.e. $\mathcal{R}_1(v_I) = 0$, and the fact that $(v - v_I)(x_j) = 0$, $j = 0, \ldots, N$, we have

$$\mathcal{R}_1(v) = \mathcal{R}_1(v - v_I) = \sum_K \int_K (f + \phi_h'' + k^2\phi_h)(\bar{v} - \bar{v}_I)\,dx$$

By Cauchy-Schwarz, and using the definition $r_K = f + \phi_h'' + k^2\phi_h$,

$$|\mathcal{R}_1(v)| \leq \sum_K \|r_K\|_{0,K}\|v - v_I\|_{0,K}$$

and using the fact that $\|v - v_I\|_{0,K} \leq h_K|v - v_I|_{1,K} \leq h_K|v|_{1,K}$, on each element K, we arrive at:

$$|\mathcal{R}_1(v)| \leq \sum_K h_K\|r_K\|_{0,K}|v|_{1,K} \leq \sqrt{\sum_K h_K^2\|r_K\|_{0,K}^2}\sqrt{\sum_K |v|_{1,K}^2}$$

Since $\sqrt{\sum_K |v|_{1,K}^2} = |v|_1$, we finally have:

$$\|\mathcal{R}_1\|_* = \sup_{v\in V\setminus\{0\}} \frac{|\mathcal{R}_1(v)|}{|v|_1} \leq \sqrt{\sum_K h_K^2\|r_K\|_{0,K}^2}$$

which is exactly what was to be proved. □

A.2 Proof of Theorem 3.

Theorem 3. *Let $\phi_h \in V^h$ be the finite element approximation of Problem (53). Then the dual norm of the residual $\mathcal{R}(v) = F(v) - A(\phi_h, v)$ defined with respect to the H^1-seminorm satisfies*

$$\|\mathcal{R}\|_* \leq C\sqrt{\sum_K h_K^2\|r_K\|_{0,K}^2 + h_K\|j_{\gamma,K}\|_{0,\partial K}^2} \tag{105}$$

where C is a constant independent of the discretization parameters h_K and the wave number k.

Proof. The residual fonctional $\mathcal{R}(v) = F(v) - A(\phi_h, v)$, where ϕ_h is a finite element approximation of Problem (53) in a suitable finite element space V^h, reads:

$$\mathcal{R}(v) = \int_\Omega f\bar{v}\,dx - \int_\Omega \nabla\phi_h\cdot\nabla\bar{v}\,dx + k^2\int_\Omega \phi_h\bar{v}\,dx + ik\int_{\Gamma_R}\phi_h\bar{v}\,ds$$

Integrating by parts the second integral over each element of the mesh gives

$$\mathcal{R}(v) = \sum_K \int_K (f + \Delta\phi_h + k^2\phi_h)\bar{v}\,dx - \sum_K\int_{\partial K}\partial_n\phi_h\bar{v}\,ds + ik\int_{\Gamma_R}\phi_h\bar{v}\,ds$$

Thus, using the definitions of the interior residuals r_K and boundary residuals $j_{\gamma,K}$, the expression for the residual reduces to:

$$\mathcal{R}(v) = \sum_K\int_K r_K\bar{v}\,dx - \sum_K\int_{\partial K} j_{\gamma,K}\bar{v}\,ds.$$

By the orthogonality property, i.e. $\mathcal{R}(v_h) = 0$ with v_h any arbitrary function in V^h, and by the Cauchy-Schwarz inequality, we have:

$$|\mathcal{R}(v)| \leq \sum_K \|r_K\|_{0,K}\|v - v_h\|_{0,K} + \sum_K \|j_{\gamma,K}\|_{0,\partial K}\|v - v_h\|_{0,\partial K}$$

In order to proceed, we need bounds on $\|v - v_h\|_{0,K}$ and $\|v - v_h\|_{0,\partial K}$. For that purpose, let $v_h = \mathcal{I}_h v$, where $\mathcal{I}_h : V \to V^h$ is a linear bounded operator such that (see Ainsworth and Oden [5]):

$$\|v - \mathcal{I}_h v\|_{0,K} \leq C h_K |v|_{1,\tilde{K}}$$
$$\|v - \mathcal{I}_h v\|_{0,\gamma} \leq C h_K^{1/2} \|v\|_{1,\tilde{K}}$$

where C is a positive constant which depends only on the regularity of the partition, γ any edge (or face) of K, $h_K = \text{dia}(K)$, and $\tilde{K}$ denotes the patch of elements associated with K. We then obtain:

$$\begin{aligned}
|\mathcal{R}(v)| &\leq C \sum_K h_K \|r_K\|_{0,K} |v|_{1,\tilde{K}} + h_K^{1/2} \|j_{\gamma,K}\|_{0,\partial K} \|v\|_{1,\tilde{K}} \\
&\leq C \sum_K \sqrt{h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2} \sqrt{|v|_{1,\tilde{K}}^2 + \|v\|_{1,\tilde{K}}^2} \\
&\leq C \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2} \sqrt{\sum_K |v|_{1,\tilde{K}}^2 + \|v\|_{1,\tilde{K}}^2}
\end{aligned}$$

Nothing that the last quantity is bounded by $\|v\|_1$ (within a constant) and using Poincaré's inequality, i.e. $\|v\|_1 \leq C|v|_1$, we finally obtain:

$$\|\mathcal{R}\|_* = \sup_{v \in V \setminus \{0\}} \frac{|\mathcal{R}(v)|}{|v|_1} \leq C \sqrt{\sum_K h_K^2 \|r_K\|_{0,K}^2 + h_K \|j_{\gamma,K}\|_{0,\partial K}^2}$$

which completes the proof. □

A.3 Proof of Theorem 4.

Theorem 4. *For each element K in the partition, let $\varphi_K \in V_K$ denote the solution of the local problem:*

$$(\varphi_K, v)_{1,K} = \mathcal{R}_{1,K}(v) + \int_{\partial K} g_K v \, ds, \qquad \forall v \in V_K, \tag{106}$$

where the flux functions g_K satisfy

$$\sum_K \int_{\partial K} g_K v_{|_K} \, ds = 0, \qquad \forall v \in V. \tag{107}$$

Define $\varphi \in$ such that $\varphi_{|_K} = \varphi_K$. Then, the function φ provides an upper bound on the residual:

$$\|\mathcal{R}_1\|_* \leq |\varphi|_{1,\mathcal{P}_h} = \sqrt{\sum_K (\phi_K, \phi_K)_{1,K}}. \tag{108}$$

Proof. Starting from the definition of the residual, using condition (107), applying the fact that $V \subset V(\mathcal{P}_h)$, and, finally, using (106) on each element, we have

$$\begin{aligned}
\|\mathcal{R}_1\|_* &= \sup_{v\in V\setminus\{0\}} \frac{|\mathcal{R}_1(v)|}{\|v\|_1} = \sup_{v\in V\setminus\{0\}} \frac{|\sum_K \mathcal{R}_{1,K}(v_{|_K})|}{\|v\|_1} \\
&= \sup_{v\in V\setminus\{0\}} \frac{|\sum_K \mathcal{R}_{1,K}(v_{|_K}) + \sum_K \int_{\partial K} g_K v \; ds|}{|v|_{1,\mathcal{P}_h}} \\
&\leq \sup_{v\in V(\mathcal{P}_h)\setminus\{0\}} \frac{|\sum_K (\mathcal{R}_{1,K}(v_{|_K}) + \int_{\partial K} g_K v \; ds)|}{|v|_{1,\mathcal{P}_h}} \\
&\leq \sup_{v\in V(\mathcal{P}_h)\setminus\{0\}} \frac{\sum_K |(\varphi_K, v_{|_K})_{1,K}|}{|v|_{1,\mathcal{P}_h}} \\
&\leq \sup_{v\in V(\mathcal{P}_h)\setminus\{0\}} \frac{\sum_K \sqrt{(\varphi_K,\varphi_K)_{1,K}}\sqrt{(v_{|_K},v_{|_K})_{1,K}}}{|v|_{1,\mathcal{P}_h}} \\
&\leq \sup_{v\in V(\mathcal{P}_h)\setminus\{0\}} \frac{|\varphi|_{1,\mathcal{P}_h}|v|_{1,\mathcal{P}_h}}{|v|_{1,\mathcal{P}_h}} \leq |\varphi|_{1,\mathcal{P}_h}
\end{aligned}$$

which is the stated result. □

A.4 Proof of Theorem 5.

Theorem 5. *With the definitions and assumptions of Section 4.3.2,*

$$\|\mathcal{R}_1\|_* \leq \sqrt{\sum_{i\leq i\leq N} (\xi_i,\xi_i)_{1,\phi_i}}. \tag{109}$$

Proof. Using the definitions and assumptions of Section 4.3.2, we have for all $v \in V$

$$\begin{aligned}
\mathcal{R}_1(v) &= \sum_{1\leq i\leq N} \mathcal{R}(v\phi_i) = \sum_{1\leq i\leq N} (\xi_i, v)_{1,\phi_i} \\
&\leq \sum_{1\leq i\leq N} \sqrt{(\xi_i,\xi_i)_{1,\phi_i}}\sqrt{(v,v)_{1,\phi_i}} \\
&\leq \sqrt{\sum_{1\leq i\leq N} (\xi_i,\xi_i)_{1,\phi_i}}\sqrt{\sum_{1\leq i\leq N} (v,v)_{1,\phi_i}}.
\end{aligned}$$

Taking $v = e$ in the previous inequality and noticing that $\sum_{1\leq i\leq N}(v,v)_{1,\phi_i} = (v,v)_1$, we obtain

$$\frac{|\mathcal{R}_1(v)|}{|v|_1} \leq \sqrt{\sum_{1\leq i\leq N} (\xi_i,\xi_i)_{1,\phi_i}}.$$

This completes the proof since the inequality holds for all $v \in V$. □

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