Computer Assisted Mechanics and Engineering Sciences, 4: 397–415, 1997.

Solution of Helmholtz problems by knowledge-based FEM

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(Received December 20, 1996)

The numerical solution of Helmholtz' equation at large wavenumber is very expensive if attempted by "traditional" discretisation methods (FDM, standard Galerkin FEM). For reliable results, the mesh has to be very fine. The bad performance of the traditional FEM for Helmholtz problems can be related to the deterioration of stability of the Helmholtz differential operator at high wavenumber. As an alternative, several non-standard FEM have been proposed in the literature. In these methods, stabilisation is either attempted directly by modification of the differential operator or indirectly, via improvement of approximability by the incorporation of particular solutions into the trial space of the FEM. It can be shown that the increase in approximability can make up for the stability loss, thus improving significantly the convergence behavior of the knowledge based FEM compared to the standard approach. In our paper, we refer recent results on stability and convergence of h- and h-p-Galerkin ("standard") FEM for Helmholtz problems. We then review, under the label of "knowledge-based" FEM, several approaches of stabilised FEM as well as high-approximation methods like the Partition of Unity and the Trefftz method. The performance of the methods is compared on a two-dimensional model problem.

1. Introduction

Due to the oscillatory character of the propagating solutions, reliable numerical methods for Helmholtz' equation

$$\Delta u + k^2 u = 0$$

become prohibitively expensive as wavenumber k grows. It is known from computational practice [8, 9, 15, 12] that the mesh has to be very fine for convergence of standard piecewise linear Galerkin FEM or FDM. In view of this, various methods have been designed that incorporate specific information about the differential operator or the exact solution ("knowledge") into the approximate solution. In this paper, we consider several of these methods on the background of the h- and h-p-FEM for Helmholtz problems.

Our analysis in [15, 17, 18] has shown that the poor performance of standard FEM at large wavenumber can be quantified by the pollution effect in the finite element error. The pollution term is related to the deterioration of stability of the Helmholtz variational form at large wavenumber.

It is well known that both stability and approximability are necessary conditions for convergence of any numerical method for PDE. Generally speaking, we approximate the solution $u \in V$ of

$$\forall v \in V: \qquad B(u,v) = F(v) \tag{1}$$

by restricting the problem (1) to a subspace $V_h \subset V$. Here, h is a parameter that is inversely proportional to the dimension of V_h. We measure *approximability* of the method in terms of the minimal error with which the solution u (if it were known) can be approximated by functions $\chi \in V_h$, defining

$$e_{ba} := \inf_{v \in V_h} \|u - \chi\|. \tag{2}$$

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This error is related only to the spaces V and V_h; it does not depend on the particular problem to solve, i.e., on the variational form B. If the infimum in (2) is reached on a unique function $\chi^* \in V_h$ then this function is called the *best approximation* of u in V_h.

On the other hand, the approximate solution of (1) is the function $u_h \in V_h$ for which $B(u_h, v_h) = F(v_h)$ holds for all $v_h \in V_h$. We say that the numerical method is *optimal* if $u_h = \chi^*$. Generally, this is not the case. The relation

$$\frac{\|u - u_h\|_V}{\inf\limits_{v \in V_h} \|u - \chi\|_V} = C(B, \|\cdot\|, h, u)$$

depends, in general, on the variational form B, on the norm of V, the choice of the subspace and also on the exact solution u. If there exists a maximal w.r. to u constant $C_s = \sup\limits_{u \in V} C$ then we have

$$\|u - u_h\|_V \le C_s \inf_{\chi \in V_h} \|u - \chi\|_V \,. \tag{3}$$

If, in addition, one can show that the *stability constant* C_s that does not depend on h then *approximability* $\inf \|u - \chi\| \to 0$ as $h \to 0$ guarantees *convergence* $\|u - u_h\| \to 0$.

Note that the stability constant C_s always depends on the variational form. If, for some particular variational form, constant C_s is very large, then convergence in practice (i.e., for finite h) will be slow despite approximability. This is exactly the case for Helmholtz' equation where $C \sim k$. From (3) we see that one has two options to improve convergence. Firstly, modification of the variational form with the goal to reduce the size of the stability constant or, secondly, the choice of the subspace V_h such that the error of approximation is small enough to equilibrate the adverse effect of poor stability (large C_s).

Methods of both kind have been proposed for the numerical solution of Helmholtz' equation. We treat these methods that employ specific information on the Helmholtz operator in the solution process under the common notion of "knowledge-based" FEM.

In the *stabilized* FEM, one modifies the variational form (and, accordingly, the right hand side) in such a way that the new variational form is coercive. The stabilized solution then satisfies (3) with a constant C_s not growing with wavenumber k. The delicate point is to choose the stabilisation term in such a way that it does not adversely influence the consistency of the method. We consider here the Galerkin-Least Squares FEM [13] and the stabilized FEM introduced in [7, 2].

Alternatively, methods have been designed that incorporate analytical information on exact solutions of Helmholtz' equation to enhance approximability of the discrete subspace.

We show that the stabilized FEM of Babuška and Sauter can be interpreted as a Galerkin FEM with analytical shape functions. However, this approach is confined to rectilinear meshes. An efficient way to use the analytical solutions in the Galerkin FEM on general mesh has recently been designed in the form of the Partition of unity method (PUM) [21]. Here, one uses standard piecewise linear shape functions for geometric approximation on irregular mesh. The patch-functions form a partition of unity that is overlayed with local approximating sets of particular solutions. Thus the approximation properties of the FEM are significantly enhanced, retaining at the same time the flexibility in shape approximation. Analytical solutions of the differential equation are traditionally used in the Trefftz-method, where the unknown coefficients are resolved on the boundary of the domain only (or, in addition, on the boundaries between superelements in the TFEM).

In this paper, we review the methods and compare their performance in numerical computations for a 2D on a model problem. We choose the problem of [2] where we analyzed numerically the various stabilized methods. The same problem was subsequently used in [22] to evaluate the PUM.

The paper is organized as follows. In Section 2, we use a simple one-dimensional model problem to expose the specifics of approximability, stability and convergence of FEM for Helmholtz problems. In Section 3, we elaborate on the application of the various methods in two dimensions. In Section 4, we compare the numerical performance of the methods on a two-dimensional model problem. The conclusions of the investigation are listed in Section 5.

2. Standard and knowledge-based FEM on a one-dimensional example

We consider the following model problem:

$$-\frac{d^2u}{dx^2}(x) - k^2u(x) = f(x)\,, \qquad x \in \Omega = (0,1) \tag{4}$$

with boundary conditions

$$u(0) = 0\,, \qquad \frac{du}{dx}(1) - iku(1) = 0\,.$$

This model problem has the essential properties (dependency on the physical parameter k and radiation damping from the Sommerfeld-type condition at $x = 1$) of the higher-dimensional case. We will thus be able to show some of the general numerical effects of the various FEM on the most simple case. However, the model is very special for the knowledge-based approaches since the fundamental system in 1D consists of only two linearly independent homogeneous solutions whereas this system is infinite-dimensional in the general case. Still, the problem is well-suited to explain the principal ideas on a simple example.

In discrete methods for Helmholtz' equation, resolution of a wave by the mesh is a critical issue. Consider a stationary sinusoidal wave $u(x)$ of wavelength $\lambda = 2\pi/k$, then the number

$$n = \frac{\lambda}{h}$$

is called the *resolution* of the wave $u(x)$ by a mesh of stepsize h. In the context of finite difference or piecewise linear finite element methods, it is customary to call $n = 2$ the *minimal resolution* of the wave. The value $n = 10$ [13], sometimes also $n = 6$ [9] is recommended as a "rule of thumb" in computational practice. These recommendations are obvious for piecewise linear approximation. It is, however, expected that the mesh-size could be increased for higher-order approximation, be it by h-p-Galerkin or other methods. This increase of mesh-size and thus reduction in DOF should also "make up" for the increased costs of development, computational implementation or evaluation that come, in general, with the higher-order methods — see [17] for an analysis of computational cost in h-p FEM.

2.1. Error estimates for h-p-FEM solutions to Helmholtz problems

To solve the model problem by a Galerkin FEM we start from the weak formulation

$$B_G(u,v) = F_G(v)\,, \tag{5}$$

where the sesquilinear form B_G is given by

$$B_G(u,v) = (u',v') - k^2(u,v) - ik\langle u,v\rangle \tag{6}$$

and the right-hand side is

$$F_G(v) = (f,v). \tag{7}$$

We use the notation of the L^2 inner product

$$(u,v) = \int_0^1 u\bar{v}\,\mathrm{d}x$$

and

$$\langle u,v\rangle = u(1)\bar{v}(1)\,.$$

We define in the usual way the Sobolev spaces $H^s(\Omega), \Omega := (0,1)$ with the norms $\|\cdot\|_s$. Specifically, $\|u\|_o = (u,u)^{1/2}$ is the L^2-norm and $(u',u')^{1/2}$ is the H^1-seminorm which is norm on the subspace $V = \{u \in H^1(\Omega) | u(0) = 0\} \subset H^1(\Omega)$. For $f \in L^2(\Omega)$, there exists a unique solution u of the variational problem: Find $u \in V$ such that $B_G(u,v) = F_G(v)$ for all $v \in V$. This solution u lies in the space $H^2(\Omega)$ and solves the boundary value problem (4).

For the numerical solution, we introduce a FE-partition $\{\Delta_i\}_1^N$ of the interval Ω into N subintervals (elements) and define the mesh-size $h = \max_i |\Delta_i|$. The FE-solution is sought as a continuous function u_h that on each element can be written as a polynomial of order p and satisfies the essential boundary condition at $x = 0$. These functions form a subspace $V_h \subset V$ and the FE-solution is then found from the variational problem: Find $u_h \in V_h$ s.t. $B_G(u_h, v_h) = F_G(v_h)$ for all $v_h \in V_h$.

We showed in [15] that, for the standard Galerkin FEM with piecewise linear approximation ($p = 1$),

(1h) the quasioptimal estimate

$$|u - u_h|_1 \le C \inf_{\chi \in V_h} |u - \chi|_1, \tag{8}$$

where C does not depend on k, h, holds only under the assumption that $k^2 h \ll 1$;

(2h) in general, i.e., with the 'rule of thumb' $kh = const.$, the error bounds in H^1-norm or L^2-norm, respectively, are

$$\frac{|u - u_h|_1}{|u|_1} \le C_1 kh + C_2 k^3 h^2\,, \tag{9}$$

$$\frac{\|u - u_h\|}{\|u\|} \le C_3 k^2 h^2 (1 + k)\,. \tag{10}$$

On the other hand, Eq. (8) yields for the relative error

$$\frac{|u - u_h|_1}{|u|_1} \le Ckh.$$

The comparison with Eq. (10) leads to the notion of *numerical pollution* introduced in [7]. The second term of estimate (10) is called the pollution term of the FE-error for Helmholtz' equation. It has been shown in numerical experiments by several authors [8, 9, 15, 2, 12] that pollution significantly increases the error of the finite element solution computed by the rule of thumb if the wavenumber grows. Physically, this effect can be related to the phase lag of the FE-solution [15, 18].

For piecewise polynomial approximation, it is shown in [17] that

(1p) the quasioptimal estimate (8) holds if $k^2 h/p$ is small;

(2p) If $hk < \pi$ and the solution u is sufficiently smooth then the relative error in H^1-norm satisfies

$$\frac{|u - u_{hp}|_1}{|u|_1} \le C_1 \left(\frac{kh}{p}\right)^p + C_2 k \left(\frac{kh}{p}\right)^{2p}\,. \tag{11}$$

Remark 1: From the well-known theory of h-p approximability, the error of best approximation of any function $u \in H^{s+1}(\Omega)$ in the h-p subspaces is given by

$$\inf \|u - \chi\|_1 \le C \left(\frac{h}{p}\right)^s \|u\|_{s+1}$$

for $s \le p$. Taking the special case $s = p$ and assuming that $\|u\|_{s+1} / \|u\|_1 \sim k^s$ we see that the first term on the rhs of (11) measures approximability. Approximability is thus improved by increasing

p for fixed kh. The second term of the right hand side can be read as wavenumber times (error of approximation) squared. Hence, in improving approximability by increasing p we decrease at the same time the pollution term, i.e., correct the adverse effect of poor stability.

Remark 2: In the special case of the one-dimensional model problem, the analytical solutions are $\{\sin kx, \cos kx\}$. This local basis can be considered as the limiting case $p \to \infty$ of p-elements. Looking under this aspect at estimate (11) we see that pollution becomes negligible for large p. Indeed, $k^2h/p \to 0$ for any fixed h, k as $p \to \infty$. Hence we expect that, by using analytical solutions as trial functions, the pollution effect is eliminated.

2.2. Stabilized FEM for Helmholtz' equation

The pollution effect in the standard Galerkin FEM is related to the degrading stability of the Helmholtz differential operator with growing k. The Babuška-Brezzi (BB-) constant of the variational form

$$\gamma = \inf_{u \in V} \sup_{v \in V} \frac{|B(u,v)|}{|u|_1 |v|_1}$$

is of order k^{-1} — cf. [15, 11]. A standard corollary [1] then yields

$$|u|_1 \leq Ck\|f\|_{-1} \,,$$

where $\|\cdot\|_{-1}$ is the norm of the dual space. In particular, the FE-error solves the residual equation and we have $|e|_1 \leq Ck\|r\|_{-1}$, where r is the residual error, characterizing the quality of approximation. The estimate shows that the FE-error can be large for large k even if the optimal approximation error is small. This observation has given rise to the idea of stabilization for Helmholtz problems. We treat these ideas on the example of the Galerkin-Least Squares (12) method — see, e.g., [13]. In this method, we solve instead of the variational problem (5) the modified problem: Find $u_h \in V_h$ such that

$$\forall v_h \in V_h : \quad B_{GLS}(u_h, v_h) = F_{GLS}(v_h) \tag{12}$$

with

$$B_{GLS}(u_h, v_h) = B_G(u_h, v_h) + \tau\,(\mathcal{L}u_h, \mathcal{L}v_h)_{\tilde{\Omega}} \tag{13}$$

and the right-hand side is

$$F_{GLS}(v) = F_G(v) + \tau\,(f, \mathcal{L}v_h)_{\tilde{\Omega}} \,, \tag{14}$$

where $\mathcal{L}$ is the Helmholtz differential operator, τ is a parameter yet to be determined and $(\cdot,\cdot)_{\tilde{\Omega}}$ is the reduced L^2 inner product where integration is carried out only on the element interiors. We remark that the singularities in $\mathcal{L}u_h$, $\mathcal{L}v_h$ at interelement boundaries are suppressed in the reduced inner product. The goal is to make, by appropriate choice of parameter τ, the form B_{GLS} unconditionally stable and thus to "circumvent the BB-condition", i.e., to avoid the stability problems of the form B_G as quantified by the BB-condition.

For a one-dimensional model problem similar to (4) it is shown in [13] that the choice

$$\tau = \frac{(kh)^2 - 6\dfrac{1-\cos kh}{2+\cos kh}}{k^4h^2} \tag{15}$$

leads to nodally exact solutions (using piecewise linear ansatz-functions for test and trial) for the homogeneous difference equations obtained from (12) if $f \equiv 0$. More precisely, it is shown that the solution of Eq. (12) coincides in the nodal points of a uniform infinite mesh (i.e., disregarding the boundary conditions an 0 and 1) with an exact solution of Helmholtz equation (4). Consequently, the stabilized FEM is not polluted in this case since the GLS-solution has no phase lag — [2]. The error then satisfies the optimal estimate (8) for all k, h such that the mesh is at least minimally resolving the exact wave.

Remark 3: It is essential that τ is not selected too large. For instance, one could select τ in such a way that the stabilization term in all elements annihilates the mass matrix. While this would certainly render a stable sesquilinear form the solution of the problem would converge to a solution of the Poisson equation instead of Helmholtz' equation.

Remark 4: The following simple argument shows where the condition on k^2h is "hidden" in the GLS-FEM. Expanding the cosines in (15) into Taylor series we see that

$$\tau = \frac{h^2}{12} + O(k^2h^4).$$

Since the Helmholtz operator $\mathcal{L}$ is of order k^2, the stabilizing term $\tau(\mathcal{L}u_h, \mathcal{L}v_h)_{\tilde{\Omega}}$ in (13) is of order $(k^2h)^2$. Consequently, if k^2h is small the form (12) can be considered identical to (5).

The parameter τ in (15) is found from discrete Fourier analysis of the Helmholtz stiffness matrix. A typical stencil of this matrix is

$$(2\alpha_G + 1)u_{j-1} + 2(4\alpha_G - 1)u_j + (2\alpha_G + 1)u_{j+1} \tag{16}$$

with $\alpha_G := (kh)^2/12$. It can be shown (see, e.g., [15]) that this stencil produces a FE-solution with discrete wavenumber $\tilde{k}$ satisfying

$$\cos \tilde{k}h = \frac{1 - 4\alpha_G}{1 + 2\alpha_G}.$$

Hence replacing α_G in (16) by a parameter α_{EX} such that

$$\cos kh = \frac{1 - 4\alpha_{EX}}{1 + 2\alpha_{EX}}$$

leads to a nodally exact discrete solution. On the other hand, the Galerkin-FEM discretisation of stabilized Eq. (12) also yields stencils (16) only that α_G is replaced by $\alpha_{GLS} := \alpha_G\,(1 - \tau k^2)$. Thus we find the optimal τ by putting $\alpha_{GLS} = \alpha_{EX}$.

A new stabilized method that leads to nodally exact solutions also on nonuniform mesh has been proposed in [7]. In this generalized FEM, the nodal values of the approximate solution u_h are computed from the algebraic system

$$\mathbf{G}^{\text{stab}}\mathbf{u}_h = Q^{\text{stab}}(f)\,, \tag{17}$$

where $\mathbf{u}_h$ is the vector of nodal values of the function u_h on the (possibly non-uniform) mesh X_h, the FE-stiffness matrix $\mathbf{G}^{\text{stab}}$ is the triangular matrix defined by

$$G_{ij} = \frac{k^2h}{2\tan\dfrac{kh}{2}} \begin{cases} \dfrac{\sin k(x_{i+1} - x_{i-1})}{\sin(x_{i+1} - x_i)\sin k(x_i - x_{i-1})} & \text{if} \quad i = j\,, \\ -\dfrac{1}{\sin k|x_i - x_j|} & \text{if} \quad i = j\,, \\ 0 & \text{else} \end{cases} \tag{18}$$

and the mapping Q^{stab} is defined by

$$\left(Q^{\text{stab}} f\right)_i = \frac{h}{2\tan\frac{kh}{2}} \sum_{m=i}^{i+1} \frac{\tan\frac{k(x_m - x_{m-1})}{2}}{x_m - x_{m-1}} \frac{\int_{x_{m-1}}^{x_m} f(x)\,\mathrm{d}x}{x_m - x_{m-1}}. \tag{19}$$

In [7], it is proven that the solution u_h obtained from (17) is nodally exact for piecewise constant data and that it is pollution-free for any data $f \in H^1(\Omega)$. We will show below that this stabilized solution is equivalently obtained from a Galerkin FEM with analytical shape functions. This establishes an interesting connection between stabilization and improved approximation, both leading to better (in this 1D case: optimal) convergence properties.

Consider the nodal functions Φ_i of the form

$$\Phi_i = \begin{cases} t_1^{(i)} & \text{on} \quad \Delta_i\,, \\ t_2^{(i-1)} & \text{on} \quad \Delta_{i-1}\,, \\ 0 & \text{else}\,, \end{cases} \tag{20}$$

where the functions t_1, t_2 are shape functions satisfying the local BVP

$$t'' + k^2 t = 0 \quad \text{on} \;\; \Delta_j \tag{21}$$

with inhomogeneous local Dirichlet data

$$t_1(x_{j-1}) = 1, \quad t_1(x_j) = 0 \tag{22}$$

or

$$t_2(x_{j-1}) = 0, \quad t_2(x_j) = 1, \tag{23}$$

respectively. In Fig. 1, we show the function Φ_i. For comparison, we also show the H^1-approximation in the usual hierarchic Lengendre-based polynomial spaces. We choose a "superelement" of size $h = 5\lambda/\pi$ and illustrate the approximation for $p = 2$, $p = 3$, resp.

The trial functions for the Galerkin FEM are written in the standard way as a linear combination of nodal functions

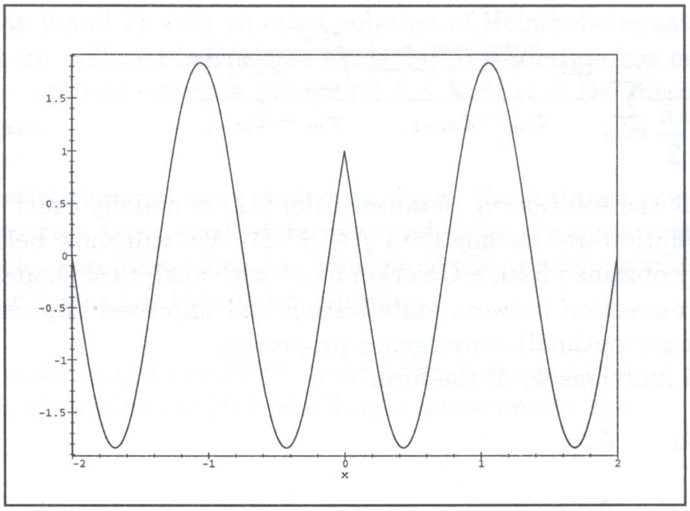
$$u_h(x) = \sum_{i=1}^{N} u_i \Phi_i(x)\,, \tag{24}$$

where u_i are the unknown nodal values of the function u_h. The connection between stabilisation and higher approximating FEM is given in

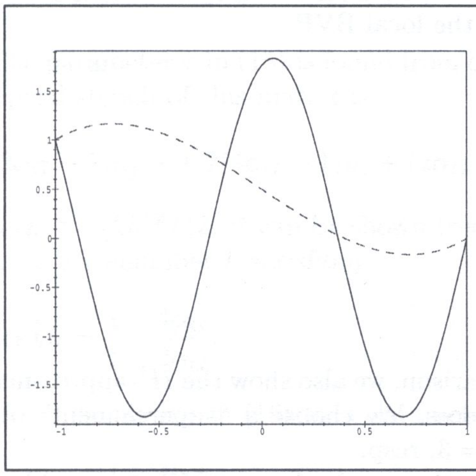
Proposition 1 *Let X_h be a finite element mesh on $\Omega = (0,1)$ and let $u_h(x)$ be given by Eq. (24). Then, for the interior mesh-points, the matrix for determination of the nodal values $\{u_i\}$ of $u_h(x)$ is identical with the matrix $\mathbf{G}_{\text{stab}}$ defined in (18). For piecewise constant data $f \in L^2(\Omega)$, the analytical shape functions yield the image $(Q^{\text{stab}} f)_i$.*

Proof: The proof is obtained by simple computation. Let t_1, t_2 be the solutions of (21) with boundary conditions (22) and (23), respectively. Then the matrix coefficient G_{ii-1} is

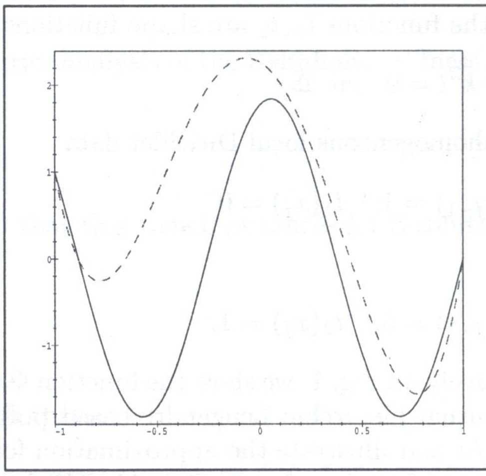
$$\begin{aligned} G_{ii-1} &= \frac{2}{x_i - x_{i-1}} \int_{-1}^{1} t_1' t_2' - \frac{x_i - x_{i-1}}{2} k^2 \int_{-1}^{1} t_1 t_2 \\ &= \frac{k}{\sin k(x_i - x_{i-1})}\,. \end{aligned}$$



a) Patch-function from exact solution



b) Shape-functions: exact vs. $p = 2$ (dashed)



c) Shape-functions: exact vs. $p = 3$ (dashed)

Fig. 1. Exact patch-function and exact shape-function compared to p-approximations

Similarly, we get

$$\begin{aligned} G_{ii} &= \frac{2}{x_i - x_{i-1}} \int_{-1}^{1} (t_2')^2 - \frac{x_i - x_{i-1}}{2} k^2 \int_{-1}^{1} (t_2)^2 \\ &\quad + \frac{2}{x_{i+1} - x_i} \int_{-1}^{1} (t_1')^2 - \frac{x_{i+1} - x_i}{2} k^2 \int_{-1}^{1} (t_1)^2 \\ &= \frac{k \sin k(x_{i+1} - x_{i-1})}{\sin k(x_i - x_{i-1}) \sin k(x_{i+1} - x_i)} . \end{aligned}$$

For the right hand side, we integrate

$$\frac{2}{x_i - x_{i-1}} \int_{-1}^{1} f t_1 + \frac{2}{x_{i+1} - x_i} \int_{-1}^{1} f t_2 = \frac{2}{k} \left(\frac{\tan k(x_i - x_{i-1})}{x_i - x_{i-1}} \frac{\int_{x_{i-1}}^{x_i} f}{x_i - x_{i-1}} + \frac{\tan k(x_{i+1} - x_i)}{x_{i+1} - x_i} \frac{\int_{x_i}^{x_{i+1}} f}{x_{i+1} - x_i} \right) .$$

Equations (18, 19) are then obtained if we multiply by a scaling factor. ◁

Remark 5: The matrix $\mathbf{G}_{\text{stab}}$ can also be regarded as the limiting case $p \to \infty$ of the condensed *h-p*-matrix for Helmholtz' equation. Indeed the *h-p*-shape functions are the Galerkin solutions of BVP (21;22) or (21;23), resp. — see also [17], proof of Theorem 3.2.

For higher-dimensional problems, stabilization is a more complicated issue — we will return to the topic in the next section.

2.3. Incorporation of particular solutions: Trefftz method

The idea of the Trefftz method [10, 26] is to find the weak solution of a boundary value problem in a class of functions that satisfy the differential equation but do not, in general, satisfy the boundary conditions of a boundary value problem (BVP). Those are included into the weak form as Lagrange multipliers. The approximate solution of the BVP is thus found from boundary integral equations, resulting from variation of the weighted residuals on the boundary of the domain. In the Trefftz FEM, this idea is extended to a partition of the solution domain into finite elements. Again the "shape-functions" satisfy the differential equation on each element; the boundary conditions and the interelement continuity are then enforced in the weak form, yielding the set of determining equations for the unknown coefficients in the trial functions.

Let us illustrate the idea on the one-dimensional model problem. As already observed, the application is somewhat trivial since the differential equation in this case has only two linearly independent particular solutions. Consider the problem

$$-u'' - k^2 u = f$$

with inhomogeneous Dirichlet and radiation boundary conditions

$$u(0) = \hat{u}\,, \qquad u'(1) - iku(1) = 0.$$

The Dirichlet condition is included in the variational form by Lagrange multiplier, yielding

$$B^*(u,v) = \int_0^1 \left(u'\bar{v}' - k^2 u\bar{v}\right) \mathrm{d}x + \lambda(u(0) - \hat{u}) + iku(1)\bar{v}(1) = \int_0^1 f\bar{v}\,\mathrm{d}x\,.$$

Integrating by parts, we obtain

$$\int_0^1 \left(-u'' - k^2 u - f\right) \bar{v}\,\mathrm{d}x + \lambda(u(0) - \hat{u}) + \chi\bar{v}(0) + (u'(1) - iku(1))\,\bar{v}(1) = 0\,,$$

where we replaced $\chi = u'(0)$. Suppose we use the trial function

$$u = u_H + u_p = \sum_{i=1}^{M} a_i \Phi_i + u_p\,,$$

where Φ_i are homogeneous solutions of Helmholtz' equation and u_p is a *known* particular solution of the inhomogeneous equation. Then the "domain" integral vanishes identically and the variational problem is stated as: Find $(u_H, \chi) \in V_1$ such that

$$B_T(u_H, \chi, v, \lambda) = \lambda u_H(0) + \chi\bar{v}(0) + (u_H'(1) - iku_H(1))\,\bar{v}(1) = F(v, \lambda)$$

with

$$F(v,\lambda) = \lambda(\hat{u} - u_p(0)) - \left(u_p'(1) - iku_p(1)\right)\bar{v}(1)$$

for all $(v, \lambda) \in V_2$ where V_1, V_2 are appropriate function spaces. These spaces are chosen on the basis of "T-complete" systems, i.e., sets of functions that are dense in the trial space. In the 1D equation, T-complete systems are for example $\{\sin kx, \cos kx\}$ or $\left\{e^{ikx}, e^{-ikx}\right\}$. If $f \equiv 0$ then, with the ansatz $u = Ae^{ikx}$, we achieve that both the domain integral and the boundary term at $x = 1$ vanish identically. The solution is thus $u = \hat{u}e^{ikx}$.

In the TFEM, we consider a FE-partition $\Omega = \{\Delta_j\}_{j=1}^{N}$ and the weighted residual equation

$$\sum_{j=1}^{N} \int_{\Delta_j} \left(-u_j'' - k^2 u_j - f_j\right) \bar{v}_j \, dx + \lambda_o(u(0) - \hat{u}) + (u'(1) - iku(1))\, \bar{v}(1)$$

$$+ \sum_{j=1}^{N-1} \left(\lambda_j (u_{j+1}^- - u_j^+) + \nu_j \left((u_{j+1}')^- - (u_j')^+\right)\right) = 0 .$$

Here, subscript j denotes restriction to element Δ_j and superscripts $+, -$ denote the left-hand and right-hand limits at nodal points j. The interelement boundaries are just points. Again the domain integrals in the first sum vanish if the ansatz is chosen on each element as the sum of a homogeneous and a particular solution of Helmholtz' equation.

2.4. Incorporation of analytical information in a piecewise Galerkin approach: Partition of Unity Method

We refer here only the most simple version of the method where the partition of unity is given by the standard nodal shape functions of the FEM. The idea is to enrich these local ansatz spaces on a *patch* by functions that contain analytical information from the differential operator. In the 1D-case, these are the homogeneous solutions of the Helmholtz equation plus polynomial degrees of freedom that *approximate* the inhomogeneity of the right hand side. For instance, if the right-hand side is constant or piecewise constant, the ansatz on patch j could be $\{1, \sin k(x-x_j), \cos k(x-x_j)\}$ — see Fig. 2. Thus assembly and geometrical approximation of the domain by elements is done in

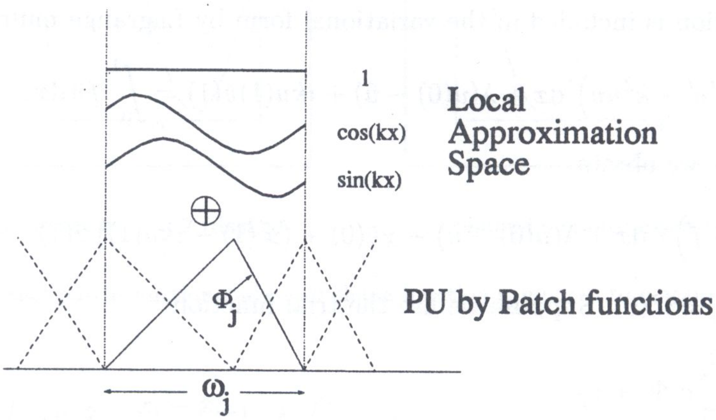


Fig. 2. Patch-function, analytical functions and polynomial ansatz for the model problem

the standard FE manner whereas improved approximability is ensured by the "knowledge-based" enrichment of the local patch-spaces. Being based on the Galerkin variational form, the method "inherits" the well-established stability and convergence theory of the finite element method. The approximability for Laplace and Helmholtz problems has been investigated in [22]. The condition that the patch-functions form a partition of unity

$$\sum_{j=1}^{N} \Phi_j(x) \equiv 1 ,$$

where the sum is taken over all patches, is crucial for the proof of approximability — see [23].

For further details, we refer to the paper by Melenk and Babuška in these proceedings. In this simple one-dimensional case, the PUM will always reproduce the exact solution if this solution is in the local subspace of approximation. In this respect, PUM and TFEM are alike. In the TFEM it is essential that a particular solution is known analytically for the given data. In the PUM, the data is approximated and analytical information is only used from the homogeneous differential operator.

3. STABILIZATION AND KNOWLEDGE-BASED APPROXIMATION IN 2D

The main difference between the 1D model case and the higher dimensional application is that the number of linearly independent particular solutions of Helmholtz equation is now infinite. For instance, all plane waves $u(x,y) = \exp(i\mathbf{k}\cdot\mathbf{x})$ with $|\mathbf{k}| = k$ are solutions of $\Delta u + k^2 u = 0$ in 2D. This has the following implications:

Stabilization: The problem is how to choose the parameter τ. The two-dimensional dispersion relation is obtained by substituting a plane-wave solution $\exp(i(\mathbf{k}^h\cdot\mathbf{x}))$ into the difference equations of the discretized finite element model — see [25]. The discrete wave-vector is $\mathbf{k}^h = |\mathbf{k}^h|\{\cos\theta_o, \sin\theta_o\}$ where θ_o is some a priori chosen direction of the plane wave. The subsequent outline of the determining equation for τ is similar to the 1D-case, yielding

$$\tau k^2 = 1 - \frac{S(kh,\theta_o)}{k^2 M(kh,\theta_o)}$$

where S, M are rational functions of $\mathbf{k}, \theta_o$ and the mesh-parameters h_x, h_y. Thompson and Pinsky [25] choose for their numerical tests $\theta_o = \pi/8$. If the exact solution is a plane wave going in that very direction, the corresponding piecewise linear FE-solution has no pollution. However, a signal is generally decomposed in plane waves going in an infinite number of directions. Even if there are directionally prevalent components in this decomposition they are not necessarily known a priori.

Babuška and Sauter show in [7] that pollution cannot be generally annihilated in the higher-dimensional case. More specifically, considering the GLS-approach as a particular case of generalized FEM (GFEM) they show that for any GFEM there exist a family of domains Ω_n and right-hand sides r_n such that the error of the GFE-solution compared to the exact solution can be estimated in a L^2-norm as

$$\|u_n^{ex} - u_n^{fe}\| \geq C k^{3.5} h^3 \tag{25}$$

whereas the minimal error of approximation is estimated in the same norm as

$$\|u_n^{ex} - u_n^{opt}\| \leq C(kh)^2$$

(C denotes generic constants not depending on k, h). Essentially one can say that if a generalized FEM is designed such that it will be very accurate in some wave direction it will still not be accurate in some other direction. Thus, in contrast to the one-dimensional case, the stabilization procedure proposed in [25] does not reduce the size of the pollution term in the error — see [2]. However, it is possible to construct a stabilized matrix such that the maximal (w.r. to the direction of all plane waves) pollution term is minimal, i.e. is of the order given by (25). Such a matrix is constructed and tested on a 2D model problem in [2] — see also Section 4 of this paper. In the 1D case we have seen that the stabilized FD-matrix on non-uniform mesh can be equivalently obtained from a FEM with analytical shape functions ("h-∞-FEM"). In the 2D-case, analytical shape functions can be constructed on rectilinear mesh (see Fig. 3) as tensor-products of the 1D-functions, $t_i(k_x x)t_j(k_y y), i,j = 1,2$. Directional enrichment of the h-∞-FEM can be achieved by superposing several products with $k_x^2 + k_y^2 = k^2$. While these shape functions will not, in general, lead to the optimally stabilized difference matrix, one expects a significant gain in approximability.

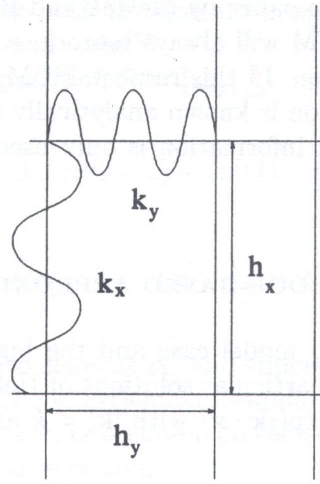


Fig. 3. Rectilinear mesh with exact shape-functions

Approximability: In 1D, any solution of the homogeneous Helmholtz equation can be written as a linear combination of functions $\exp(ikx), \exp(-ikx)$. In 2D, the question is if there exists a set of particular solutions such that any solution of Helmholtz' equation can be approximated by a linear combination of functions from this set. Such sets exist, examples are (cf. [14, 22])

$$V = \left\{ J_n(kr)e^{in\theta}, n = 0, \pm 1, \pm 2, \dots \right\}, \tag{26}$$

$$W = \left\{ \left\{ \exp(ik(x\cos\frac{2\pi m}{n} + y\sin\frac{2\pi m}{n})), m = 0, 1, \dots, n-1 \right\}, n = 1, 2, \dots \right\}. \tag{27}$$

By J_n, we denote the cylindrical Bessel functions of the first kind. In Fig. 4, we depict the local approximation space on a patch ω_j arising from overlaying a patch-function which is constructed from the piecewise linear shape functions with a linear combinations of plane waves from W, being directed in angels $\theta_1, \dots \theta_4$. In a finite element context, one expects that, by incorporation

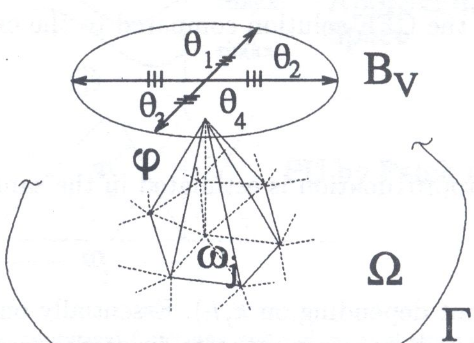


Fig. 4. Local PUM-Ansatz

of functions from V or W into the FEM ansatz space, the quality of approximation is increased significantly. This is confirmed by Melenk and Babuška [21] who prove the approximation estimate

$$\|u_H - u_m\| \leq C(\Omega, k, s)\left(\frac{\ln^2 m}{m}\right)^s \|u_H\|_s. \tag{28}$$

Here, m is the number of basis functions from W that are used in the approximation ansatz. The approximated function u_H is any homogeneous solution of Helmholtz' equation on a bounded

Lipschitz domain $\Omega \subset \mathbf{R}^2$. While this is the same convergence rate as for the p-version, the increase from m to $m+1$ adds only one DOF whereas an ever increasing number of DOF is added if advancing by degree in the p-version with polynomial approximation. While thus the question of approximability is favorably settled, the problem is how to execute the standard FEM technologies of element assembly and boundary fitting when using knowledge-based shape functions.

Variational form: Consider the boundary value problem

$$-\Delta u - k^2 u = 0 \qquad \text{on } \Omega\,, \tag{29}$$

$$u = \hat{u}_o \qquad \text{on } \Gamma_o\,, \tag{30}$$

$$\frac{\partial u}{\partial n} = \hat{u}_1 \qquad \text{on } \Gamma_1\,, \tag{31}$$

where Ω is a domain in $\mathbf{R}^2$ with boundary $\Gamma = \Gamma_0 \cup \Gamma_1$. The FEM equations are found from the weak form

$$\int_\Omega \left(\nabla u \nabla \bar{v} - k^2 u \bar{v}\right)\, dxdy + \int_{\Gamma_o} (u - \hat{u}_o)\bar{\lambda}\, ds + \int_{\Gamma_o} \bar{v}\chi\, ds = \int_{\Gamma_1} \hat{u}_1 \bar{v}\, ds\,,$$

where λ, χ are Lagrange multipliers. This equation is obtained by applying Green's theorem of partial integration to the weighted residual ansatz

$$\int_\Omega (-\Delta u - k^2 u)\bar{v}\, dxdy + \int_{\Gamma_o} (u - \hat{u}_o)\bar{\lambda}\, ds = 0$$

and replacing $\chi = \dfrac{\partial u}{\partial n}$ on Γ_o.

In the Trefftz method, one includes the non-essential boundary conditions into the weighted residual ansatz, yielding

$$\int_\Omega (-\Delta u - k^2 u)\bar{v}\, dxdy + \int_{\Gamma_o} (u - \hat{u})\bar{\lambda}\, ds + \int_{\Gamma_1} \chi \left(\frac{\partial u}{\partial n} - \hat{u}_1\right) ds = 0\,.$$

Again one chooses the trial functions for u such that the domain integral vanishes and only the integral on the boundary has to be resolved.

4. Numerical evaluation

Model problem: We solve the Helmholtz equation in 2D on the square $\Omega = [0,1] \times [0,1]$. Figure 5 (a) shows the domain and a partition into uniform finite elements as used in [2]. The problem is formulated as

$$-\Delta u - k^2 u = 0 \quad \text{in } \Omega$$

with boundary conditions

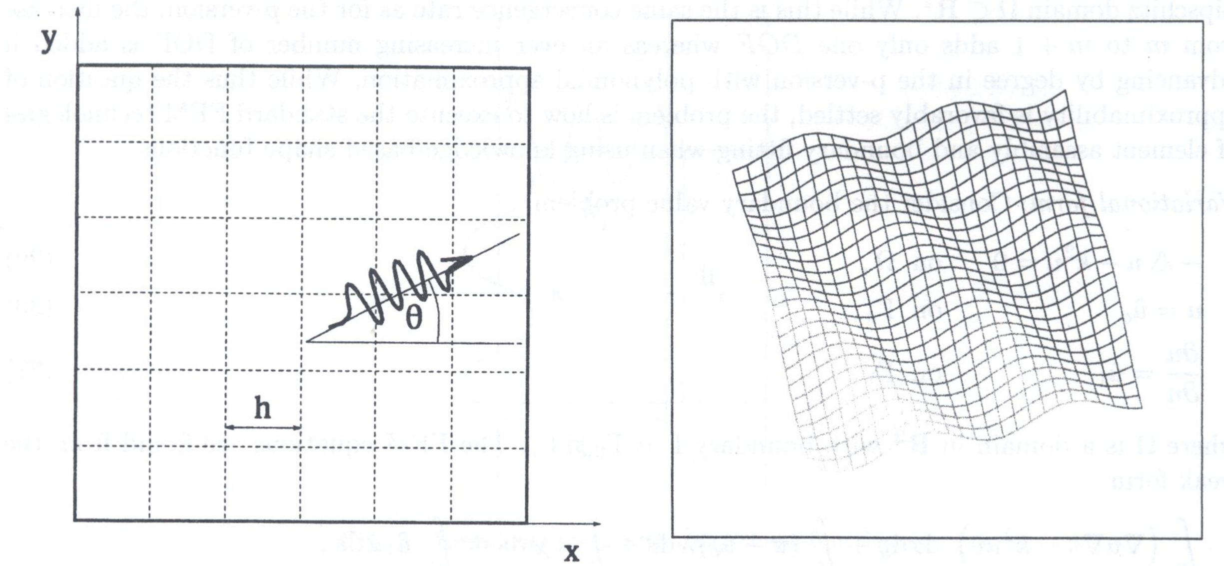
$$iku + \frac{\partial u}{\partial n} = g \quad \text{on } \Gamma\,,$$

where the function g is chosen such that the exact solution is a plane wave

$$u_{ex} = e^{i\mathbf{k}\cdot\mathbf{x}}$$

propagating in direction θ, i.e., $\mathbf{k} = k\{\cos\theta, \sin\theta\}$.

This problem has been solved in [2], using the Galerkin FEM, Galerkin Least-Squares and the Quasistabilized Galerkin FEM with piecewise linear trial functions. Furthermore, the same problem



a) FE-mesh b) Plane wave in direction θ

Fig. 5. Domain, FE mesh and exact solution

was solved in [21] (cf. also [22]) by the PUM using approximation space W from Eq. (27) — plane waves.

Trefftz Method: For comparison, we implemented the solution by Trefftz method, using the trial function

$$u_T = \sum_{m=1}^{N} u_m \phi_m(x,y)\,, \tag{32}$$

where $\phi_m \in W_N$ are plane waves in direction $\theta_m = 2\pi m/N$. For simplicity, we replaced the Sommerfeldt-type boundary condition on Γ with a Dirichlet condition $u = \hat{u}$, assuming $\hat{u} = e^{\mathbf{ik}\cdot\mathbf{x}}$, $x \in \Gamma$. We assume that wavenumber k is not close to any of the discrete eigenvalues of the Dirichlet problem. Testing subsequently with $\bar{\phi}_m, m = 1 \dots N$, we solve the variational problem: Find u_T such that

$$\int_\Gamma (u_T - \hat{u})\bar{\phi}_n = 0 \tag{33}$$

for all $n = 1, 2, \dots, N$. This leads to the algebraic system

$$\mathbf{T}\,\mathbf{u} = \mathbf{g} \tag{34}$$

with a dense $N \times N$-matrix $\mathbf{T}$ the entries of which are $t_{mn} = \int_\Gamma \phi_m \bar{\phi}_n$. Vector $\mathbf{u}$ contains the unknown coefficients u_m; the entries of the rhs vector are $g_m = \int_\Gamma \hat{u}\bar{\phi}_n$. Once $\mathbf{u}$ is computed, function u_T can be evaluated at any interior point. We measure the domain error in L^2 norm

$$e_\Omega = \left(\int_\Omega |u_{ex} - u_T|^2 \right)^{1/2}\,. \tag{35}$$

Convergence: It is easy to see that the solution of eq (33) is equivalent to the minimization problem:

$$\min_{v \in \partial W} \int_\Gamma |v - \hat{u}|^2\,. \tag{36}$$

Here, ∂W denotes the traces of functions $w \in W \subset H^1(\Omega)$ on Γ; obviously $\partial W \subset L^2(\Gamma)$. The solution $v = u_T$ of Eq. (36) is unique. By the approximation result (28), convergence $u_T \to \hat{u}$ is assured on Γ. Further, the domain error $u_{ex} - u_T$ solves on Ω the Helmholtz equation with the Dirichlet boundary condition $e|_\Gamma = (\hat{u} - u_T)|_\Gamma$. Then by Proposition 8.1.4 of [22][1] we have the estimate

$$\|e\|_{L^2(\Omega)} \leq \|e\|_{H^1(\Omega)} \leq C(\Omega)\|\hat{u} - u_T\|_{L^2(\Gamma)},$$

yielding convergence in the domain if convergence on the boundary is assured. For a similar method to solve elasticity problems, see [6, 3.16; 3.20].

Remark 6: In this case, no loss of stability occurs with growing wavenumber k since one effectively solves a least squares minimization problem with BB-constant 1 (independently of k). However the situation changes if, instead of a Trefftz method over the whole domain, one applies a TFEM. This leads to mixed FEM [5] where the question of stability arises and needs careful consideration.

Implementation: The algorithm has been implemented in double precision Fortran. The boundary integrals are evaluated numerically using h-p- Gauss quadrature, i.e., the Gauss-rule with $p = 50$ nodes is applied on $1/h$ boundary elements. The same rule is used in 2D to evaluate numerically the error e_T in (35). We verify that the error is zero if the approximated exact solution lies in the trial space. See, for example, Fig. 6 for $\theta = \pi/3$: the error vanishes for $m = 6$ and $m = 12$.

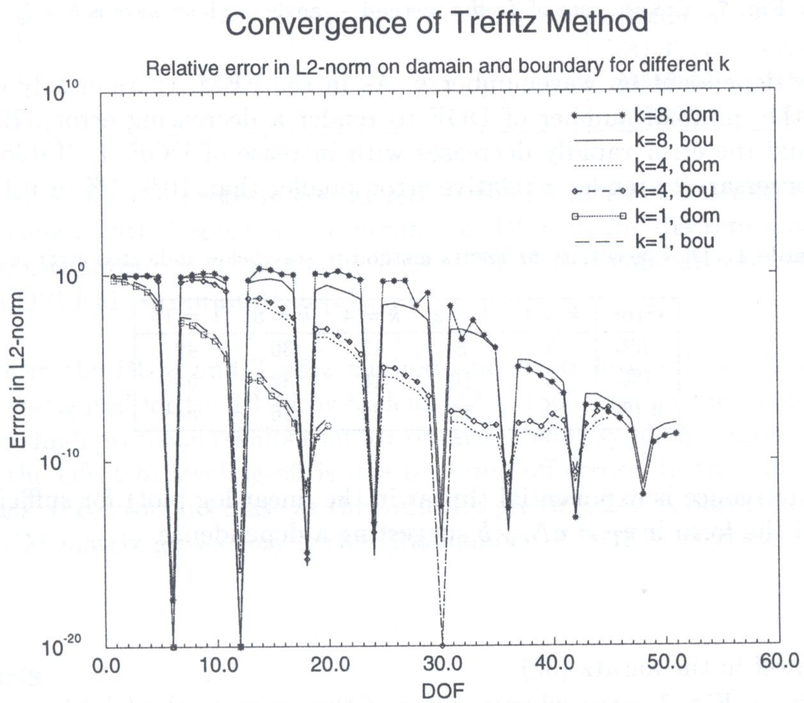


Fig. 6. Convergence of Trefftz method — angle of plane wave is $\theta = \frac{\pi}{3}$

Observations and discussion: We are interested in the rate of convergence and in the influence of wavenumber k on convergence. We chose $\theta = \frac{\pi}{e}$ to make sure that the approximated wave does not lie in the trial space. The convergence rates for different k is shown in Fig. 7. The convergence

[1]This proposition is shown for the Robin boundary conditions. In the Dirichlet case, it holds only with the assumption that k is not close to a discrete eigenvalue

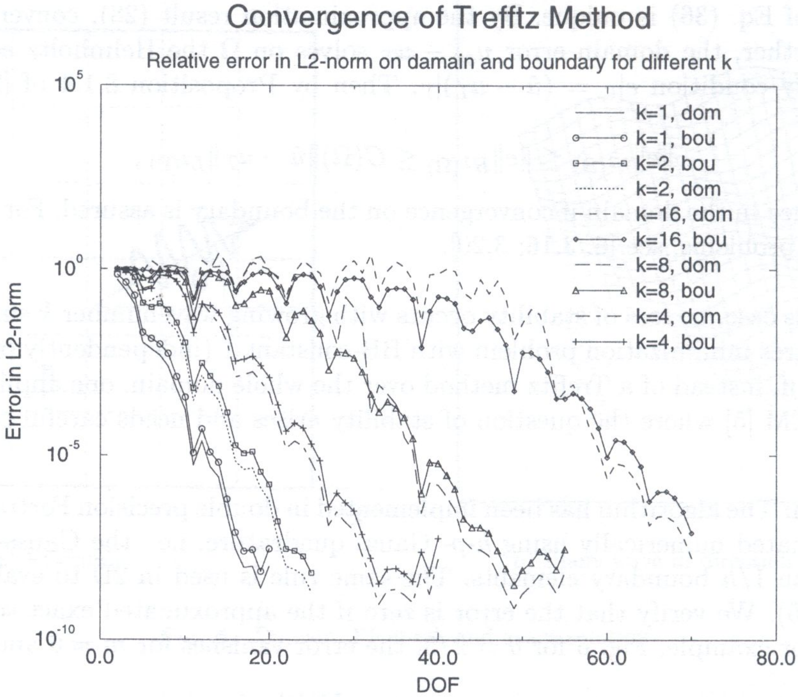


Fig. 7. Convergence of Trefftz method — angle of plane wave is $\theta = \frac{\pi}{3}$

behavior is highly dependent on wavenumber k. As in the FEM, there clearly exists a "minimal resolution" (i.e., the minimal number of DOF to render a decreasing error). If the resolution is larger than minimal the error rapidly decreases with increase of DOF. In Table 1, we collect the number of DOF necessary to render a relative error smaller than 10%, 1% or 0.1%, resp.

Table 1. DOF necessary in Trefftz method to stay below indicated error level

error	$k = 1$	$k = 2$	$k = 4$	$k = 8$	$k = 16$
10%	5	8	12	30	49
1%	6	10	18	32	54
0.1%	9	13	22	36	54

The rate of convergence is exponential (linear in the linear-log plot) for sufficiently large DOF. The behavior is of the form $\ln e_T = aN + b$ suggesting a dependence

$$e_T \sim Ce^{aN}$$

where N is the cutoff in the ansatz (32).

The lower peaks in Fig. 7 occur whenever one of the waves in the trial basis has a wavevector that is directionally very close to the exact wavevector — cf. the observation for $\theta = \pi/3$ in Fig. 6.

Finally, let us compare the Trefftz method with the methods in [2] and [22], see also [21]. As in these references, we chose the incoming wave with angle $\theta = \pi/16$. In Table 2, we compare the number of DOF needed for accuracy ϵ. The DOF for FEM and QSFEM have been estimated in [22] from the examples in [2]. We give the results for the PUM on one and on 64 square elements, corresponding to $n = 1$ or $n = 8$ subdivisions of the sides, respectively. In both cases, convergence is achieved by increasing the number of "analytical" DOF within the patches. Note that the PUM in the case $n = 8$ leads to a banded system matrix similarly to the FEM. Both in the Trefftz method and the PUM, we use the approximation space W. However, in the PUM, the Helmholtz sesquilinear

Table 2. DOF necessary in different methods to stay below indicated error level, $k = 32$.

ϵ	10%	1%	0.1%	0.01%
FEM	5900	5800	580000	5800000
QSFEM	840	8400	82000	800000
PUM, $n = 1$	88	104	120	120
Trefftz	88	92	94	95
PUM, $n = 8$	162	486	1134	1134

form extends over the domain whereas in the Trefftz method, integration is performed only on the boundary. For both methods, we tabulate the relative errors in L^2-norm over the domain Ω.

We observe that the Trefftz method needs the least number of DOF. A direct comparison of results PUM/Trefftz is given in Table 3. We compare for three wavenumbers, $k = 1, 4, 32$, respectively, the results of PUM vs. Trefftz method. The dashes in the table indicate that no further convergence was observed beneath an error level of E-07 ... E-08 — see the remark below.

Table 3. PUM vs. Trefftz method: comparison of results for different wavenumber and DOF.

	$k = 1$		$k = 4$		$k = 32$	
DOF	PUM	Trefftz	PUM	Trefftz	PUM	Trefftz
8	.2092E-02	.1793E-02	.3103E-01	.4191E+00	.9923E+00	.1119E+01
24	.2047E-06	.1232E-08	.9917E-3	.1284E-04	.9971E+00	.1150E+01
40	.1801E-08	.1608E-07	.8764E-6	.5094E-08	.106E+01	.8811E+00
56	.8868E-08	–	.99108E-09	.5416E-08	.1087E+01	.8006E+00
72	–	–	.8158E-8	.2579E-08	.4484E+00	.5362E+00
88	–	–	–	–	.6413E-01	.1605E+00
104	–	–	–	–	.3755E-02	.8164E-05
120	–	–	–	–	.1320E-05	.2829E-08

We observe that — for the problem considered — the PUM for $n = 1$ and the Trefftz method are of similar efficiency with respect to the number of DOF in the discrete model. An effectivity analysis that also estimates operation counts for the PUM and compares to respective estimates for the FEM and QSFEM is contained in [21].

Remark 7: Both in the PUM and Trefftz method, the errors level off at 1.E-07 ... 1.E-08. This effect has been investigated for the PUM by Melenk [22, p.150]. Comparing the FORTRAN double-precision results to high precision results that are obtained using symbolic manipulation in MAPLE, it is shown that the effect of leveling-off is due to round-off errors. In the evaluation of the symbolic computations, the errors decrease as theoretically predicted. It is observed that the condition number of the PUM matrix grows very fast as the number of DOF is increased.

5. Conclusions

The growing awareness that the standard h-version of the FEM performs poorly for the solution of the Helmholtz equation has led to different propositions and investigations of improved methods. The Helmholtz sesquilinear form — which is the starting point for Galerkin-type approximations — loses stability as wavenumber k grows. We recall that both good stability and approximability are necessary to get fast convergence of a numerical method. From this angle, our overview of different methods shows that the convergence can be equally well improved by *either* enhancing stability *or* approximability of the standard method. We considered two stabilized methods which we compared to methods that include the fundamental solution into the ansatz space. In 1D, one can design by both approaches a FEM with optimal convergence (no pollution). In a special case, the stabilized stiffness matrix is equivalently obtained from an approximation ansatz using analytical shape-functions. The analytical shape functions are the limiting case for the h-p-version of the FEM. Thus the FEM with analytical shape functions is called here h-∞-FEM. This FEM trivially yields the exact solution in 1D. In 2D, we proposed a h-∞ FEM with directional enrichment on rectilinear grids. In two dimensions, stabilization is, in general, more complicated whereas approximation enhancement by h-p-FEM is well researched and can be performed in the standard way. A way to further enhance approximability is to include analytical solutions of Helmholtz' equation into the trial space. This is done in the traditional Trefftz method and in the recently proposed Partition of Unity Method (PUM). Comparison of implementations on a simple 2D model problem shows that both methods are equally efficient, compared to the standard and stabilized h-version FEM. It seems very promising to test these high-approximating methods on more realistic problems. However, applying the Trefftz approach on super-elements (Trefftz-FEM) leads to a mixed-hybrid formulation for which the question of stability is still open. The PUM, on the other hand, is a Galerkin method based on the bilinear form. Stability, approximability and convergence are well-researched. The open questions concern conditioning and efficient implementation.

ACKNOWLEDGEMENTS

The first author (F.I.) is visiting at the Texas Institute for Computational and Applied Mathematics (TICAM). The support of the Deutsche Forschungsgemeinschaft under Grant Ih-23 and the hospitability of the Institute are greatly acknowledged. Special thanks to Prof. Ch. Schwab and Dr. J.M. Melenk of the Seminar Applied Mathematics, ETH Zürich, and to Dr. S.A. Sauter, Kiel University, for inspiring discussions on various topics presented in this paper.

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