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# OPTIMIZATION OF PLANE WAVE DIRECTIONS IN PLANE WAVE DISCONTINUOUS GALERKIN METHODS FOR THE HELMHOLTZ EQUATION

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Abstract. Recently, the use of special local test functions other than polynomials in Discontinuous Galerkin (DG) approaches has attracted a lot of attention and became known as DG-Trefftz methods. In particular, for the 2D Helmholtz equation plane waves have been used in [10] to derive an Interior Penalty (IP) type Plane Wave DG (PWDG) method and to provide an a priori error analysis of its *p*-version with respect to equidistributed plane wave directions. However, the dependence on the distribution of the plane wave directions has not been studied. In this contribution, we study this dependence by formulating the choice of the directions as an optimal control problem with a tracking type objective functional and the variational formulation of the PWDG method as a constraint. The necessary optimality conditions are derived and numerically solved by a projected gradient method. Numerical results are given which illustrate the benefits of the approach.

Key words. Plane Wave Discontinuous Galerkin methods, optimization of plane wave directions, Helmholtz equation

#### AMS subject classifications. 65N30;35J20;74J20

1. Introduction. The use of plane waves in the finite element approximation of the Helmholtz equation goes back to the ultra weak variational formulation of the problem by Cessenat and Després [3]. The approach can be interpreted as a Discontinuous Galerkin (DG) approximation and is therefore referred to as the Plane Wave Discontinuous Galerkin (PWDG) method. Since it uses local trial spaces consisting of plane waves, it is also a particular example of a Trefftz-type finite element approximation and hence called a Trefftz-type DG method. Due to its superior performance compared to standard finite element approximations which suffer from the so-called pollution effect, it has been studied extensively in the literature (cf., e.g., [1, 2, 4, 6, 7, 9]). In particular, the h-version and the p-version of the PWDG method have been analyzed in [8] and in [10], whereas the exponential convergence of the hp-version has been established in [11].

The PWDG method features a triangulation  $\mathcal{T}_h(\Omega)$  of the computational domain  $\Omega \subset \mathbb{R}^2$  and the use of a certain number  $p = 2m + 1, m \in \mathbb{N}$ , of plane waves in each element  $K \in \mathcal{T}_h(\Omega)$  which compose the local trial spaces. The plane waves are of the form  $\exp(ik\mathbf{d}_\ell \cdot \mathbf{x}), \mathbf{d}_\ell = (\cos(\theta_\ell), \sin(\theta_\ell))^T, -m \leq \ell \leq +m, \mathbf{x} \in K$ , where k stands for the wavenumber. It is known from the convergence analysis of the PWDG method [10] that the p directions  $\mathbf{d}_\ell, -m \leq \ell \leq +m$ , should be chosen in such a way that the minimum angle between two different directions is greater or equal  $2\pi\eta/p$  for some  $\eta \in (0, 1]$ . An issue that has not been considered so far is how to choose the directions (for fixed  $\mathcal{T}_h(\Omega)$  and  $m \in \mathbb{N}$ ) in order to minimize the discretization error.

In this paper, we formulate this problem as a constrained optimal control problem with

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a tracking type objective functional and the variational formulation of the PWDG method as a constraint, where the controls are the p angles  $\theta_{\ell}, -m \leq \ell \leq +m$ . We derive the first order necessary optimality conditions by means of the Lagrange multiplier approach [13] and derive a projected gradient type method with Armijo line search to compute an optimal solution. Numerical results illustrate the dependence of the discretization error on the choice of the plane wave directions.

**2. The PWDG Method.** For a bounded convex polygonal domain  $\Omega \subset \mathbb{R}^2$  with boundary  $\Gamma = \partial \Omega$  we consider the Helmholtz equation

$$-\Delta u - \omega^2 u = 0 \quad \text{in } \Omega, \tag{2.1a}$$

$$\mathbf{n} \cdot \nabla u + i\omega u = g \quad \text{on } \Gamma = \partial \Omega. \tag{2.1b}$$

where  $\omega > 0$  is the wavenumber,  $g \in L^2(\Gamma)$  is a given function, and **n** denotes the exterior unit normal vector on  $\Gamma$ . We rewrite (2.1) as the first order system:

$$i\omega\boldsymbol{\sigma} - \nabla u = \mathbf{0} \quad \text{in } \Omega,$$
 (2.2a)

$$-\nabla \cdot \boldsymbol{\sigma} + i\omega u = 0 \quad \text{in } \Omega, \tag{2.2b}$$

$$i\omega \mathbf{n} \cdot \boldsymbol{\sigma} + i\omega u = g \quad \text{on } \Gamma.$$
 (2.2c)

The variational formulation of (2.2) reads: Find  $(\sigma, u) \in \mathbf{H}(\operatorname{div}, \Omega) \times H^1(\Omega)$  such that for all  $(\boldsymbol{\tau}, v) \in \mathbf{H}(\operatorname{div}, \Omega) \times H^1(\Omega)$  it holds

$$(i\omega \ \boldsymbol{\sigma}, \boldsymbol{\tau})_{0,\Omega} + (u, \nabla \cdot \boldsymbol{\tau})_{0,\Omega} = \langle u, \mathbf{n} \cdot \boldsymbol{\tau} \rangle_{H^{1/2}(\Gamma), H^{-1/2}(\Gamma)},$$
(2.3a)

$$(\boldsymbol{\sigma}, \nabla v)_{0,\Omega} + (u, v)_{0,\Gamma} + (i\omega \ u, v)_{0,\Omega} = (\frac{1}{i\omega} \ g, v)_{0,\Gamma}.$$
(2.3b)

We consider a shape regular family of geometrically conforming, quasi-uniform simplicial triangulations  $\mathcal{T}_h(\Omega)$  of the computational domain  $\Omega$ . For  $D \subset \overline{\Omega}$  we denote by  $\mathcal{E}_h(D)$  the set of edges of the triangulation in D. For  $T \in \mathcal{T}_h(\Omega)$ , we refer to  $h_T$  as the diameter of T and set  $h := \max \{h_T \mid T \in \mathcal{T}_h(\Omega)\}$ . For  $E \in \mathcal{E}_h(\overline{\Omega})$ , the length of Ewill be denoted by  $h_E$ . For functions  $v \in \prod_{T \in \mathcal{T}_h(\Omega)} H^1(T)$  the trace of v on  $E \in \mathcal{E}_h(\Omega)$ may exhibit a jump across E. For  $E \in \mathcal{E}_h(\Omega)$  with  $E = T_+ \cap T_-, T_\pm \in \mathcal{T}_h(\Omega)$  and  $E \in \mathcal{E}_h(\Gamma)$  we define

$$\{v\}_E := \begin{cases} (v|_{T_+\cap E} + v|_{T_-\cap E})/2 , E \in \mathcal{E}_h(\Omega) \\ v|_E , E \in \mathcal{E}_h(\Gamma) \end{cases},$$

$$[v]_E := \begin{cases} v|_{T_+\cap E} - v|_{T_-\cap E} , E \in \mathcal{E}_h(\Omega) \\ v|_E , E \in \mathcal{E}_h(\Gamma) \end{cases}.$$

$$(2.4)$$

For vector-valued functions we use an analogous notation.

We approximate (2.3a),(2.3b) by introducing the following local spaces spanned by plane waves

$$V_p(T) := \{ v(\mathbf{x}) := \sum_{\ell=1}^p \alpha_\ell \exp(i\omega \mathbf{d}_\ell \cdot \mathbf{x}) \}, \quad p \in \mathbb{N},$$

$$\mathbf{V}_p(T) := V_p(T)^2,$$
(2.5)

where  $\alpha_{\ell} \in \mathbb{C}$  and  $\mathbf{d}_{\ell}, 1 \leq \ell \leq p$ , are p different unit directions

$$\mathbf{d}_{\ell} = (\cos(\theta_{\ell}), \sin(\theta_{\ell}))^T, \quad 1 \le \ell \le p = 2m + 1, \ m \in \mathbb{N}.$$

$$(2.6)$$

We set  $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_p)^T$  such that  $\theta_\ell, 1 \leq \ell \leq p$ . Setting  $\theta_{p+1} = \theta_1 + 2\pi$  we require that

$$\boldsymbol{\theta} \in \mathbf{K} := \{ \boldsymbol{\theta} \in [0, 2\pi)^p \mid \theta_{min} \le \theta_{\ell+1} - \theta_{\ell} \le \theta_{max}, \ 1 \le i \le p \},$$
(2.7)  
$$\theta_{min} := (2\pi\eta_1)/p, \ \theta_{max} := (2\pi\eta_2)/p, \ 0 < \eta_1 < 1 < \eta_2 < 3/2.$$

The associated global spaces are given by

$$V_h := \{ v_h \in L^2(\Omega) \mid v_h \mid_T \in V_p(T), \ T \in \mathcal{T}_h(\Omega) \},$$
  
$$\mathbf{V}_h := \{ \boldsymbol{\tau}_h \in L^2(\Omega)^2 \mid \boldsymbol{\tau}_h \mid_T \in \mathbf{V}_p(T), \ T \in \mathcal{T}_h(\Omega) \}.$$
  
(2.8)

Then, the PWDG approximation of (2.1a),(2.1b) amounts to the computation of  $(u_h, \boldsymbol{\sigma}_h) \in V_h \times \mathbf{V}_h$  such that for all  $(v_h, \boldsymbol{\tau}_h) \in V_h \times \mathbf{V}_h$  it holds

$$\sum_{T\in\mathcal{T}_{h}(\Omega)} \left( (i\omega\boldsymbol{\sigma}_{h},\boldsymbol{\tau}_{h})_{0,T} + (u_{h},\nabla\cdot\boldsymbol{\tau}_{h})_{0,T} \right) - \sum_{T\in\mathcal{T}_{h}(\Omega)} (\hat{u}_{h},\mathbf{n}_{\partial T}\cdot\boldsymbol{\tau}_{h})_{0,\partial T} = 0, \quad (2.9a)$$
$$\sum_{T\in\mathcal{T}_{h}(\Omega)} \left( (\boldsymbol{\sigma}_{h},\nabla v_{h})_{0,T} + (i\omega u_{h},v_{h})_{0,T} \right) - \sum_{T\in\mathcal{T}_{h}(\Omega)} (\mathbf{n}_{\partial T}\cdot\hat{\boldsymbol{\sigma}}_{h},v_{h})_{0,\partial T} = 0. \quad (2.9b)$$

Here, the PWDG flux functions  $\hat{u}_h$  and  $\hat{\boldsymbol{\sigma}}_h$  are given by

$$\hat{u}_{h}|_{E} := \begin{cases} \{u_{h}\}_{E} - \frac{\beta}{i\omega} [\nabla u_{h}]_{E}, E \in \mathcal{E}_{h}(\Omega) \\ u_{h} - \delta \left(\frac{1}{i\omega} \mathbf{n}_{E} \cdot \nabla u_{h} + u_{h} - \frac{1}{i\omega} g\right), E \in \mathcal{E}_{h}(\Gamma) \end{cases},$$
(2.10a)

$$\hat{\boldsymbol{\sigma}}_{h}|_{E} := \begin{cases} \frac{1}{i\omega} \{\nabla u_{h}\}_{E} - \alpha[u_{h}]_{E}, E \in \mathcal{E}_{h}(\Omega) \\ \frac{1}{i\omega} \nabla u_{h} - (1-\delta) \left(\frac{1}{i\omega} \nabla u_{h} + \mathbf{n}_{E} u_{h} - \frac{1}{i\omega} \mathbf{n}_{E} g\right), E \in \mathcal{E}_{h}(\Gamma) \end{cases}, \quad (2.10b)$$

where  $\mathbf{n}_E$  is the exterior unit normal on E and  $\alpha > 0, \beta > 0, \delta \in (0, 1)$  are flux parameters independent of h, p, and  $\omega$ .

By choosing  $\boldsymbol{\tau}_h = \nabla v_h$  in (2.9a), we can eliminate  $\boldsymbol{\sigma}_h$  from (2.9a),(2.9b) and obtain the following primal variational formulation of the PWDG method: Find  $u_h \in V_h$ such that for all  $v_h \in V_h$  it holds

$$\sum_{T \in \mathcal{T}_h(\Omega)} \left( (\nabla u_h, \nabla v_h)_{0,T} - \omega^2 (u_h, v_h)_{0,T} \right) -$$

$$\sum_{T \in \mathcal{T}_h(\Omega)} \left( (u_h - \hat{u}_h, \mathbf{n}_{\partial T} \cdot \nabla v_h)_{0,\partial T} + i\omega (\mathbf{n}_{\partial T} \cdot \hat{\boldsymbol{\sigma}}_h, v_h)_{0,\partial T} \right) = 0.$$
(2.11)

Moreover, using Green's formula for the first term on the left-hand side in (2.11) and observing  $(-\Delta - \omega^2 I)u_h|_T = 0$ ,  $T \in \mathcal{T}_h(\Omega)$ , we are led to a formulation of the PWDG method involving only integrals over edges  $E \in \mathcal{E}_h(\overline{\Omega})$ : Find  $u_h \in V_h$  such that

$$a_h(u_h, v_h) = \ell_h(v_h), \quad v_h \in V_h, \tag{2.12}$$

where the sesquilinear form  $a_h(\cdot, \cdot) : V_h \times V_h \to \mathbb{C}$  and the functional  $\ell_h : V_h \to \mathbb{C}$  are given by

$$a_{h}(u_{h}, v_{h}) := \sum_{E \in \mathcal{E}_{h}(\Omega)} \left( (\{u_{h}\}_{E}, \mathbf{n}_{E} \cdot [\nabla v_{h}]_{E})_{0,E} + i\beta\omega^{-1}(\mathbf{n}_{E} \cdot [\nabla u_{h}]_{E}, \mathbf{n}_{E} \cdot [\nabla v_{h}]_{E})_{0,E} - (\mathbf{n}_{E} \cdot \{\nabla u_{h}\}_{E}, [v_{h}]_{E})_{0,E} + i\alpha\omega([u_{h}]_{E}, [v_{h}]_{E})_{0,E}) \right)$$
$$\sum_{E \in \mathcal{E}_{h}(\Gamma)} \left( (1 - \delta)(u_{h}, \mathbf{n}_{E} \cdot \nabla v_{h})_{0,E} + i\delta\omega^{-1}(\mathbf{n}_{E} \cdot \nabla u_{h}, \mathbf{n}_{E} \cdot \nabla v_{h})_{0,E} - \delta(\mathbf{n}_{E} \cdot \nabla u_{h}, v_{h})_{0,E} + i(1 - \delta)\omega(u_{h}, v_{h})_{0,E}) \right), \qquad (2.13a)$$

$$\ell_h(v_h) := \sum_{E \in \mathcal{E}_h(\Gamma)} \left( i\delta\omega^{-1}(g, \mathbf{n}_E \cdot \nabla v_h)_{0,E} + (1-\delta)(g, v_h)_{0,E} \right).$$
(2.13b)

As has been shown in [10], the variational equation (2.12) admits a unique solution  $u_h \in V_h$ . Moreover, if the solution u of (2.1a),(2.1b) satisfies  $u \in H^{k+1}(\Omega), k \in \mathbb{N}$ , and if the mesh width h of the triangulation  $\mathcal{T}_h(\Omega)$  satisfies  $\omega h \leq \kappa$  for some  $\kappa > 0$ , then there exists a constant C > 0, independent of p and u, but depending on  $\kappa$ , such that the following a priori error estimate holds true (cf. Theorem 3.14 in [10])

$$\|u - u_h\|_{0,\Omega} \le C\omega^{-1} \operatorname{diam}(\Omega) h^{k-1} \left(\frac{\log p}{p}\right)^{k-1/2} \|u\|_{k+1,\omega,\Omega},$$
(2.14)

where  $\|\cdot\|_{k+1,\omega,\Omega}$  stands for the  $\omega$ -weighted Sobolev norm

$$\|v\|_{k+1,\omega,\Omega} := \left(\sum_{j=0}^{k+1} \omega^{2(k+1-j)} |v|_{j,\Omega}^2\right)^{1/2}, \quad v \in H^{k+1}(\Omega).$$

Setting  $N := \operatorname{card}(\mathcal{T}_h(\Omega))$  and  $\boldsymbol{\theta} := (\theta_1, \cdots, \theta_p)^T$ , the global PWDG space  $V_h$  is spanned by Np basis functions

$$V_{h} = \operatorname{span}(\varphi_{h}^{(1)}, \cdots, \varphi_{h}^{(Np)}),$$

$$\varphi_{h}^{((k-1)p+\ell)} := \exp(i\omega(\cos(\theta_{\ell}), \sin(\theta_{\ell}))^{T} \cdot \mathbf{x})|_{T_{k}}, \ 1 \le k \le N, 1 \le \ell \le p.$$

$$(2.15)$$

Then,  $u_h \in V_h$  can be written as

$$u_h = \sum_{j=1}^{N_p} u_j \ \varphi_h^{(j)}, \quad u_j \in \mathbb{C}, \ 1 \le j \le Np.$$
 (2.16)

Further, setting  $\mathbf{y} := (y_1, \cdots, y_{Np})^T \in \mathbb{C}^{Np}$  with  $y_j := u_j, 1 \leq j \leq Np$ , the PWDG approximation (2.12) represents a complex linear algebraic system

$$\mathbf{A}(\boldsymbol{\theta})\mathbf{y} = \mathbf{b}(\boldsymbol{\theta}),\tag{2.17}$$

where the matrix  $\mathbf{A}(\boldsymbol{\theta}) = (a_{k\ell}(\boldsymbol{\theta}))_{k,\ell=1}^{N_p} \in \mathbb{C}^{N_p \times N_p}$  and the vector  $\mathbf{b}(\boldsymbol{\theta}) = (b_1(\boldsymbol{\theta}), \cdots, b_{N_p}(\boldsymbol{\theta}))^T \in \mathbb{C}^{N_p}$  are given by

$$a_{k\ell}(\boldsymbol{\theta}) := a_h(\varphi_h^{(\ell)}(\boldsymbol{\theta}), \varphi_h^{(k)}(\boldsymbol{\theta})), \quad 1 \le k, \ell \le Np,$$

$$b_\ell(\boldsymbol{\theta}) := \ell_h(\varphi_h^{(\ell)}), \quad 1 \le \ell \le Np.$$
(2.18)

3. Optimization of the plane wave directions. The a priori estimate (2.14) for the  $L^2$ -norm of the global discretization error tells us how the error depends on the number p of plane wave directions, but is does not provide any information on the appropriate choice of the directions  $\mathbf{d}_{\ell} = (\cos(\theta_{\ell}), \sin(\theta_{\ell}))^T, 1 \leq \ell \leq p$ , except that they are supposed to satisfy assumption (2.7). In fact, since

$$V_h = \operatorname{span}(\exp(i\omega \mathbf{d}_1 \cdot \mathbf{x})|_{T_1}, \cdots, \exp(i\omega \mathbf{d}_p \cdot \mathbf{x})|_{T_N}),$$
(3.1)

where  $N := \operatorname{card}(\mathcal{T}_h(\Omega))$ , the solution  $u_h \in V_h$  of (2.12) depends on  $\boldsymbol{\theta} := (\theta_1, \cdots, \theta_p)^T \in \mathbf{K}$  according to

$$u_h(\boldsymbol{\theta}) = \sum_{k=1}^N \sum_{\ell=1}^p u_{k\ell} \exp(i\omega \mathbf{d}_\ell \cdot \mathbf{x})|_{T_k}, \quad u_{k\ell} \in \mathbb{C}.$$
 (3.2)

We attempt to choose  $\boldsymbol{\theta} \in \mathbf{K}$  such that with respect to the  $L^2$ -norm the solution  $u_h(\boldsymbol{\theta})$  of (2.12) is as close as possible to a given desired state  $u^d \in L^2(\Omega)$ . This can be formulated as the optimal control problem

$$\min_{u_h \in V_h, \ \boldsymbol{\theta} \in \mathbf{K}} J(u_h, \boldsymbol{\theta}) := \frac{1}{2} \| u_h(\boldsymbol{\theta}) - u^d \|_{0,\Omega}^2, \tag{3.3a}$$

subject to the PWDG constraint

$$a_h(u_h(\theta), v_h(\theta)) = \ell_h(v_h(\theta)), \quad v_h(\theta) \in V_h.$$
 (3.3b)

Introducing the Hermitian matrix  $\mathbf{M}(\boldsymbol{\theta}) = (m_{k\ell}(\boldsymbol{\theta}))_{k,\ell=1}^{N_p} \in \mathbb{C}^{N_p \times N_p}$  and the vector  $\mathbf{c}(\boldsymbol{\theta}) = (c_1(\boldsymbol{\theta}), \cdots, c_{N_p}(\boldsymbol{\theta}))^T$  according to

$$m_{k\ell}(\boldsymbol{\theta}) := (\varphi_h^{(k)}, \varphi_h^{(\ell)})_{0,\Omega}, \quad 1 \le k, \ell \le Np,$$
  
$$c_\ell(\boldsymbol{\theta}) := (u^d, \varphi_h^{(\ell)})_{0,\Omega}, \quad 1 \le \ell \le Np,$$
  
(3.4)

the algebraic formulation of (3.3a),(3.3b) turns out to be

$$\min_{\boldsymbol{\in}\mathbb{C}^{N_{p}}, \boldsymbol{\theta}\in\mathbf{K}} J(\mathbf{y},\boldsymbol{\theta}) := \frac{1}{2} \langle \mathbf{M}(\boldsymbol{\theta})\mathbf{y},\mathbf{y}\rangle - \operatorname{Re}(\langle \mathbf{c}(\boldsymbol{\theta}),\mathbf{y}\rangle), \qquad (3.5a)$$

subject to the state equation

у

$$e(\mathbf{y}, \boldsymbol{\theta}) := \mathbf{A}(\boldsymbol{\theta})\mathbf{y} - \mathbf{b}(\boldsymbol{\theta}) = 0.$$
(3.5b)

We further denote by  $\mathbf{G} : \mathbf{K} \to \mathbb{C}^{Np}$  the control-to-state map which assigns to the control  $\boldsymbol{\theta} \in \mathbf{K}$  the unique solution  $\mathbf{y} \in \mathbb{C}^{Np}$  of the state equation (3.5b) and by  $J_{red} : \mathbf{K} \to \mathbb{R}$  the reduced objective functional

$$J_{red}(\boldsymbol{\theta}) := J(\mathbf{G}(\boldsymbol{\theta}), \boldsymbol{\theta}).$$

Then, the control-reduced formulation of the optimal control problem (3.5a),(3.5b) reads as follows

$$\min_{\boldsymbol{\theta} \in \mathbf{K}} J_{red}(\boldsymbol{\theta}). \tag{3.6}$$

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THEOREM 3.1. The optimal control problem (3.5a),(3.5b) admits an optimal solution  $(\mathbf{y}^*, \boldsymbol{\theta}^*) \in \mathbb{C}^{Np} \times \mathbf{K}$ .

*Proof.* Let  $\{\boldsymbol{\theta}^{(n)}\}_{\mathbb{N}}, \boldsymbol{\theta}^{(n)} \in \mathbf{K}, n \in \mathbb{N}$ , be a minimizing sequence, i.e., it holds

$$J_{red}(\boldsymbol{\theta}^{(n)}) \to \min_{\boldsymbol{\theta} \in \mathbf{K}} J_{red}(\boldsymbol{\theta}) \text{ as } n \to \infty.$$
 (3.7)

Obviously, the sequence  $\{\boldsymbol{\theta}^{(n)}\}_{\mathbb{N}}$  is bounded and hence, there exist a subsequence  $\mathbb{N}' \subset \mathbb{N}$  and  $\boldsymbol{\theta}^* \in \mathbb{R}^p$  such that

$$\boldsymbol{\theta}^{(n)} \to \boldsymbol{\theta}^*, \quad \mathbb{N}' \ni n \to \infty.$$

In view of the closedness of  $\mathbf{K}$ , we have  $\boldsymbol{\theta}^* \in \mathbf{K}$ . Moreover, due to the continuity of both the control-to-state map  $\mathbf{G}$  and of the reduced objective functional  $J_{red}$  we deduce

$$\mathbf{G}(\boldsymbol{\theta}^{(n)}) \to \mathbf{G}(\boldsymbol{\theta}^*), \ J_{red}(\boldsymbol{\theta}^{(n)}) \to J_{red}(\boldsymbol{\theta}^*) \quad \mathbb{N}' \ni n \to \infty.$$

Consequently, from (3.7) we have

$$J_{red}(\boldsymbol{\theta}^*) = \min_{\boldsymbol{\theta} \in \mathbf{K}} J_{red}(\boldsymbol{\theta}),$$

and with  $\mathbf{y}^* := \mathbf{G}(\boldsymbol{\theta}^*)$  it follows that the pair  $(\mathbf{y}^*, \boldsymbol{\theta}^*) \in \mathbb{C}^{N_p} \times \mathbf{K}$  is an optimal solution of (3.5a), (3.5b).  $\Box$ 

REMARK 3.2. Since the control-to-state map **G** is a non-convex function of the control  $\boldsymbol{\theta}$ , we do not have uniqueness of an optimal solution.

4. First order necessary optimality conditions. We will derive the first order necessary optimality conditions for the optimal control problem (3.5a),(3.5b) by the method of Lagrange multipliers which is justified if the linear independence constraint qualification holds true. To this end, we note that the bound constraints on the control can be expressed as the inequalities  $\mathbf{g}(\boldsymbol{\theta}) \leq \mathbf{0}$ , where the mapping  $\mathbf{g} = (\mathbf{g}_1, \mathbf{g}_2) : \mathbb{R}^p \to \mathbb{R}^p \times \mathbb{R}^p$  is defined by means of

$$\mathbf{g}_{1}(\boldsymbol{\theta}) := (\theta_{2} - \theta_{1} - \theta_{max}, \cdots, \theta_{p+1} - \theta_{p} - \theta_{max}),$$

$$\mathbf{g}_{2}(\boldsymbol{\theta}) := (\theta_{min} - (\theta_{2} - \theta_{1}), \cdots, \theta_{min} - (\theta_{p+1} - \theta_{p})).$$
(4.1)

For a local minimum  $(\mathbf{y}^*, \boldsymbol{\theta}^*) \in \mathbb{C}^{Np} \times \mathbf{K}$  of (3.5a),(3.5b) the active set is given by  $A(\boldsymbol{\theta}^*) = A_1(\boldsymbol{\theta}^*) \cup A_2(\boldsymbol{\theta}^*)$  where

$$A_1(\boldsymbol{\theta}^*) := \{ q \in \{1, \cdots, p\} \mid \theta_{q+1}^* - \theta_q^* - \theta_{max} = 0 \},$$
(4.2a)

$$A_2(\theta^*) := \{ q \in \{1, \cdots, p\} \mid \theta_{min} - (\theta_{q+1}^* - \theta_q^*) = 0 \}.$$
(4.2b)

We refer to  $I(\boldsymbol{\theta}^*) := \{1, \dots, p\} \setminus A(\boldsymbol{\theta}^*)$  as the inactive set. The linear independence constraint qualification requires the linearization of  $(e, (\mathbf{g}_1)_{A_1(\boldsymbol{\theta}^*)}, (\mathbf{g}_2)_{A_2(\boldsymbol{\theta}^*)})$  at  $(\mathbf{y}^*, \boldsymbol{\theta}^*)$  to be surjective.

THEOREM 4.1. Let  $p_i^* := card(A_i(\boldsymbol{\theta}^*)), 1 \leq i \leq 2$  and assume  $I(\boldsymbol{\theta}^*) \neq \emptyset$ . The mapping

$$(\nabla e(\mathbf{y}^*, \boldsymbol{\theta}^*), \nabla \mathbf{g}_{1, A_1(\boldsymbol{\theta}^*)}(\boldsymbol{\theta}^*), \nabla \mathbf{g}_{2, A_2(\boldsymbol{\theta}^*)}(\boldsymbol{\theta}^*)) : \mathbb{C}^{Np} \times \mathbb{R}^p \to \mathbb{C}^{Np} \times \mathbb{R}^{p_1^*} \times \mathbb{R}^{p_2^*}$$

is surjective. In particular, for any  $(\mathbf{r}, \mathbf{s}_1, \mathbf{s}_2) \in \mathbb{C}^{Np} \times \mathbb{R}^{p_1^*} \times \mathbb{R}^{p_2^*}$  there exists a unique solution  $(\delta \mathbf{y}, \delta \boldsymbol{\theta}) \in \mathbb{C}^{Np} \times \mathbb{R}^p$  of the equation

$$(\nabla e(\mathbf{y}^*, \boldsymbol{\theta}^*)(\delta \mathbf{y}, \delta \boldsymbol{\theta}), \nabla \mathbf{g}_{1, A_1(\boldsymbol{\theta}^*)}(\boldsymbol{\theta}^*) \delta \boldsymbol{\theta}, \nabla \mathbf{g}_{2, A_2(\boldsymbol{\theta}^*)}(\boldsymbol{\theta}^*) \delta \boldsymbol{\theta}) = (\mathbf{r}, \mathbf{s}_1, \mathbf{s}_2).$$

*Proof.* For  $k \in A_1(\theta^*)$  we obviously have

$$\nabla g_{1,k'}(\boldsymbol{\theta}^*) = \begin{cases} -1 , k' = k \\ +1 , k' = k + 1 \\ 0 , \text{ otherwise} \end{cases}$$
(4.3)

whereas for  $k \in A_2(\theta^*)$ 

$$\nabla g_{2,k'}(\boldsymbol{\theta}^*) = \begin{cases} +1 , k' = k \\ -1 , k' = k + 1 \\ 0 , \text{ otherwise} \end{cases}$$
(4.4)

Since  $I(\boldsymbol{\theta}^*) \neq \emptyset$ , there exists  $q \in \{1, \dots, p\}$  such that  $q \in I(\boldsymbol{\theta}^*)$ . We renumber the controls according to  $\hat{\theta}_k^* := \theta_{q+k-1}^*, \hat{\theta}_{k+p}^* = \hat{\theta}_k^* + 2\pi, 1 \leq k \leq p$ , and set  $(\delta \boldsymbol{\theta})_k = 0$  for  $k \in I(\hat{\boldsymbol{\theta}}^*)$ . If  $A(\hat{\boldsymbol{\theta}}^*) = \emptyset$ , there is nothing to show. If  $A(\hat{\boldsymbol{\theta}}^*) \neq \emptyset$ , there exists

$$k_{min} := \min\{k \in \{2, \cdots, p\} \mid k \in A(\hat{\boldsymbol{\theta}}^*)\},\$$

Moreover, in view of  $p + 1 \in I(\hat{\boldsymbol{\theta}}^*)$ , there also exists

$$k_{max} := \min\{k \in \{k_{min} + 1, \cdots, p+1\} \mid k \in I(\hat{\boldsymbol{\theta}}^*)\}.$$

In view of (4.3),(4.4),  $(\delta \theta)_k, k_{min} \leq k \leq k_{max} - 1$ , is the unique solution of a linear algebraic system with a regular upper triangular matrix. For the computation of  $(\delta \theta)_k \in A(\hat{\theta}^*) \setminus \{k_{min}, \cdots, k_{max} - 1\}$  we proceed in the same way.

On the other hand, the equation  $\nabla e(\mathbf{y}^*, \boldsymbol{\theta}^*)(\delta \mathbf{y}, \delta \boldsymbol{\theta}) = \mathbf{r}$  can be equivalently written as

$$\mathbf{A}(\boldsymbol{\theta})\delta\mathbf{y} = \nabla_{\boldsymbol{\theta}} \Big( \mathbf{b}(\boldsymbol{\theta}^*) - \mathbf{A}(\boldsymbol{\theta}^*)\mathbf{y}^* \Big) \ \delta\boldsymbol{\theta},$$

which has a unique solution  $\delta \mathbf{y} \in \mathbb{C}^{Np}$ .  $\Box$ 

Due to Theorem 4.1, the necessary optimality conditions can be derived by the method of Lagrange multipliers.

THEOREM 4.2. Assume that  $(\mathbf{y}^*, \boldsymbol{\theta}^*) \in \mathbb{C}^{N_p} \times \mathbf{K}$  is an optimal solution of (3.5a),(3.5b). Then there exist an adjoint state  $\mathbf{p}^* \in \mathbb{C}^{N_p}$  and a multiplier  $\boldsymbol{\mu}^* = (\boldsymbol{\mu}_{1,1}^*, \boldsymbol{\mu}_{2}^*) \in \mathbb{R}^{2p}_+, \boldsymbol{\mu}_{i}^* = (\mu_{i,1}^*, \cdots, \mu_{i,p}^*)^T, 1 \leq i \leq 2$ , such that the state equation, the adjoint state equation and the gradient equation

$$\begin{split} \mathbf{A}(\boldsymbol{\theta}^*)\mathbf{y}^* - \mathbf{b}(\boldsymbol{\theta}^*) &= \mathbf{0},\\ \mathbf{A}^H(\boldsymbol{\theta}^*)\mathbf{p}^* + \mathbf{M}(\boldsymbol{\theta}^*)\mathbf{y}^* - Re(\mathbf{c}(\boldsymbol{\theta}^*)) &= \mathbf{0},\\ \nabla_{\boldsymbol{\theta}}J(\mathbf{y}^*,\boldsymbol{\theta}^*) + Re(\langle \nabla_{\boldsymbol{\theta}}(\mathbf{A}(\boldsymbol{\theta}^*)\mathbf{y}^* - \mathbf{b}(\boldsymbol{\theta}^*)),\mathbf{p}^* \rangle) + \nabla_{\boldsymbol{\theta}}\mathbf{g}_1(\boldsymbol{\theta}^*)^T\boldsymbol{\mu}_1^* + \nabla_{\boldsymbol{\theta}}\mathbf{g}_2(\boldsymbol{\theta}^*)^T\boldsymbol{\mu}_2^* &= \mathbf{0}. \end{split}$$

are satisfied as well as the complementarity conditions

$$g_{i,q}(\boldsymbol{\theta}^*) \le 0, \ \mu_{i,q}^* \ge 0, \ g_{i,q}(\boldsymbol{\theta}^*)\mu_{i,q}^* = 0, \ 1 \le q \le p, \ 1 \le i \le 2.$$

*Proof.* We introduce the Lagrangian  $L: \mathbb{C}^{Np} \times \mathbb{R}^p \times \mathbb{C}^{Np} \times \mathbb{R}^2_+$  according to

$$L(\mathbf{y},\boldsymbol{\theta},\mathbf{p},\boldsymbol{\mu}) := J(\mathbf{y},\boldsymbol{\theta}) + \operatorname{Re}(\langle e(\mathbf{y},\boldsymbol{\theta}),\mathbf{p}\rangle) + \mathbf{g}_1(\boldsymbol{\theta})^T \boldsymbol{\mu}_1 + \mathbf{g}_2(\boldsymbol{\theta})^T \boldsymbol{\mu}_2.$$

Setting  $\mathbf{x} := (\mathbf{y}, \boldsymbol{\theta}, \mathbf{p})$  and  $\mathbf{x}^* := (\mathbf{y}^*, \boldsymbol{\theta}^*, \mathbf{p}^*)$ , the first order necessary optimality conditions are given by

$$\frac{\partial L}{\partial \mathbf{y}}(\mathbf{x}^*, \boldsymbol{\mu}^*) = \mathbf{0}, \quad \frac{\partial L}{\partial \boldsymbol{\theta}}(\mathbf{x}^*, \boldsymbol{\mu}^*) = \mathbf{0}, \quad \frac{\partial L}{\partial \mathbf{p}}(\mathbf{x}^*, \boldsymbol{\mu}^*) = \mathbf{0}, \quad (4.5a)$$

$$\frac{\partial L}{\partial \boldsymbol{\mu}_i} (\mathbf{x}^*, \boldsymbol{\mu}^*)^T (\boldsymbol{\nu}_i - \boldsymbol{\mu}_i^*) \le 0, \quad \boldsymbol{\nu}_i \in \mathbb{R}^p_+, \ 1 \le i \le 2.$$
(4.5b)

The state equation, the adjoint state equation, and the gradient equation result from the third, first, and second equation in (4.5a), whereas the complementarity conditions are a consequence of (4.5b).  $\Box$ 

5. Projected gradient method. The projected gradient method is based on the formulation of the gradient equation as the variational inequality

$$-\nabla_{\theta} J(\mathbf{y}^*, \boldsymbol{\theta}^*) + \operatorname{Re}(\langle \nabla_{\theta} (\mathbf{b}(\boldsymbol{\theta}^*) - \mathbf{A}(\boldsymbol{\theta}^*) \mathbf{y}^*), \mathbf{p}^* \rangle) \in \partial I_{\mathbf{K}},$$

where  $\partial I_{\mathbf{K}}$  is the subdifferential of the indicator function of the constraint set  $\mathbf{K}$ .

## **Projected Gradient Method:**

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**Step 1:** Choose an initial control  $\boldsymbol{\theta}^{(0)} \in \mathbf{K}$  and a tolerance TOL > 0 and set n = 0. **Step 2.1:** Set n = n + 1 and compute  $\mathbf{y}^{(n)} \in \mathbb{C}^{Np}$  and  $\mathbf{p}^{(n)} \in \mathbb{C}^{Np}$  as the unique solutions of the state equation

$$\mathbf{A}(\boldsymbol{\theta}^{(n-1)})\mathbf{y}^{(n)} = \mathbf{b}(\boldsymbol{\theta}^{(n-1)})$$

and of the adjoint state equation

$$\mathbf{A}^{H}(\boldsymbol{\theta}^{(n-1)})\mathbf{p}^{(n)} = \operatorname{Re}(\mathbf{c}(\boldsymbol{\theta}^{(n-1)})) - \mathbf{M}(\boldsymbol{\theta}^{(n-1)})\mathbf{y}^{(n)}.$$

**<u>Step 2.2</u>**: Compute  $\tilde{\boldsymbol{\theta}}^{(n)} \in \mathbb{R}^p$  according to

$$\tilde{\boldsymbol{\theta}}^{(n)} = \boldsymbol{\theta}^{(n-1)} - \kappa \left( \nabla_{\boldsymbol{\theta}} J(\mathbf{y}^{(n)}, \boldsymbol{\theta}^{(n-1)}) + \operatorname{Re}(\langle \nabla_{\boldsymbol{\theta}} (\mathbf{A}(\boldsymbol{\theta}^{(n-1)}) \mathbf{y}^{(n)}) - \mathbf{b}(\boldsymbol{\theta}^{(n-1)}) \right), \mathbf{p}^{(n)} \rangle),$$

where  $\kappa > 0$  is the Armijo line search parameter.

**Step 2.3:** Compute  $\theta^{(n)}$  as the projection of  $\tilde{\theta}^{(n)}$  onto the constraint set **K**. **Step 2.4:** If n > 1 and

$$|J(\mathbf{y}^{(n)}, \boldsymbol{\theta}^{(n)}) - J(\mathbf{y}^{(n-1)}, \boldsymbol{\theta}^{(n-1)})| < TOL,$$

stop the algorithm. Otherwise, go to Step 2.1.

We will provide some details regarding the numerical realization of **Step 2.2**. For the update formula we need to compute the following quantity:

$$abla_{ heta} J\left(oldsymbol{y},oldsymbol{ heta}
ight) + \operatorname{Re}\left(\left< 
abla_{ heta} oldsymbol{A}\left(oldsymbol{ heta}
ight) oldsymbol{y} - oldsymbol{b}\left(oldsymbol{ heta}
ight), oldsymbol{p}
ight
angle
ight).$$

For the computation of  $\nabla_{\theta} J(\boldsymbol{y}, \boldsymbol{\theta})$  we recall from (3.5a) that

$$J(\boldsymbol{y},\boldsymbol{\theta}) = \frac{1}{2} \langle \boldsymbol{M}(\boldsymbol{\theta}) \, \boldsymbol{y}, \boldsymbol{y} \rangle - \operatorname{Re}\left( \langle \boldsymbol{c}(\boldsymbol{\theta}), \boldsymbol{y} \rangle \right), \qquad (5.1)$$

where the  $Np \times Np$  matrix  $\boldsymbol{M}(\boldsymbol{\theta})$  and the Np vector  $\boldsymbol{c}(\boldsymbol{\theta})$  are given by (3.4). Moreover, according to (3.5b) the vector  $\boldsymbol{y} = (y_1, \cdots, y_{Np})^T$  is the unique solution of

$$\boldsymbol{A}\left(\boldsymbol{\theta}\right)\boldsymbol{y}=\boldsymbol{b}\left(\boldsymbol{\theta}\right),$$

where the  $Np \times Np$  matrix  $\boldsymbol{A}(\boldsymbol{\theta})$  and the Np vector  $\boldsymbol{b}(\boldsymbol{\theta})$  are given by (2.18). We note that for any two given basis functions  $\phi_h^{(k)}$  and  $\phi_h^{(\ell)}$  either,

$$\mu\left(\operatorname{supp}\left(\phi_{h}^{(k)}\right)\cap\operatorname{supp}\left(\phi_{h}^{(\ell)}\right)\right)=0$$

or,

$$\operatorname{supp}\left(\phi_{h}^{(k)}\right)\cap\operatorname{supp}\left(\phi_{h}^{(\ell)}\right)=T\in\mathcal{T}_{h}(\Omega),$$

where  $\mu$  is the 2-D Lebesgue measure. Let  $T_{k,\ell}, 1 \leq k, \ell \leq Np$ , be defined as

$$T_{k,\ell} := \begin{cases} \emptyset & , \text{ if } \mu\left(\sup\left(\phi_h^{(k)}\right) \cap \sup\left(\phi_h^{(\ell)}\right)\right) = 0\\ \sup\left(\phi_h^{(k)}\right) \cap \sup\left(\phi_h^{(\ell)}\right) & , \text{ otherwise} \end{cases}$$

and let  $T_{\ell}, 1 \leq \ell \leq Np$  be given by

$$T_{\ell} := \operatorname{supp}\left(\phi_{h}^{(\ell)}\right) \in \mathcal{T}_{h}(\Omega).$$

Hence, we can rewrite (3.4) as

$$m_{k\ell}(\boldsymbol{\theta}) := \int_{T_{k,\ell}} \exp\left(i\omega \boldsymbol{d}_k \cdot \boldsymbol{x}\right) \overline{\exp\left(i\omega \boldsymbol{d}_\ell \cdot \boldsymbol{x}\right)} d\boldsymbol{x} \quad , \quad 1 \le k, \ell \le Np,$$

$$c_{\ell}(\boldsymbol{\theta}) := \int_{T_{\ell}} u_d \overline{\exp\left(i\omega \boldsymbol{d}_\ell \cdot \boldsymbol{x}\right)} d\boldsymbol{x} \quad , \quad 1 \le \ell \le Np.$$
(5.2)

In view of (5.1) we obtain

$$\nabla_{\theta} J\left(\boldsymbol{y}, \boldsymbol{\theta}\right) = \nabla_{\theta} \left( \frac{1}{2} \sum_{k,\ell=1}^{N_{p}} m_{k\ell}(\boldsymbol{\theta}) y_{k} \overline{y_{\ell}} \right) - \nabla_{\theta} \left( \operatorname{Re} \sum_{k=1}^{N_{p}} c_{k}(\boldsymbol{\theta}) \overline{y_{k}} \right).$$
(5.3)

,

Differentiating (5.2) with respect to  $\theta_j$  it follows that

$$\frac{\partial}{\partial \theta_{j}} \left( \frac{1}{2} \sum_{k,\ell=1}^{N_{p}} m_{kl}(\theta) y_{\ell} \overline{y_{k}} \right) = \\
\frac{1}{2} \left( \sum_{\ell=1}^{N_{p}} y_{j} \overline{y_{\ell}} \int_{T_{j,\ell}} \left( i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{j} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{\ell} \cdot \boldsymbol{x})} d\boldsymbol{x} + \\
\sum_{\ell=1}^{N_{p}} y_{\ell} \overline{y_{j}} \int_{T_{j,\ell}} \left( -i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{\ell} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{j} \cdot \boldsymbol{x})} d\boldsymbol{x} \right) = \\
\frac{1}{2} \left( \sum_{\ell=1}^{N_{p}} y_{j} \overline{y_{\ell}} \int_{T_{j,\ell}} \left( i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{j} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{\ell} \cdot \boldsymbol{x})} d\boldsymbol{x} + \\
\sum_{\ell=1}^{N_{p}} \overline{y_{j} \overline{y_{\ell}}} \int_{T_{j,\ell}} \left( i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{j} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{\ell} \cdot \boldsymbol{x})} d\boldsymbol{x} + \\
\sum_{\ell=1}^{N_{p}} \overline{y_{j} \overline{y_{\ell}}} \int_{T_{j,\ell}} \left( i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{j} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{\ell} \cdot \boldsymbol{x})} d\boldsymbol{x} \right) = \\
\operatorname{Re} \sum_{\ell=1}^{N_{p}} y_{j} \overline{y_{\ell}} \int_{T_{j,\ell}} \left( i \omega d_{j}^{*} \cdot \boldsymbol{x} \right) \exp(i \omega d_{j} \cdot \boldsymbol{x}) \cdot \overline{\exp(i \omega d_{\ell} \cdot \boldsymbol{x})} d\boldsymbol{x} , \\$$

where  $d_j^* = (-\sin(\theta_j), \cos(\theta_j))^T$ . Moreover, we obtain

$$\frac{\partial}{\partial \theta_j} \left( \operatorname{Re} \sum_{k=1}^{Np} c_k(\boldsymbol{\theta}) \overline{y_k} \right) = \operatorname{Re} \left( \overline{y_j} \int_{\Omega} \left( -i\omega \boldsymbol{d}_j^* \cdot \boldsymbol{x} \right) u_d \overline{\exp(i\omega \boldsymbol{d}_j \cdot \boldsymbol{x})} d\boldsymbol{x} \right).$$
(5.5)

On the other hand, for  $\operatorname{Re}\left( \nabla_{\theta} \left\langle \boldsymbol{A}\left( \boldsymbol{\theta} \right) \boldsymbol{y} - \boldsymbol{b}\left( \boldsymbol{\theta} \right), \boldsymbol{p} \right\rangle \right)$  we have

$$\operatorname{Re}\left(\frac{\partial}{\partial\theta_{j}}\left\langle \boldsymbol{A}\left(\boldsymbol{\theta}\right)\boldsymbol{y}-\boldsymbol{b}\left(\boldsymbol{\theta}\right),\boldsymbol{p}\right\rangle\right)=\operatorname{Re}\left(\frac{\partial}{\partial\theta_{j}}\sum_{k,\ell=1}^{Np}\left(a_{k\ell}(\boldsymbol{\theta})\boldsymbol{y}_{\ell}-b_{k}(\boldsymbol{\theta})\right)\overline{p_{k}}\right)=$$

$$\operatorname{Re}\left(\sum_{k,\ell=1}^{Np}\left(\frac{\partial a_{kl}(\boldsymbol{\theta})}{\partial\theta_{j}}\boldsymbol{y}_{l}-\frac{\partial b_{k}(\boldsymbol{\theta})}{\partial\theta_{j}}\right)\overline{p_{k}}\right).$$
(5.6)

We obtain the derivatives  $\frac{\partial a_{kl}(\theta)}{\partial \theta_j}$  and  $\frac{\partial b_k(\theta)}{\partial \theta_j}$  by directly differentiating the formulas in (2.18).

Using (5.4)-(5.6) provides the update formula in **Step 2.2** of the projected gradient method.

6. Numerical results. As in [9, 10] we consider the Helmholtz problem (2.1a), (2.1b) in  $\Omega = (0, 1) \times (-0.5, +0.5)$  with  $\omega = 10$  and g in (2.1b) being chosen such that the exact solution u (in polar coordinates) is given by

$$u(r,\varphi) = J_{\xi}(\omega r) \cos(\xi \varphi), \quad \xi \ge 0,$$

where  $J_{\xi}$  stands for the Bessel function of the first kind and order  $\xi$ . We note that for  $\xi \in \mathbb{N}$  the solution is regular, whereas for  $\xi \notin \mathbb{N}$  the solution satisfies  $u \in H^{1+\xi-\varepsilon}(\Omega)$ 



FIG. 6.1. Example 1: The computational domain  $\Omega$  and the simplicial triangulation  $\mathcal{T}_h(\Omega)$  for the PWDG method (top left). The exact solution for  $\xi = 1$  (top right),  $\xi = 2/3$  (bottom left), and  $\xi = 3/2$  (bottom right).

for any  $\varepsilon > 0$  and its derivatives have a singularity at the origin. Figure 6.1 displays the exact solution for  $\xi = 1$  (top right),  $\xi = 2/3$  (bottom left), and  $\xi = 3/2$  (bottom right).

For  $\xi = 1$ ,  $\xi = 2/3$ , and  $\xi = 3/2$  the PWDG method has been implemented with respect to a geometrically conforming simplicial triangulation  $\mathcal{T}_h(\Omega)$  consisting of eight isosceles triangles (cf. Figure 6.1 (top left)). The parameters  $\alpha, \beta$ , and  $\delta$  in the PWDG method (2.9a),(2.9b) are chosen either according to

$$\alpha = \beta = \delta = 0.5 \tag{6.1}$$

as in the ultraweak variational formulation by Cessenat and Després [3] or by means of

$$\alpha = \beta^{-1} = \delta^{-1} = \frac{10p}{\omega h \log(p)} \tag{6.2}$$

as suggested in [10]. For the optimization of the plane wave directions, the desired state  $u^d$  in the objective functional J (cf. (3.3a)) has been chosen as the exact solution, and for the projected gradient method the initial distribution  $\theta_0$  has been chosen as either uniform as in [10] or random as suggested by Cessenat and Després. We note that the optimization problem has multiple local minima and hence, starting at different initial distributions the algorithm may terminate at different local minima. For  $\xi = 1$  Figure 6.2 and for  $\xi = 2/3$  Figure 6.3 display the global discretization error  $u - u_h$  in the L<sup>2</sup>-norm  $\|\cdot\|_{0,\Omega}$  as a function of the number p of plane wave basis functions. For the choice of the parameters  $\alpha, \beta$ , and  $\delta$  according to (6.1), the results A. Agrawal and R.H.W. Hoppe



FIG. 6.2. Example 1: The  $L^2$ -error  $||u - u_h||_{0,\Omega}$  as a function of the number p of plane wave basis functions for  $\xi = 1$ : Parameter choice (6.1) and uniform initial distribution  $\theta_0$  (top left), parameter choice (6.1) and random initial distribution  $\theta_0$  (top right), parameter choice (6.2) and uniform initial distribution  $\theta_0$  (bottom left), parameter choice (6.2) and random initial distribution  $\theta_0$  (bottom right).

for a uniform initial distribution  $\theta_0$  of the plane wave directions are top left and for a random initial distribution  $\theta_0$  they are shown top right. On the other hand, if the parameters  $\alpha, \beta$ , and  $\delta$  are chosen by means of (6.2), the results for a uniform initial distribution  $\theta_0$  are displayed bottom left, whereas for a random initial distribution  $\theta_0$ they are shown bottom right. We see that both in case of a regular solution ( $\xi = 1$ ) and of a singular solution ( $\xi = 2/3$ ) the uniform distribution of  $\theta_0$  is optimal except for p = 3, 5, 7, 9 where it is almost optimal (cf. Figure 6.4 for  $\xi = 2/3$  and p = 5). However, for a random initial distribution  $\theta_0$  the computed optimal distribution yields a reduction in the L<sup>2</sup>-error  $||u-u_h||_{0,\Omega}$  up to one order of magnitude. Figure 6.5 shows the randomly chosen initial distribution and the computed optimal distribution for  $\xi = 1$  and p = 7.

The (almost) optimality of the uniform distribution of the plane wave directions is probably due to the fact that the solution is symmetric (with respect to the  $x_1$ -axis). Moreover, we see that the difference between the two parameter choices (6.1) and (6.2) is only marginal. The results for the case  $\xi = 3/2$  are very similar and are thus omitted.

We note that the condition number of the matrix  $\mathbf{A}(\boldsymbol{\theta})$  deteriorates with increasing number p of plane wave basis functions so that roundoff errors may effect the convergence. For  $\xi = 1$  we observe such a behavior for  $p \geq 23$  (cf. Figure 6.2), whereas in the singular case  $\xi = 2/3$  a slowdown of the convergence can already be seen for  $p \geq 17$  (cf. Figure 6.3).



FIG. 6.3. Example 1: The  $L^2$ -error  $||u - u_h||_{0,\Omega}$  as a function of the number p of plane wave basis functions for  $\xi = 2/3$ : Parameter choice (6.1) and uniform initial distribution  $\theta_0$  (top left), parameter choice (6.1) and random initial distribution  $\theta_0$  (top right), parameter choice (6.2) and uniform initial distribution  $\theta_0$  (bottom left), parameter choice (6.2) and random initial distribution  $\theta_0$  (bottom right).



FIG. 6.4. Example 1: Uniform initial distribution  $\theta_0$  of the plane wave directions (red dotted line) and the computed optimal distribution (blue solid line) for  $\xi = 2/3$  and p = 5: Parameter choice (6.1) left and parameter choice (6.2) right.

Example 2: The second example deals with a screen problem which describes an



FIG. 6.5. Example 1: Randomly chosen initial distribution  $\theta_0$  of the plane wave directions (red dotted line) and the computed optimal distribution (blue solid line) for  $\xi = 1$  and p = 7: Parameter choice (6.1) left and parameter choice (6.2) right.

acoustic wave scattered at a sound-soft scatterer:

$$-\Delta u - \omega^2 u = f \quad \text{in } \Omega, \tag{6.3a}$$

$$\mathbf{n} \cdot \nabla u + i\omega u = g \quad \text{on } \Gamma_R,\tag{6.3b}$$

$$u = 0 \quad \text{on } \Gamma_D, \tag{6.3c}$$

The computational domain is given by  $\Omega := (-1, +1)^2 \setminus (S_1 \cup S_2)$  where

$$S_1 := \operatorname{conv}((0,0), (-0.25, +0.50), (-0.50, +0.50)),$$
  

$$S_2 := \operatorname{conv}((0,0), (+0.25, -0.50), (+0.50, -0.50)).$$

Moreover,  $\Gamma_R = \partial (-1, +1)^2$  and  $\Gamma_D := \partial S_1 \cup \partial S_2$ . The right-hand sides f and g are chosen according to  $f \equiv 0$  and

$$g = \cos(\omega x_2) + i\sin(\omega x_2).$$

The exact solution u is not known explicitly. As a substitute for the exact solution we have used an approximate solution  $u_s$  computed by the adaptive Interior Penalty Discontinuous Galerkin method from [12] with a sufficiently large number of refinement steps. For  $\omega = 15$ , the approximate solution  $u_s$  is displayed in Figure 6.6 (right).

The PWDG method has been implemented with respect to a geometrically conforming simplicial triangulation  $\mathcal{T}_h(\Omega)$  shown in Figure 6.6 (left). The parameters  $\alpha, \beta$ , and  $\delta$ of the PWDG method have been chosen according to (6.1). For the optimization, we have chosen  $u_d$  in the objective functional as the substitute solution  $u_s$ . Moreover, for the projected gradient method the initial distribution  $\boldsymbol{\theta}_0$  of the plane wave directions has been chosen as a uniform distribution.

In this example, the effect of roundoff errors due to ill-conditioned PWDG matrices  $\mathbf{A}(\boldsymbol{\theta})$  already sets in for  $p \geq 11$  so that we restrict the numerical results to  $3 \leq p \leq 9$ . Figure 6.7 shows the uniformly chosen initial distribution  $\boldsymbol{\theta}_0$  and the computed optimal distribution of the plane wave directions for p = 3, 5, 7, and p = 9 (from top left to bottom right). In these cases the L<sup>2</sup> error  $||u - u_h||_{0,\Omega}$  is reduced by up to 20 %. Compared to Example 1, the non-optimality of the uniform distribution is due to the fact that the solution of the screen problem is not symmetric.



FIG. 6.6. Example 2: The computational domain  $\Omega$  and the simplicial triangulation  $\mathcal{T}_h(\Omega)$  for the PWDG method (left; the sound-soft scatterer is shown in blue). The substitute solution  $u_s$  computed by the adaptive Interior Penalty Discontinuous Galerkin method from [12] (right).



FIG. 6.7. Example 2: Uniform initial distribution  $\theta_0$  of the plane wave directions (red dotted line) and the computed optimal distribution (blue solid line) for p = 3 (top left), p = 5 (top right), p = 7 (bottom left), and p = 9 (bottom right).

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