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# Approximation of constrained problems using the PGD method with application to pure Neumann problems

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## Abstract

In this paper we introduce, analyze, and compare several approaches designed to incorporate a linear (or affine) constraint within the Proper Generalized Decomposition framework. We apply the considered methods and numerical strategies to two classes of problems: the pure Neumann case where the role of the constraint is to recover unicity of the solution; and the Robin case, where the constraint forces the solution to move away from the already existing unique global minimizer of the energy functional.

**Keywords:** Model Reduction, Separation of Variables, Low-rank Approximation, Tensor Product Approximation, Proper Generalized Decomposition (PGD), Constrained Problem, Mixed Formulation

## 1 Introduction

The need for fast evaluation of surface responses in parametric analyses has spurred the development of novel model reduction methods to construct, in an effective manner, solutions to boundary-value problems. One such method is the Proper Generalized Decomposition (PGD) framework [10, 11], in which the solution is sought numerically using the concept of separation of variables. The PGD approximation scheme allows one to simplify a complex problem into a set of coupled problems, defined with respect to each spatial and/or parametric variable, which can be further decoupled using the so-called Alternated Directions scheme [2, 11]. There exist to date a variety of PGD methods [22], which have been adapted to the nature of the problem at hand and which have been successfully tested on a wide range of applications and model problems, see e.g. [3, 5, 6, 8, 9, 12, 23, 26, 28]. Yet, and to the best of the authors' knowledge, none of these applications include problems subjected to constraints defined on the solution space, except, maybe, the case of the incompressible Navier-Stokes equations, for which the divergence-free constraint is treated using a fractional-step or projection method [14, 15]. We also mention the works presented in [1, 17] and

the references therein where a penalization formulation is used to circumvent the mixed formulation arising from the constrained problem.

The objective of the paper is therefore to study how a general boundary-value problem involving a linear or affine constraint can be treated within the PGD setting. For the sake of simplicity in the exposition, but without loss of generality, the model problem that we have chosen to focus on consists of a two-dimensional Poisson equation with pure Neumann boundary conditions prescribed on the whole boundary of the domain. It is well-known that the solution of such a problem is given only within a constant and that one needs to prescribe an extra constraint on the solution in order to fix the constant [4]. The main challenge in applying a constraint functional within the PGD framework arises from the fact that the coupled problem is decoupled into subproblems with respect to each spatial and/or parametric variable while the constraint should be applied to the solution globally. Classical methods to enforce constraints are the Penalization, Lagrange Multiplier, and Augmented Lagrangian methods [24]. Our goal here is to see if and how these methods and their numerical implementations (direct, Uzawa, iterative Uzawa) can be extended to the case of PGD formulations.

The paper is organized as follows: In Section 2, we first describe the model problem, namely a pure Neumann boundary-value problem in terms of the Poisson equation. We then review different approaches, namely Penalization, Lagrange Multiplier, and Augmented Lagrangian methods, to impose a constraint in order to recover the unicity of the solution. We also introduce a Robin boundary-value problem as a perturbation of the Neumann problem. The main difference with the latter is that it already admits a unique solution without resorting to any constraint on the solution. We will nevertheless consider a constrained Robin problem in order to compare the influence of the methods on the behavior of the solution with the case of the pure Neumann problem. In Section 3, we briefly describe the finite element discretization of the constrained problems and review some classical numerical strategies for solving these problems. In Section 4, we recall the Proper Generalized Decomposition framework and extend above methods and strategies to the PGD formulation of the constrained problems. Numerical examples are presented in Section 5 to analyze the performance of each of the methods to the Neumann and Robin problems. We finally provide some concluding remarks in Section 6.

## 2 Model problem

Let  $d \in \mathbb{N}$  be such that  $d \geq 2$  and let  $\Omega_i$  be open intervals  $(a_i, b_i) \subset \mathbb{R}$ ,  $i = 1, \dots, d$  such that the domain  $\Omega = \prod_{i=1}^d \Omega_i$  forms an open, hyper-rectangular, bounded subset of  $\mathbb{R}^d$  with boundary  $\partial\Omega$ . We shall denote by  $\mathbf{n}$  the outward normal unit vector to  $\Omega$  and by  $|\Omega|$  a measure of  $\Omega$ .

We consider in this paper the so-called pure Neumann boundary-value problem:

$$\text{Find } u \text{ such that } \begin{cases} -\nabla \cdot (a\nabla u) = f, & \text{in } \Omega, \\ \mathbf{n} \cdot a\nabla u = g, & \text{on } \partial\Omega, \end{cases} \quad (2.1)$$

where  $a = a(x) \in L^\infty(\Omega)$  is strictly positive and the data  $f \in L^2(\Omega)$  and  $g \in H^{1/2}(\partial\Omega)$  are given such that the so-called compatibility condition

$$\int_{\Omega} f \, dx + \int_{\partial\Omega} g \, ds = 0, \quad (2.2)$$

is satisfied. In that case, the Fredholm alternative implies that above problem admits solutions up to an additive constant [4].

A weak formulation associated with Problem (2.1) reads:

$$\text{Find } u \in H^1(\Omega) \text{ such that } b(u, v) = \ell(v), \quad \forall v \in H^1(\Omega), \quad (2.3)$$

where the bilinear form  $b$  and linear form  $\ell$  continuous on  $H^1(\Omega)$  are given by

$$\begin{aligned} b(u, v) &= \int_{\Omega} a\nabla u \cdot \nabla v \, dx, \\ \ell(v) &= \int_{\Omega} f v \, dx + \int_{\partial\Omega} g v \, ds. \end{aligned} \quad (2.4)$$

Alternatively, Problem (2.3) can be recast as a minimization problem by introducing the energy functional

$$J(u) = \frac{1}{2}b(u, u) - \ell(u), \quad (2.5)$$

and minimizing  $J$  over  $H^1(\Omega)$ .

Solutions to Problems (2.3) or (2.5) are not unique in  $H^1(\Omega)$  since the bilinear form  $b$  fails to be coercive in that space. In practice, unicity of the solution is often recovered by imposing the value of the solution at a given point in  $\Omega$  or on  $\partial\Omega$ . Unfortunately, this approach yields an ill-posed problem as the point-value functional is not well defined for functions of  $H^1(\Omega)$  when  $d \geq 2$ . A proper way to proceed is to search solutions in the subspace  $V$  of  $H^1(\Omega)$  of zero-mean functions [4]

$$V = \left\{ v \in H^1(\Omega); \frac{1}{|\Omega|} \int_{\Omega} v \, dx = 0 \right\}, \quad (2.6)$$

often referred to as the quotient space and denoted by  $V = H^1(\Omega)/\mathbb{R}$ . Since the bilinear form  $b$  is coercive over  $V$ , the problem

$$\text{Find } u \in V \text{ such that } b(u, v) = \ell(v), \quad \forall v \in V, \quad (2.7)$$

is now well-posed. However, when considering discretization methods such as the Finite Element Method, Problem (2.7) is never solved as is, as it is difficult to construct trial and test functions

with zero-mean. Instead, one reformulates the problem as a constrained problem by minimizing  $J$  over  $V$ , that is, by minimizing  $J$  over  $H^1(\Omega)$  subjected to the constraint that the solution has zero-mean. Let  $q$  denote the functional in  $H^{-1}(\Omega)$  such that

$$q(v) = \frac{1}{|\Omega|} \int_{\Omega} v \, dx. \quad (2.8)$$

The zero-mean constraint on function  $u \in H^1(\Omega)$  now reads  $q(u) = 0$ .

In this paper we shall consider a class of problems that is slightly larger in two respects. First, the linear constraint  $q(u) = 0$  will be replaced by the affine constraint  $q(u) = \gamma$ , where  $\gamma \in \mathbb{R}$  is a prescribed mean. Secondly, the constraint will be further extended to the case where the solution has a prescribed mean on a subset  $\omega \subset \Omega$ , which will be denoted as  $q_{\omega}(u) = \gamma$  where

$$q_{\omega}(v) = \frac{1}{|\omega|} \int_{\omega} v \, dx. \quad (2.9)$$

For simplicity, we will drop the  $q_{\omega}$  notation and simply refer to this linear functional as  $q$ .

In this setting, the strong form of the constrained pure Neumann problem reads

$$\text{Find } u \text{ such that } \begin{cases} -\nabla \cdot (a \nabla u) = f, & \text{in } \Omega, \\ \mathbf{n} \cdot a \nabla u = g, & \text{on } \partial\Omega, \\ q(u) = \gamma. \end{cases} \quad (2.10)$$

The standard way to impose constraints is by the introduction of the Lagrangian functional: for  $(u, \lambda) \in H^1(\Omega) \times \mathbb{R}$  consider the functional

$$\mathcal{L}(u, \lambda) = J(u) + \lambda(q(u) - \gamma), \quad (2.11)$$

where  $\lambda \in \mathbb{R}$  is the so-called Lagrange multiplier.

The saddle-point formulation of  $\mathcal{L}$  over  $H^1(\Omega) \times \mathbb{R}$  yields the mixed problem

$$\text{Find } (u, \lambda) \in H^1(\Omega) \times \mathbb{R} \text{ such that } \begin{cases} b(u, v) + \lambda q(v) = \ell(v), & \forall v \in H^1(\Omega), \\ \tau q(u) = \tau \gamma, & \forall \tau \in \mathbb{R}. \end{cases} \quad (2.12)$$

**Remark 1** An alternative approach is to take into account the constraint  $q(u) = \gamma$ , although not exactly, by considering a penalized formulation where the goal is to minimize  $J(u) + \frac{\beta}{2}(q(u) - \gamma)^2$  over  $H^1(\Omega)$ , with  $\beta > 0$  a fixed penalization parameter. In that case, the penalization problem reads

$$\text{Find } u_{\beta} \in H^1(\Omega) \text{ such that } b(u_{\beta}, v) + \beta q(u_{\beta})q(v) = \ell(v) + \beta \gamma q(v), \quad \forall v \in H^1(\Omega), \quad (2.13)$$

where the bilinear form on the left-hand side is coercive over  $H^1(\Omega)$  due to the addition of the “mass-term” governed by parameter  $\beta$ . The penalization problem (2.13) is thus well-posed.

The corresponding strong form of the problem reads in that case

$$\text{Find } u_{\beta} \text{ such that } \begin{cases} -\nabla \cdot (a \nabla u_{\beta}) + \frac{\beta}{|\omega|} q(u_{\beta}) = f + \frac{\beta}{|\omega|} \gamma, & \text{in } \Omega, \\ \mathbf{n} \cdot a \nabla u_{\beta} = g, & \text{on } \partial\Omega. \end{cases} \quad (2.14)$$

**Remark 2** *The so-called Augmented Lagrangian method is yet another way of taking the constraint  $q(u) = \gamma$  into account and can be seen as a trade-off between the Lagrangian and the penalization methods. In this method, the mixed problem to be solved is*

$$\text{Find } (u, \lambda) \in H^1(\Omega) \times \mathbb{R} \text{ such that} \quad \begin{cases} b(u, v) + \lambda q(v) + \beta q(u)q(v) = \ell(v) + \beta\gamma q(v), & \forall v \in H^1(\Omega), \\ \tau q(u) = \tau\gamma, & \forall \tau \in \mathbb{R}. \end{cases} \quad (2.15)$$

In order to highlight the performances of the different methods and numerical strategies for solving (2.12), e.g. the Lagrangian or Uzawa methods, we also introduce a class of perturbed problems where the pure Neumann boundary condition in (2.10) is replaced by a Robin boundary condition with an impedance coefficient controlled by a parameter  $\varepsilon > 0$ , i.e. the strong form of the Robin problem reads

$$\text{Find } u \text{ such that} \quad \begin{cases} -\nabla \cdot (a\nabla u) = f, & \text{in } \Omega, \\ \mathbf{n} \cdot a\nabla u + \varepsilon u = g, & \text{on } \partial\Omega, \\ q(u) = \gamma. \end{cases} \quad (2.16)$$

In this Robin problem, the role of the constraint is not to enforce unicity: the mass term on the boundary controlled by  $\varepsilon$  provides a coercive bilinear form on  $H^1(\Omega)$  so the solution of the unconstrained Robin problem is unique for any fixed  $\varepsilon$ . The role of the constraint is to force the unconstrained solution to move away from the global minimum of the energy functional  $J$ . For any fixed  $\varepsilon$ , the solution of the constrained Robin problem (2.16) is unique and the standard Lagrangian approach yields the mixed problem:

$$\text{Find } (u, \lambda) \in H^1(\Omega) \times \mathbb{R} \text{ such that} \quad \begin{cases} b_\varepsilon(u, v) + \lambda q(v) = \ell(v), & \forall v \in H^1(\Omega), \\ \tau q(u) = \tau\gamma, & \forall \tau \in \mathbb{R}, \end{cases} \quad (2.17)$$

where  $b_\varepsilon(u, v) = b(u, v) + \varepsilon \int_{\partial\Omega} uv \, ds$ . For simplicity, we will drop the  $b_\varepsilon$  notation and simply refer to this bilinear form by  $b$  when the context is clear.

The perturbed problem (2.16) provides a solution  $u_\varepsilon$  that converges to the solution  $u$  of (2.10) as  $\varepsilon$  goes to zero. The fact that we introduce this problem here will become clear when we consider the Uzawa method, which is introduced in Section 3.3.

### 3 Finite element formulations of constrained problems

In this section, we derive the finite element formulations of the above constrained problems. Whenever relevant, we also highlight the differences between the Neumann and Robin problems. Here, and in the remainder of the paper, we consider a general conforming finite element space  $V_h = \text{span} \{ \varphi_i \} \subset H^1(\Omega)$  where the  $\varphi_i$ 's define  $n$  basis functions, i.e.  $n = \dim V_h$ . We also assume that the corresponding mesh satisfies the usual regularity properties, see [13].

### 3.1 Penalization method

The finite element problem corresponding to the penalization approach (2.13) is given by

$$\text{Find } u_h \in V_h \text{ such that } b(u_h, v_h) + \beta q(u_h)q(v_h) = \ell(v_h) + \beta\gamma q(v_h), \quad \forall v_h \in V_h. \quad (3.1)$$

The linear system associated with this finite-dimensional problem is of the form

$$(K + \beta QQ^T)U = F + \beta\gamma Q, \quad (3.2)$$

where  $K_{ij} = b(\varphi_j, \varphi_i)$ ,  $Q_i = q(\varphi_i)$ ,  $F_i = \ell(\varphi_i)$  and the solution vector  $U$  collects the degrees of freedom of  $u_h$ , i.e.  $u_h = \sum_{i=1}^n U_i \varphi_i$ . The rank-one matrix  $\beta QQ^T$  can be viewed as a correction to the original (unconstrained) stiffness matrix  $K$ . In the pure Neumann case, the original stiffness matrix  $K$  is positive semi-definite, with a rank deficiency of one, while the matrix  $K + \beta QQ^T$  is positive definite.

Drawbacks of the penalization approach are now briefly recalled. First, the choice of  $\beta$  has a strong influence on the numerical solution. Second, depending on the value of  $\beta$ , the condition number of the matrix can become very high and adversely affect the accuracy of the approach. Asymptotically, we observed in the considered numerical experiments that  $\kappa = \mathcal{O}(\beta)$ , where  $\kappa$  denotes the scaled condition number of the stiffness matrix based on the  $\|\cdot\|_2$  vector norm. Third, due to the addition of the term  $QQ^T$  in the stiffness matrix, the sparsity of the matrix is lost and the cost of the method increases. Finally, we mention that one can recover an approximation of the Lagrange multiplier  $\lambda$  by computing  $\beta(Q^T U - \gamma)$ .

### 3.2 Lagrangian method

The mixed finite element problem on  $V_h \times \mathbb{R}$  corresponding to the Lagrangian approach (2.12) or (2.17) is given by

$$\text{Find } (u_h, \lambda) \in V_h \times \mathbb{R} \text{ such that } \begin{cases} b(u_h, v_h) + \lambda q(v_h) = \ell(v_h), & \forall v_h \in V_h, \\ \tau q(u_h) = \tau\gamma, & \forall \tau \in \mathbb{R}. \end{cases} \quad (3.3)$$

The linear system associated with this finite-dimensional problem is in this case of the form

$$\begin{bmatrix} K & Q \\ Q^T & 0 \end{bmatrix} \begin{bmatrix} U \\ \lambda \end{bmatrix} = \begin{bmatrix} F \\ \gamma \end{bmatrix}. \quad (3.4)$$

The system could be directly solved as given since the augmented matrix is indeed non-singular. However, its size is also larger, which results in higher computational cost, as the constraint is globally applied to the solution. Our goal is nevertheless to decouple the system in order to preserve the efficiency of the PGD approximation solution process. This issue will be dealt with in Section 4.2.

The presence of the entry zero on the diagonal of the resulting matrix prevents one from uncoupling the solution  $U$  from the Lagrange multiplier  $\lambda$ . The next method aims at circumventing this issue.



### 3.3 Uzawa method

The Uzawa method [24, 25] is a numerical strategy aiming at decoupling the constraint from the original problem in (3.4). Two versions of the method are available: the first one, referred to as direct Uzawa, relies on the evaluation of the Schur complement to compute the Lagrange multiplier; the second one, the so-called iterative Uzawa, computes a sequence approximating the Lagrange multiplier within an iterative scheme. However, both methods need for  $K$  to be invertible, which is the case for the Robin problem, but not for the Neumann problem. *In the rest of this section, we will thus consider only the Robin problem.*

**Direct Uzawa:** let us develop the linear system of equations for (3.4) as

$$\begin{cases} KU + Q\lambda = F, \\ Q^T U = \gamma. \end{cases} \quad (3.5)$$

Since  $K$  is invertible, one can manipulate the first equation to get  $U = K^{-1}(F - Q\lambda)$ . Then, using this result in the second equation yields

$$\gamma = Q^T(K^{-1}(F - Q\lambda)) = Q^T K^{-1}F - Q^T K^{-1}Q\lambda. \quad (3.6)$$

Denoting the Schur complement by  $S = Q^T K^{-1}Q$ , one gets

$$S\lambda = Q^T K^{-1}F - \gamma. \quad (3.7)$$

In other words, the Lagrangian formulation (3.4) has been recast as

$$\begin{bmatrix} K & Q \\ 0 & S \end{bmatrix} \begin{bmatrix} U \\ \lambda \end{bmatrix} = \begin{bmatrix} F \\ Q^T K^{-1}F - \gamma \end{bmatrix}, \quad (3.8)$$

where the matrix is now upper triangular: direct Uzawa performs a triangularization by blocks, as a result, the constraint is indeed decoupled from the rest of the problem and the system can be solved by a backward substitution by blocks. However, it still requires us to explicitly invert the stiffness matrix  $K$ . Iterative Uzawa provides a means to avoid explicitly calculating the inverse  $K^{-1}$ .

**Iterative Uzawa:** in the iterative Uzawa method, the system (3.8), and most particularly the constraint equation, is solved in an iterative manner. The corresponding algorithm, given here in its most simple form using for example the linear descent, is described in Algorithm 1. In this algorithm, the residual bypasses the use of  $K^{-1}$  and  $S$ , indeed

$$r^{(k)} = Q^T K^{-1}(F - Q\lambda^{(k)}) - \gamma = Q^T U^{(k)} - \gamma, \quad (3.9)$$

which corresponds to the constraint residual of the original Lagrangian system (3.5).

The step length  $\alpha^{(k)} \in \mathbb{R}$  can be taken as a constant or be evaluated using a (conjugate-)gradient approach to improve the performance of the method. In [24], bounds for the step length are provided

**Algorithm 1:** Iterative Uzawa method.

```

1 Initialize  $\lambda^{(0)}$ ,  $k = 0$ 
2 while convergence not reached do
3   Solve for  $U^{(k)}$ :  $KU^{(k)} = F - Q\lambda^{(k)}$ 
4   Compute the residual  $r^{(k)} = Q^T U^{(k)} - \gamma$ 
5   Compute the step length  $\alpha^{(k)}$ 
6   Update  $\lambda^{(k+1)} = \lambda^{(k)} + \alpha^{(k)} r^{(k)}$ 
7    $k \leftarrow k + 1$ 
8 end

```

in order for the method to converge and optimal step lengths are given, for the case where  $K$  is symmetric positive-definite and  $Q$  is full rank. These bounds and the optimal step length are

$$0 < \alpha^{(k)} < \frac{2}{\lambda_{\max}(S)} \quad \text{and} \quad \alpha_{\text{opt}} = \frac{2}{\lambda_{\min}(S) + \lambda_{\max}(S)}, \quad (3.10)$$

where  $\lambda_{\max}(S)$  (resp.  $\lambda_{\min}(S)$ ) denotes the largest (resp. smallest) eigenvalue of the Schur complement  $S$ . In the present case, since the constraint is scalar, we have that  $Q$  is a (non-zero) column-vector, and so it has full-rank (equal to one). Moreover,  $K$  is positive definite, so that  $S$  is a strictly positive scalar and  $\lambda_{\max}(S) = \lambda_{\min}(S) = S > 0$ . The conditions (3.10) reduce to

$$0 < \alpha^{(k)} < \frac{2}{S} \quad \text{and} \quad \alpha_{\text{opt}} = \frac{1}{S}. \quad (3.11)$$

Note that the optimal step length is not used in practice since it requires the Schur complement  $S$ . A classical refinement concerning the step length  $\alpha^{(k)}$  is to use a gradient descent on the constraint equation (3.7), in which case the step length would be given by

$$\alpha^{(k)} = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k)}, S r^{(k)} \rangle}. \quad (3.12)$$

To avoid the use of  $S$ , one can write

$$S r^{(k)} = Q^T K^{-1} Q r^{(k)} = Q^T w^{(k)}, \quad (3.13)$$

where  $w^{(k)}$  is the solution of the auxiliary problem  $K w^{(k)} = Q r^{(k)}$ . Finally, one can use this auxiliary solution  $w^{(k)}$  and the step length  $\alpha^{(k)}$  to update all variables in the Uzawa algorithm. Indeed, updating  $\lambda^{(k+1)} = \lambda^{(k)} + \alpha^{(k)} r^{(k)}$  results in an update of the constraint residual as

$$r^{(k+1)} = Q^T K^{-1} (F - Q \lambda^{(k+1)}) - \gamma = r^{(k)} - \alpha^{(k)} S r^{(k)} = r^{(k)} - \alpha^{(k)} Q^T w^{(k)}, \quad (3.14)$$

and similarly for the solution vector

$$U^{(k+1)} = K^{-1} (F - Q \lambda^{(k+1)}) = U^{(k)} - \alpha^{(k)} K^{-1} Q r^{(k)} = U^{(k)} - \alpha^{(k)} w^{(k)}. \quad (3.15)$$

<b>Algorithm 2:</b> Uzawa method with gradient descent.	
1	Initialize $\lambda^{(0)}, k = 0$
2	Solve for $U^{(0)}$ : $KU^{(0)} = F - Q\lambda^{(0)}$
3	Compute the constraint residual $r^{(0)} = Q^T U^{(0)} - \gamma$
4	<b>while</b> <i>convergence not reached</i> <b>do</b>
5	Solve for $w^{(k)}$ : $Kw^{(k)} = Qr^{(k)}$
6	Compute the step length $\alpha^{(k)} = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k)}, Q^T w^{(k)} \rangle}$
7	Update $\lambda^{(k+1)} = \lambda^{(k)} + \alpha^{(k)} r^{(k)}$
8	Update $r^{(k+1)} = r^{(k)} - \alpha^{(k)} Q^T w^{(k)}$
9	Update $U^{(k+1)} = U^{(k)} - \alpha^{(k)} w^{(k)}$
10	$k \leftarrow k + 1$
11	<b>end</b>

In the end, the iterative Uzawa algorithm with gradient descent is described by Algorithm 2. This algorithm has thus eliminated all uses of  $K^{-1}$  and  $S$ .

**Uzawa Adjoint:** The constraint considered in this paper is scalar and so is  $r^{(k)}$ , as a result Algorithm 2 can be further simplified introducing the adjoint problem associated to the constraint functional

$$\text{Find } p \in H^1(\Omega) \text{ such that } b(v, p) = q(v), \quad \forall v \in H^1(\Omega). \quad (3.16)$$

This problem is well-posed since bilinear form  $b$  is coercive (recall we are only considering the Robin problem in this section) and  $q$  is continuous, so that there is a unique solution  $p \in H^1(\Omega)$ . Note that this approach cannot be applied to the pure Neumann problem since the loading of the adjoint problem  $q$  does not satisfy the compatibility condition (2.2). Now, going back to the mixed-weak formulation arising from the Lagrangian method (2.12) and denoting its solution by  $(u_\lambda, \lambda)$ , we have

$$\begin{cases} b(u_\lambda, v) + \lambda q(v) = \ell(v), & \forall v \in H^1(\Omega), \\ q(u_\lambda) = \gamma. \end{cases} \quad (3.17)$$

Then, using the adjoint problem  $b(v, p) = q(v)$  we obtain

$$b(u_\lambda, v) + \lambda b(v, p) = \ell(v), \quad \forall v \in H^1(\Omega). \quad (3.18)$$

Now, making use of the fact that  $b$  is bilinear and symmetric yields

$$b(u_\lambda + \lambda p, v) = \ell(v), \quad \forall v \in H^1(\Omega). \quad (3.19)$$

Finally, the Lax-Milgram theorem applied to the unconstrained Robin problem ensures unicity of the solution so that

$$u_\lambda + \lambda p = u_0, \quad (3.20)$$

where  $u_0 \in H^1(\Omega)$  denotes the unconstrained solution. We see that the scalar constraint allows one to simplify the problem, since the Lagrange multiplier  $\lambda$  can readily be obtained by applying the functional  $q$  to (3.20) and rearranging the terms, that is

$$\lambda = \frac{q(u_0) - q(u_\lambda)}{q(p)} = \frac{q(u_0) - \gamma}{q(p)}, \quad (3.21)$$

where  $q(p) \neq 0$  since  $q(p) = b(p, p)$ . As a result, one only needs to compute the unconstrained solution  $u_0$ , the adjoint solution  $p$  and the Lagrange multiplier  $\lambda$  to solve the constrained problem. We will subsequently refer to this approach as ‘‘Uzawa Adjoint’’.

### 3.4 Augmented Lagrangian method

The mixed finite element problem on  $V_h \times \mathbb{R}$  corresponding to the Augmented Lagrangian approach (2.15) is given by

$$\text{Find } (u_h, \lambda) \in V_h \times \mathbb{R} \text{ such that} \quad \begin{cases} b(u_h, v_h) + \lambda q(v_h) + \beta q(u_h)q(v_h) = \ell(v_h) + \beta\gamma q(v_h), & \forall v_h \in V_h, \\ \tau q(u_h) = \tau\gamma, & \forall \tau \in \mathbb{R}. \end{cases} \quad (3.22)$$

The linear system associated with this finite-dimensional problem is

$$\begin{bmatrix} K + \beta QQ^T & Q \\ Q^T & 0 \end{bmatrix} \begin{bmatrix} U \\ \lambda \end{bmatrix} = \begin{bmatrix} F + \beta\gamma Q \\ \gamma \end{bmatrix}. \quad (3.23)$$

Since the matrix  $K + \beta QQ^T$  is positive-definite, and thus invertible, one can apply the Uzawa method here to both the Neumann and Robin problems. The direct Uzawa method yields the block triangular system

$$\begin{bmatrix} K + \beta QQ^T & Q \\ 0 & S_\beta \end{bmatrix} \begin{bmatrix} U \\ \lambda \end{bmatrix} = \begin{bmatrix} F + \beta\gamma Q \\ Q^T(K + \beta QQ^T)^{-1}(F + \beta\gamma Q) - \gamma \end{bmatrix}, \quad (3.24)$$

where  $S_\beta$  denotes the Schur complement of the perturbed matrix, i.e.  $S_\beta = Q^T(K + \beta QQ^T)^{-1}Q$ .

The derivation of the iterative Uzawa scheme is constructed *mutatis mutandis* as the earlier one. However, some simplifications can be made to compute the step length  $\alpha^{(k)}$  (see steps 5 and 6 in Algorithm 2) assuming, for instance, that  $K + \beta QQ^T \approx \beta QQ^T$ . The auxiliary problem in step 5 then reduces to finding  $w^{(k)}$  such that  $\beta QQ^T w^{(k)} = Qr^{(k)}$ . Viewing now  $Q \in \mathbb{R}^n$  as a linear application from  $\mathbb{R}$  to  $\mathbb{R}^n$ , by the rank-nullity theorem,  $\dim(\text{Ker } Q) = \dim(\mathbb{R}) - \text{rk}(Q) = 1 - \text{rk}(Q^T) = 1 - 1 = 0$ . As a result,  $Q$  is injective and  $\beta QQ^T w^{(k)} = Qr^{(k)}$  implies that  $\beta Q^T w^{(k)} = r^{(k)}$ . Then, in step 6 of Algorithm 2, the step length  $\alpha^{(k)}$  is approximately  $\beta$ ; in other words, the auxiliary problem has been avoided. As a result, the Augmented Lagrangian method reduces to an Uzawa method on the penalized bilinear form with a constant step length  $\beta$ , see Algorithm 1.

**Remark 3** For the Robin case, in which the matrix  $K$  is invertible, one can rely on the Sherman-Morrison-Woodbury matrix identity [18] instead of the quite sloppy  $K + \beta QQ^T \approx \beta QQ^T$ . In the present context, the identity states

$$(K + \beta QQ^T)^{-1} = K^{-1} - \frac{\beta K^{-1} QQ^T K^{-1}}{1 + \beta Q^T K^{-1} Q}, \quad (3.25)$$

which allows one to write the Schur complement of the perturbed matrix  $S_\beta$  in terms of  $S$  as

$$S_\beta = Q^T \left( K^{-1} - \frac{\beta K^{-1} QQ^T K^{-1}}{1 + \beta Q^T K^{-1} Q} \right) Q = S - \frac{\beta S^2}{1 + \beta S} = \frac{S}{1 + \beta S}. \quad (3.26)$$

According to Saad [24], the optimal step length  $\alpha_{opt}$  is then given by the inverse of the Schur complement:  $\frac{1}{S_\beta} = \beta + \frac{1}{S}$ . Taking  $\beta$  large enough, we obtain  $\alpha_{opt} \approx \beta$ .

Similarly to the penalization approach discussed in Section 3.1, the choice of the penalization parameter  $\beta$  has some influence on the performance of the algorithm. First, the stiffness matrix loses its sparsity pattern resulting in higher computational costs. Secondly, the condition number of the matrix may increase significantly. Finally, choosing  $\beta$  too large may result in round-off errors, which could affect the accuracy of the method, while choosing  $\beta$  too small may result in an incorrect step length  $\alpha$ , leading to an increased number of iterations needed to reach convergence. Note however that the Augmented Lagrangian approach is consistent with the Lagrangian method so that the solution of the former coincides with that of the latter.

## 4 PGD formulations of constrained problems

The objective in this section is to apply the above formulations to the Proper Generalized Decomposition (PGD) framework. For the sake of simplicity, we will consider here the so-called progressive Galerkin version of the PGD, but the ideas naturally extend to other types of PGD formulations. For completeness, we first describe the PGD formulation in the unconstrained setting for the pure Neumann Problem (2.3). This will allow us to introduce notations and to recall the main concepts behind the PGD scheme. The interested reader is referred to [10, 22] for a more in-depth analysis of the method and its variants.

In order to compare the results of the PGD algorithms with both the exact solution  $u$  and the finite element solution  $u_h$ , we will consider that the mesh associated to  $V_h$  is obtained by the tensor product of one-dimensional meshes along each of the  $d$  directions of  $\Omega \subset \mathbb{R}^d$ . As a result  $V_h$  is a tensor product of  $d$  one-dimensional FE spaces:  $V_h = \bigotimes_{i=1}^d V_h^{(i)}$ .

We introduce the set of elementary rank-one tensors  $\mathcal{S}_1 = \left\{ \bigotimes_{i=1}^d v_i \in V_h; v_i \in V_h^{(i)}, i = 1, \dots, d \right\}$ . For a given  $\bigotimes_{i=1}^d z_i \in \mathcal{S}_1$  and a given direction  $j \in \{1, \dots, d\}$ , we denote the vector space of ‘‘admissible variations’’ around  $\bigotimes_{i=1}^d z_i$  in the  $j$ -th direction defined by

$$\mathcal{T}^{(j)}(\bigotimes_{i=1}^d z_i) = \left\{ \bigotimes_{i=1}^d v_i \in \mathcal{S}_1; v_i = z_i, i = 1, \dots, d, i \neq j \right\} = z_1 \otimes z_2 \otimes \dots \otimes V_h^{(j)} \otimes \dots \otimes z_d. \quad (4.1)$$

Considering now all directions, we denote the tangent space to the elementary tensor  $\otimes_{i=1}^d z_i$  by  $\mathcal{T}(\otimes_{i=1}^d z_i) = \sum_{j=1}^d \mathcal{T}^{(j)}(\otimes_{i=1}^d z_i) \subset V_h$ . Note that the functions  $v \in \mathcal{T}(\otimes_{i=1}^d z_i)$  are of the form

$$v = \underbrace{v_1 \otimes z_2 \otimes \cdots \otimes z_d}_{\psi_1 \in \mathcal{T}^{(1)}(\otimes_{i=1}^d z_i)} + \underbrace{z_1 \otimes v_2 \otimes \cdots \otimes z_d}_{\psi_2 \in \mathcal{T}^{(2)}(\otimes_{i=1}^d z_i)} + \cdots + \underbrace{z_1 \otimes z_2 \otimes \cdots \otimes v_d}_{\psi_d \in \mathcal{T}^{(d)}(\otimes_{i=1}^d z_i)}, \quad (4.2)$$

where the  $v_i$ 's are arbitrary (one-dimensional test functions in  $V_h^{(i)}$ ).

Starting from a given approximation  $u_{m-1}$ , the goal of PGD is to compute a rank-one update  $\delta u = \otimes_{i=1}^d z_i \in \mathcal{S}_1$ , or correction, such that the updated solution  $u_m = u_{m-1} + \delta u$  minimizes the energy functional  $J$  over the set of rank-one tensors

$$\text{Find } \delta u \in \mathcal{S}_1 \text{ such that } J(u_{m-1} + \delta u) = \min_{v \in \mathcal{S}_1} J(u_{m-1} + v). \quad (4.3)$$

The weak formulation (necessary condition) associated to this non-linear problem reads

$$\text{Find } \delta u \in \mathcal{S}_1 \text{ such that } b(u_{m-1} + \delta u, v) = \ell(v), \quad \forall v \in \mathcal{T}(\delta u). \quad (4.4)$$

Problem (4.4) naturally leads to the set of coupled one-dimensional problems

$$\text{Find } \otimes_{i=1}^d z_i \in \mathcal{S}_1 \text{ such that } \begin{cases} b(\otimes_{i=1}^d z_i, \psi_1) = R_{m-1}(\psi_1), & \forall \psi_1 \in \mathcal{T}^{(1)}(\otimes_{i=1}^d z_i), \\ b(\otimes_{i=1}^d z_i, \psi_2) = R_{m-1}(\psi_2), & \forall \psi_2 \in \mathcal{T}^{(2)}(\otimes_{i=1}^d z_i), \\ \vdots \\ b(\otimes_{i=1}^d z_i, \psi_d) = R_{m-1}(\psi_d), & \forall \psi_d \in \mathcal{T}^{(d)}(\otimes_{i=1}^d z_i), \end{cases} \quad (4.5)$$

where  $R_{m-1}$  denotes the residual  $R_{m-1}(v) = \ell(v) - b(u_{m-1}, v)$ . Problem (4.5) is obviously non-linear.

An approach for solving (4.5) is the so-called Alternated Directions scheme, a fixed-point algorithm in which one successively solves each of the previous equations. To be more precise, each iteration of the Alternated Directions scheme is as follows: from the current iterate  $z_1^{(k)}, \dots, z_d^{(k)}$ , compute the new  $z_1^{(k+1)}$  using  $z_2^{(k)}, \dots, z_d^{(k)}$  by solving the first equation of (4.5). Then, compute the new  $z_2^{(k+1)}$  using the just computed  $z_1^{(k+1)}$  and  $z_3^{(k)}, \dots, z_d^{(k)}$  by solving the second equation of (4.5). All the  $d$  problems are thus solved until the last one, where we compute  $z_d^{(k+1)}$  using the already computed  $z_1^{(k+1)}, \dots, z_{d-1}^{(k+1)}$  by solving the last equation of (4.5). This process repeats  $k^*$  times until the fixed point  $\otimes_{i=1}^d z_i^{(k^*)}$  is (approximately) reached, then we set  $u_m = u_{m-1} + \otimes_{i=1}^d z_i^{(k^*)}$  and repeat the search for the next rank-one update until convergence.

Before investigating the constrained approaches, we propose to examine the properties of the linear systems arising from the PGD algorithm when applied to the unconstrained pure Neumann problem (2.3). For simplicity, we consider  $d = 2$ , that is  $\Omega = \Omega_1 \times \Omega_2 \subset \mathbb{R}^2$ , with a diffusivity constant  $a$  equal to unity throughout  $\Omega$ , and  $m = 1$ , i.e. we want to compute a rank-one

solution  $u_1 = z_1 \otimes z_2$ . In this case, problem (4.5) simplifies to

$$\text{Find } (z_1, z_2) \in V_h^{(1)} \times V_h^{(2)} \text{ such that } \begin{cases} b(z_1 \otimes z_2, v_1 \otimes z_2) = \ell(v_1 \otimes z_2), & \forall v_1 \in V_h^{(1)}, \\ b(z_1 \otimes z_2, z_1 \otimes v_2) = \ell(z_1 \otimes v_2), & \forall v_2 \in V_h^{(2)}. \end{cases} \quad (4.6)$$

Recalling the definition of the bilinear form, at a given iteration of the Alternated Directions scheme, the first equation of (4.6) is found to be:

$$\text{Given } z_2 \in V_h^{(2)}, \text{ find } z_1 \in V_h^{(1)} \text{ such that} \\ b(z_1 \otimes z_2, v_1 \otimes z_2) = \|z_2\|_{L^2(\Omega_2)}^2 \left( \int_{\Omega_1} z_1' v_1' dx \right) + |z_2|_{H^1(\Omega_2)}^2 \left( \int_{\Omega_1} z_1 v_1 dx \right), \quad \forall v_1 \in V_h^{(1)}, \quad (4.7)$$

where  $\|z_2\|_{L^2(\Omega_2)}^2$  and  $|z_2|_{H^1(\Omega_2)}^2$  appear as known constant coefficients in front of what are essentially a stiffness matrix and a mass matrix, respectively.

From (4.7), we can already make some simple observations about system (4.6). First, in the case where  $|z_2|_{H^1(\Omega_2)} \neq 0$ , i.e.  $z_2$  is not constant over  $\Omega_2$ , then the matrix arising from the FE formulation of problem (4.7) over  $\Omega_1$  will be positive-definite, even though the solution of the original Neumann problem was only defined up to a constant. As a result, the PGD sets for itself an additive constant during the process. However, this value depends, among other things, on the initialization of the fixed-point algorithm and it is not clear how or even if it can be controlled.

Second, if  $|z_2|_{H^1(\Omega_2)} \approx 0$ , i.e.  $z_2$  is almost constant over  $\Omega_2$  or the variations of  $z_2$  are small compared to its magnitude, then the matrix arising from the FE formulation of the problem over  $\Omega_1$  will be ill-conditioned, or sometimes non-invertible with a rank deficiency of one (just like the matrix  $K$  from Section 3 was). This is precisely the degenerate case of PGD the authors came across and the motivation for this paper. Nevertheless, it is worth mentioning that even in that case, the compatibility condition is inherited from the original problem so that solutions do exist.

We now assume that the input data admit affine representations [7], meaning that the diffusivity coefficient  $a$ , as well as the loadings  $f$  and  $g$ , admit exact separated representations. As a consequence, the bilinear form  $b$  and linear form  $\ell$  can be separated accordingly. In addition, we also require the subset  $\omega$  (and consequently the linear functional  $q$  too) to admit a separated representation. For  $\omega$ , this means that the domain can be written as a (possibly non-disjoint) union of  $d$ -dimensional hyper-rectangles, while for  $q$  this means it can be written in tensor form. The reader is referred to [27] for the case where the input data is not separable.

#### 4.1 Penalization method

Since the penalization approach is nothing but an *ad-hoc* stabilization of the bilinear form together with a consistent correction of the right-hand side, the PGD formulation of this problem can readily

be established: given a previously computed numerical approximation  $u_{m-1}$

$$\begin{aligned} &\text{Find } \delta u \in \mathcal{S}_1 \text{ such that} \\ &b(u_{m-1} + \delta u, v) + \beta q(u_{m-1} + \delta u)q(v) = \ell(v) + \beta \gamma q(v), \quad \forall v \in \mathcal{T}(\delta u). \end{aligned} \quad (4.8)$$

Rearranging the terms in the equation, the problem can be recast:

$$\begin{aligned} &\text{Find } \delta u \in \mathcal{S}_1 \text{ such that} \\ &b(\delta u, v) + \beta q(\delta u)q(v) = R_{m-1}(v) + \beta(\gamma - q(u_{m-1}))q(v), \quad \forall v \in \mathcal{T}(\delta u). \end{aligned} \quad (4.9)$$

With the assumed separation of the input data and  $q$ , this leads to a problem which possesses the same structure as problem (4.5), namely

$$\begin{aligned} &\text{Find } \delta u \in \mathcal{S}_1 \text{ such that} \\ &\begin{cases} b(\delta u, \psi_1) + \beta q(\delta u)q(\psi_1) = R_{m-1}(\psi_1) + \beta(\gamma - q(u_{m-1}))q(\psi_1), & \forall \psi_1 \in \mathcal{T}^{(1)}(\delta u), \\ b(\delta u, \psi_2) + \beta q(\delta u)q(\psi_2) = R_{m-1}(\psi_2) + \beta(\gamma - q(u_{m-1}))q(\psi_2), & \forall \psi_2 \in \mathcal{T}^{(2)}(\delta u), \\ \vdots \\ b(\delta u, \psi_d) + \beta q(\delta u)q(\psi_d) = R_{m-1}(\psi_d) + \beta(\gamma - q(u_{m-1}))q(\psi_d), & \forall \psi_d \in \mathcal{T}^{(d)}(\delta u). \end{cases} \end{aligned} \quad (4.10)$$

Each of these equations is solved in an Alternated Directions manner until convergence of the new mode  $\delta u = \otimes_{i=1}^d z_i$ , after which one can set  $u_m = u_{m-1} + \otimes_{i=1}^d z_i$ .

Following [16] and under the assumption on weak closedness therein, the penalized PGD converges towards the penalized FEM, at least in the norm induced by the penalized bilinear form.

## 4.2 Lagrangian method

Once again, using a progressive approach, we assume that  $u_{m-1}$  is given and we seek for a next mode  $\delta u$  and Lagrange multiplier  $\lambda$  satisfying

$$\text{Find } (\delta u, \lambda) \in \mathcal{S}_1 \times \mathbb{R} \text{ such that } \begin{cases} b(u_{m-1} + \delta u, v) + \lambda q(v) = \ell(v), & \forall v \in \mathcal{T}(\delta u), \\ \tau q(u_{m-1} + \delta u) = \tau \gamma, & \forall \tau \in \mathbb{R}. \end{cases} \quad (4.11)$$

Note that in this paper we have not studied the existence nor the unicity of the solution  $(\delta u, \lambda)$  and are only concerned with finding critical points of the Lagrangian functional.

Rearranging the terms, we have

$$\text{Find } (\delta u, \lambda) \in \mathcal{S}_1 \times \mathbb{R} \text{ such that } \begin{cases} b(\delta u, v) + \lambda q(v) = R_{m-1}(v), & \forall v \in \mathcal{T}(\delta u), \\ \tau q(\delta u) = \tau(\gamma - q(u_{m-1})), & \forall \tau \in \mathbb{R}, \end{cases} \quad (4.12)$$



leading to the following problem

Find  $(\delta u, \lambda) \in \mathcal{S}_1 \times \mathbb{R}$  such that

$$\begin{cases} b(\delta u, \psi_1) + \lambda q(\psi_1) = R_{m-1}(\psi_1), & \forall \psi_1 \in \mathcal{T}^{(1)}(\delta u), \\ b(\delta u, \psi_2) + \lambda q(\psi_2) = R_{m-1}(\psi_2), & \forall \psi_2 \in \mathcal{T}^{(2)}(\delta u), \\ \vdots \\ b(\delta u, \psi_d) + \lambda q(\psi_d) = R_{m-1}(\psi_d), & \forall \psi_d \in \mathcal{T}^{(d)}(\delta u), \\ \tau q(\delta u) = \tau(\gamma - q(u_{m-1})), & \forall \tau \in \mathbb{R}. \end{cases} \quad (4.13)$$

It is interesting to observe that problem (4.13) has a structure that is clearly different from that of (4.5) or (4.10) due to the constraint equation and the Lagrange multiplier  $\lambda$ . In the spirit of the Alternated Directions scheme, one would be tempted to associate the constraint with one (or more) of the  $d$  other equations and perform the Alternated Directions as usual until convergence. However, this approach raises several questions: does the method converge? Does the choice of the coupling have an influence on convergence?

From our preliminary experiments, it turns out that none of these approaches yield satisfactory results. To be more specific, the constraint  $q(u_{m-1} + \delta u) = \gamma$  is satisfied, but as we increase the number of modes  $m$ , the PGD solution does not converge towards the FE solution of the original Lagrangian problem (3.3). Furthermore, depending on the choice adopted when coupling the constraint with one of the  $d$  problems, we obtain different results. Finally, the Lagrange multiplier  $\lambda$  does not converge either.

In order to solve (4.13) efficiently, it appears there are two options: either associate the constraint with all the  $d$  problems, or fully decouple the constraint from the other equations, as the Uzawa and Augmented Lagrangian methods do. In the rest of this section, we will investigate the first option: the goal is to solve (4.13) in such a way that the constraint equation is evenly associated to the other problems.

The approach considered in this section differs from the classical Alternated Directions scheme in that we update simultaneously all the  $z_i^{(k+1)}$ ,  $i = 1, \dots, d$  using the previous iterates  $z_j^{(k)}$ ,  $j = 1, \dots, d$ ,  $j \neq i$ . If one were to make an analogy between the classical Alternated Directions scheme and the block Gauss-Seidel method, then the present approach could be viewed as a block Jacobi method. Since we update each function  $z_i^{(k+1)}$  using only information that is already available from the previous iterate  $k$ , one could do this process in parallel, but this is not the approach we take. Instead, we assemble a global block-diagonal system whose unknown is the concatenation of all the  $z_i^{(k+1)}$ ,  $i = 1, \dots, d$ . This way, we have a system where all the  $d$  functions are updated simultaneously. Finally, we incorporate the constraint into this global system, after having linearized it around the current iterate  $\delta u^{(k)} = \otimes_{i=1}^d z_i^{(k)}$ , e.g. by the Newton method. Therefore, instead of

$$q\left(\otimes_{i=1}^d z_i^{(k+1)}\right) = \gamma - q(u_{m-1}), \quad (4.14)$$

we consider

$$\begin{aligned} & q\left(z_1^{(k+1)} \otimes z_2^{(k)} \otimes \cdots \otimes z_d^{(k)} + z_1^{(k)} \otimes z_2^{(k+1)} \otimes \cdots \otimes z_d^{(k)} + \cdots + z_1^{(k)} \otimes z_2^{(k)} \otimes \cdots \otimes z_d^{(k+1)}\right) \\ & = \gamma - q\left(u_{m-1} + (1-d) \otimes_{i=1}^d z_i^{(k)}\right). \end{aligned} \quad (4.15)$$

In the end, each fixed-point iteration consists in solving a linear system where all the  $d$  functions are updated simultaneously and in which the constraint couples the one-dimensional problems.

The finite element counterpart yields the following system of equations, where  $z_i^{(k+1)}$  defines the vectors of unknown in each direction  $i$ :

$$\begin{bmatrix} K^{(1,k)} & 0 & \cdots & 0 & Q^{(1,k)} \\ 0 & K^{(2,k)} & \cdots & 0 & Q^{(2,k)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & K^{(d,k)} & Q^{(d,k)} \\ Q^{(1,k)T} & Q^{(2,k)T} & \cdots & Q^{(d,k)T} & 0 \end{bmatrix} \begin{bmatrix} z_1^{(k+1)} \\ z_2^{(k+1)} \\ \vdots \\ z_d^{(k+1)} \\ \lambda \end{bmatrix} = \begin{bmatrix} F^{(1,k)} \\ F^{(2,k)} \\ \vdots \\ F^{(d,k)} \\ \tilde{\gamma} \end{bmatrix}, \quad (4.16)$$

with, for each  $i = 1, \dots, d$

$$\begin{cases} K_{ln}^{(i,k)} = b(z_1^{(k)} \otimes z_2^{(k)} \otimes \cdots \otimes \varphi_n^{(i)} \otimes \cdots \otimes z_d^{(k)}, z_1^{(k)} \otimes z_2^{(k)} \otimes \cdots \otimes \varphi_l^{(i)} \otimes \cdots \otimes z_d^{(k)}), \\ Q_l^{(i,k)} = q(z_1^{(k)} \otimes z_2^{(k)} \otimes \cdots \otimes \varphi_l^{(i)} \otimes \cdots \otimes z_d^{(k)}), \\ F_l^{(i,k)} = R_{m-1}(z_1^{(k)} \otimes z_2^{(k)} \otimes \cdots \otimes \varphi_l^{(i)} \otimes \cdots \otimes z_d^{(k)}), \end{cases} \quad (4.17)$$

where  $V_h^{(i)} = \text{span} \left\{ \varphi_j^{(i)} \right\}_{j=1}^{\dim V_h^{(i)}}$ , and  $\tilde{\gamma} = \gamma - q\left(u_{m-1} + (1-d) \otimes_{i=1}^d z_i^{(k)}\right)$ .

It is worth mentioning here that the method needs help with convergence. We noticed in our numerical experiments that starting each fixed-point problem with a few iterations using the penalized version PGD (or the forthcoming Uzawa or Augmented Lagrangian methods) provides a remedy to this issue. It is likely because these few iterations bring the iterates closer to the attraction basin of the solution.

### 4.3 Uzawa method

In this section and the next, we show how system (4.13) can be solved by decoupling the constraint from the other equations. In Section 3.3, we described three versions for the Uzawa method: Algorithm 1, where the step length  $\alpha$  was not elaborated upon (one can take  $\alpha$  constant for a first grab at the method, note however that it cannot be too large, otherwise the method will not converge, according to [24]); Algorithm 2, where the step length  $\alpha$  was computed using a gradient algorithm, which required the solution of an auxiliary problem (step 5); and the so-called Uzawa Adjoint method. We will now adapt those to the PGD setting.

We start by mentioning that the linearization of the constraint equation displayed in (4.15) is consistent with (3.9).

As far as Algorithm 1 is concerned, step 3 has to be adapted to the PGD framework. For simplicity, this step can be written in weak form, leading to, for an already computed approximate value of  $\lambda$ :

$$\text{Find } \delta u \in \mathcal{S}_1 \text{ such that } b(\delta u, v) = R_{m-1}(v) - \lambda q(v), \quad \forall v \in \mathcal{T}(\delta u). \quad (4.18)$$

Since  $\lambda$  is (approximately) known at this stage, this problem is of the same form as the problem arising from classical PGD, and is solved using the Alternated Directions scheme.

Then, several choices are available for the update of the Lagrange multiplier  $\lambda$  (step 6): it could be updated after reaching the fixed point satisfying (4.18), i.e. for the current approximation of  $\lambda$ , or more often such as after one full Alternated Directions iteration, or even more often after each problem in the Alternated Directions scheme. In the present paper we did not study in detail the influence of this feature and simply chose to update after one full Alternated Directions iteration.

Concerning Algorithm 2, some more in-depth modifications need to be made since we cannot afford to solve the auxiliary problem  $Kw^{(k)} = Qr^{(k)}$  which lives in the fully discretized space (in fact this approach would be the so-called Uzawa Adjoint which we will investigate at the end of this subsection). Instead, we proceed as follows: for the current approximate value of the Lagrange multiplier  $\lambda$  we perform one full Alternated Directions iteration on (4.18) and we compute the constraint residual  $r^{(k)}$ . For the step length  $\alpha$ , the analysis of [24] is again required because we are no longer working with system (3.3) but with (4.16) instead, having uncoupled the  $d$  problems by the Alternated Directions and linearized the constraint equation by Newton's method. As a consequence, the Schur complement is now the sum of  $d$  "unidimensional Schur complements"

$$S = \sum_{i=1}^d S_i, \text{ where } S_i = Q^{(i,k^*)T} \left( K^{(i,k^*)} \right)^{-1} Q^{(i,k^*)}, \quad (4.19)$$

where these vectors and matrices were defined in (4.17). Note that each matrix  $K^{(i,k^*)}$  is associated with a one-dimensional problem in  $V_h^{(i)}$ ,  $i = 1, \dots, d$ .

Then, the optimal step length is given by  $\alpha_{\text{opt}} = \frac{1}{S} = \frac{1}{\sum_{i=1}^d S_i}$ , and to approximate it, one can use a gradient descent on the constraint equation, in which the step length would be given by

$$\alpha = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k)}, Sr^{(k)} \rangle}. \quad (4.20)$$

To avoid the use of  $S$ , one can write

$$Sr^{(k)} = \sum_{i=1}^d Q^{(i,k^*)T} \left( K^{(i,k^*)} \right)^{-1} Q^{(i,k^*)} r^{(k)} = \sum_{i=1}^d Q^{(i,k^*)T} w_i, \quad (4.21)$$

where each  $w_i$  is the solution of an auxiliary one-dimensional problem  $K^{(i,k^*)} w_i = Q^{(i,k^*)} r^{(k)}$ .

Finally, the extension of the Uzawa Adjoint method to the PGD setting is relatively straightforward, since one only needs to compute the unconstrained and adjoint solutions as well as the

Lagrange multiplier using (3.21). One iteration of the PGD version of this algorithm is as follows: compute one more mode  $\delta u$  for the unconstrained solution, one more mode  $\delta p$  for the adjoint solution, and the approximate Lagrange multiplier

$$\lambda = \frac{q(u_{m-1} + \delta u) - \gamma}{q(p_{m-1} + \delta p)}. \quad (4.22)$$

#### 4.4 Augmented Lagrangian method

The Augmented Lagrangian method is essentially the same as the Uzawa method but with the bilinear form replaced by its penalized version. We only state in this subsection the simplifications associated with the step length  $\alpha$ . Similarly to what was derived in Section 3.4, when  $\beta$  is large enough, the auxiliary problems can be circumvented assuming  $\beta Q^{(i,k^*)T} w_i = r^{(k)}$ . The step length is then computed from

$$\alpha = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k)}, \sum_{i=1}^d \frac{r^{(k)}}{\beta} \rangle} = \frac{\beta}{d}, \quad (4.23)$$

instead of (4.20)–(4.21). Here again, the auxiliary problems have been avoided. Note that the Sherman-Morrison-Woodbury matrix identity applied to each (penalized) term in the sum (4.19) yields the same result.

## 5 Numerical Examples

In this section, we apply above methods to the two model problems considered in this paper, namely the constrained pure Neumann problem (2.10) and the constrained Robin problem (2.16).

For the numerical simulations, we consider  $d = 2$  and  $\Omega = \omega = (0, 1)^2$  and choose a point  $(p_x, p_y) \in \Omega$  so that  $\Omega$  is split into two regions:  $\Omega_1 = \{(x, y) \in \Omega; x > p_x \text{ and } y > p_y\}$ , and the complementary region  $\Omega_0 = \Omega \setminus \Omega_1$ . Then  $a$  is chosen piecewise constant in each  $\Omega_i, i = 0, 1$ . We chose  $p_x = 7/32$ ,  $p_y = 19/32$ ,  $a_0 = 1$  and  $a_1 = 10$ . Finally, we take  $\gamma = 0$ . The exact solution  $u$  of the constrained pure Neumann problem (2.10) is constructed using the so-called manufactured solution method, and is chosen to be harmonic of the form

$$u = \begin{cases} A_0 r^\mu \cos(\mu\theta) + B_0 r^\mu \sin(\mu\theta) + C, & \text{in } \Omega_0, \\ A_1 r^\mu \cos(\mu\theta) + B_1 r^\mu \sin(\mu\theta) + C, & \text{in } \Omega_1, \end{cases} \quad (5.1)$$

where  $(r, \theta)$  is the polar coordinate centered at  $(p_x, p_y)$ . The constants  $\mu, A_0, B_0, A_1$  and  $B_1$  are chosen such that  $u$  is continuous in  $\Omega$  and  $a \frac{\partial u}{\partial n}$  is continuous across the interface between  $\Omega_0$  and  $\Omega_1$ . Finally,  $C$  is chosen so that  $u$  satisfies the constraint  $q(u) = 0$ . We mention that  $\mu$  is chosen greater than the degree of the shape functions considered in the numerical experiments so that the manufactured solution has sufficient regularity and cannot be represented exactly by the

FE basis functions. The loadings  $f$  and  $g$  are derived using (2.1). We mention that  $f = 0$  because  $u$  is taken to be harmonic in  $\Omega$ . Table 1 collects the values of the constant parameters  $\mu, A_0, B_0$  and  $C$  while we have  $A_1 = A_0$  and  $B_1 = (a_0/a_1)B_0$ .

$\mu$	$A_0$	$B_0$	$C$
2.7317	0.1526	0.9883	0.0534

Table 1: Values of the parameters  $\mu, A_0, B_0$  and  $C$  used for the numerical experiments.

In order to compare the numerical solutions we will use the semi-norm induced by  $b$ , denoted by  $|\cdot|_b$ , and the mean-functional  $q$ . Concerning the Robin problem (2.16), we consider the same loadings  $f$  and  $g$  as for the pure Neumann problem (2.10), independently of  $\varepsilon$ . As a result, the exact solution  $u_\varepsilon$  of the Robin problem (2.16) is unknown, but this is not the focus of the present paper (it was verified though that for every value of  $\varepsilon$ , the unconstrained finite element solution of the Robin problem did not already satisfy the constraint). Furthermore, we will also use the semi-norm induced by  $b$  and the mean-functional  $q$  for the Robin problem. Finally, a regular mesh of square elements with associated mesh size  $h = 1/32$  is used, and the bilinear Lagrange polynomials are chosen as basis functions.

First, in the framework of the FE approaches described in Section 3 we start by illustrating some properties of the Robin problem when the impedance coefficient  $\varepsilon$  goes to zero. Afterwards, we present some results for the penalized FEM and compare the Neumann and Robin problems. Finally, we present results for the constrained PGD approaches introduced in Section 4.

## 5.1 Constrained FEM solutions

As stated in Section 2, for any  $\varepsilon > 0$  the Schur complement  $S$  for the Robin problem exists and is finite. However, as Figure 1 shows, when  $\varepsilon$  goes to zero,  $S^{-1}$  goes to zero as well, with a slope of one. On the same figure, we also collected

- the algebraic error  $|u_{\varepsilon,h} - u_h|_b$  between the FE solutions of the Robin problem and the Neumann problem, both obtained by the Lagrangian method (3.4); as  $\varepsilon$  goes to zero, Figure 1 shows that the constrained Robin solution converges towards the constrained Neumann solution, at least in terms of the semi-norm  $|\cdot|_b$ ;
- the absolute value of the mean-value of the Robin solution  $|q(u_{\varepsilon,h})|$ ; Figure 1 shows that the constraint is numerically enforced for all values of  $\varepsilon$ , so that, together with the previous point,  $u_{\varepsilon,h}$  does converge towards  $u_h$ ;
- the absolute value of the Lagrange multiplier  $|\lambda|$ ; Figure 1 shows that it has the same behavior as  $\varepsilon$ . From our numerical experiments, there could be two reasons (or a combination of both):

as  $\varepsilon$  goes to zero, either the unconstrained solution progressively satisfies the zero-mean condition, or the matrix  $K$  becomes more and more numerically singular;

- the inverse of the scaled condition number of matrix  $K$ , denoted by  $\kappa^{-1}$ ; Figure 1 shows that, as  $\varepsilon$  goes to zero, the matrix becomes numerically singular, reflecting that the underlying bilinear form progressively loses coercivity;
- the absolute value of the mean-value of the unconstrained Robin solution  $|q(\tilde{u}_{\varepsilon,h})|$ ; Figure 1 shows that it is bounded away from zero for any  $\varepsilon$ , and so we can conclude that  $|\lambda|$  goes to zero because of the lost coercivity.

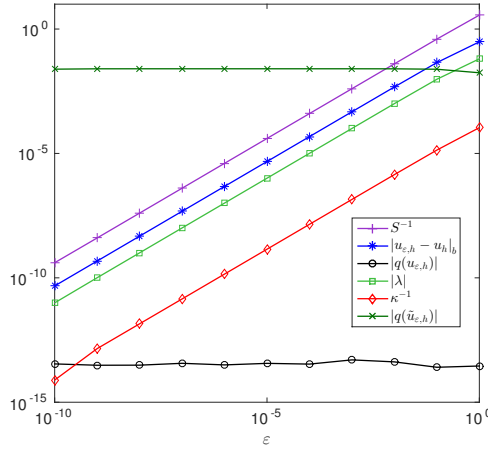


Figure 1: Evolution of some outputs of the Robin problem solved by the Lagrangian method with respect to the impedance coefficient  $\varepsilon$ .

Following (3.11), in order for the Uzawa method to converge, the upper bound for the step length  $\alpha$  is given by  $\frac{2}{S}$ , which is of the order of  $\varepsilon$ . Therefore, when  $\varepsilon$  goes to zero, the convergence of the Uzawa method deteriorates. At the limit  $\varepsilon = 0$ , which is the pure Neumann case,  $S$  does not exist and one cannot use the Uzawa method.

We now consider the penalized FE methods and compare the Robin problem (with fixed impedance parameter  $\varepsilon = 1$ ) and the Neumann problem when the penalization coefficient  $\beta$  varies. The results are collected in Figure 2 where we show

- the algebraic error between the penalized solution and the Lagrangian solution  $|u_{\beta,h} - u_h|_b$ ;
- the absolute value of the mean-value  $|q(u_{\beta,h})|$ ;

- the error in the post-processed Lagrange multiplier  $|\beta q(u_{\beta,h}) - \lambda|$ ;
- the inverse of the scaled condition number of the penalized matrix  $\kappa^{-1}$ ;
- for the Robin problem only, the algebraic error between the penalized solution and the unconstrained solution  $|u_{\beta,h} - \tilde{u}_h|_b$ .

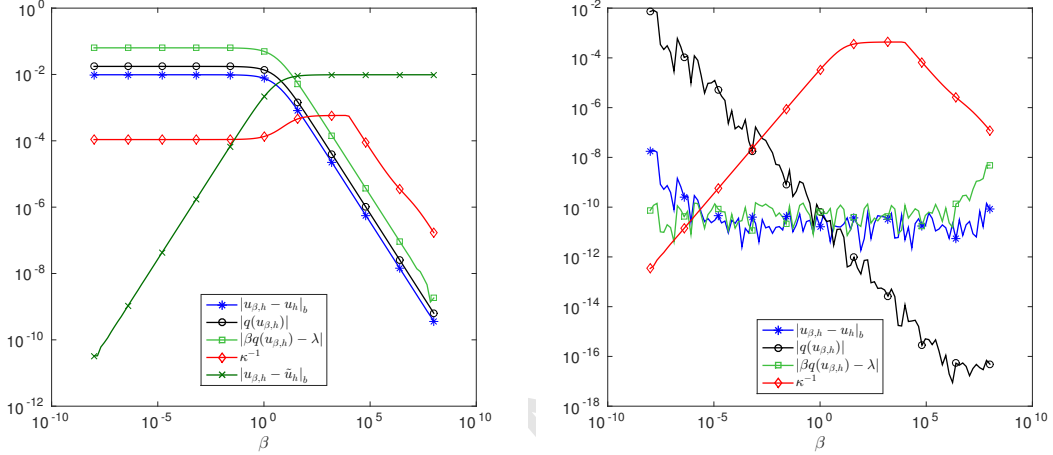


Figure 2: Evolution of some outputs of the penalization approach with respect to the penalization parameter  $\beta$ . Left: Robin problem. Right: Neumann problem.

We observe strikingly different results between the two problems. For the Robin case, the choice of  $\beta$  has evidently a strong influence on the solution: it has to be sufficiently large to enforce the constraint. This is because the unconstrained Robin problem already has a unique solution, and the penalization method is nothing but a trade-off between this unconstrained solution and the solution of the Lagrangian method. This is in contrast with the Neumann problem, for which the unconstrained solution is not unique, as a result, there is no trade-off where the energy would have to be sacrificed in favor of the constraint. To some extent, as  $K$  is singular and thus not coercive, any  $\beta > 0$  is large enough to impose the constraint so that the penalized solution coincides with the Lagrangian solution. However, for small values of the parameter  $\beta$  the constraint is not quite enforced, this is simply caused by the penalized matrix  $K$  becoming more and more singular as  $\beta$  goes to zero, so that the numerical solutions become polluted by round-off errors.

Based on the results collected in Figure 2, we will now set  $\beta = 10^2$  for the penalization and Augmented Lagrangian approaches. We purposely take  $\beta$  not too large in order to observe the limitations of the penalization approach. We emphasize here that the penalization parameter  $\beta$  in the Augmented Lagrangian approach has to be chosen large enough to ensure the precision of

the step length  $\alpha$  and, thus, the fast convergence of the solution, but not too large to avoid that round-off errors pollute the numerical solution.

## 5.2 Constrained PGD solutions

We now turn our attention to the constrained PGD solutions. In Section 4, we introduced five different methods, namely the penalization method; the Lagrangian method with simultaneous update of the functions by a block Jacobi method; the iterative Uzawa and the Uzawa Adjoint methods (recall that they can only be applied to the Robin case where the Schur complement exists); and the Augmented Lagrangian method. For completeness, we also consider the classical (unconstrained) PGD method, which can equivalently be seen as a penalization method with  $\beta = 0$ . We mention that in these experiments, the step length for the iterative Uzawa method was chosen as  $\alpha = 1$ . We will subsequently analyze the influence of this parameter on the convergence of the method. We recall that for the iterative Uzawa and Augmented Lagrangian methods, the Lagrange multiplier  $\lambda$  is updated after each Alternated Direction iteration. Finally, the PGD algorithms were initialized with  $\lambda = 1$  and with random modes.

For each method and each problem, we measure the truncation error in the semi-norm induced by  $b$  between the FE solution of the Lagrangian problem and the PGD solution, displayed in Figure 3, as well as the absolute value of the mean-value, displayed in Figure 4, and the error in the Lagrange multiplier, displayed in Figure 5.

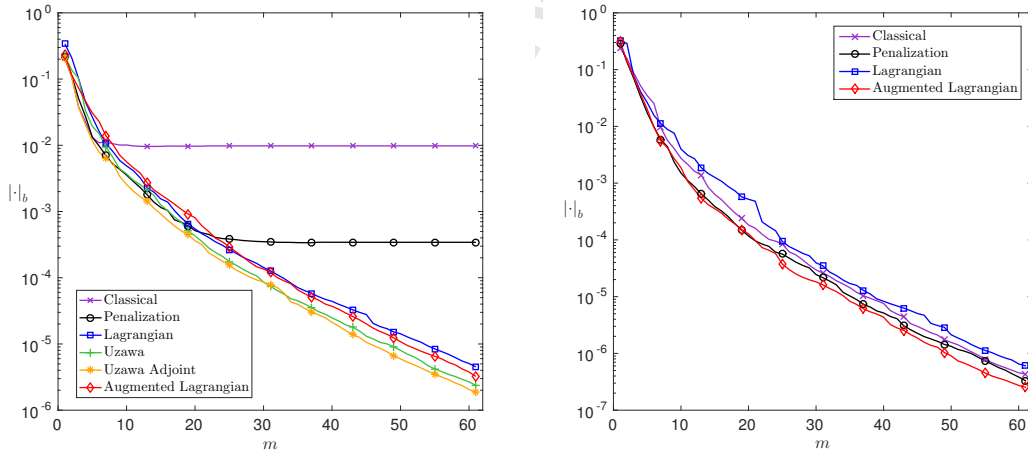


Figure 3: Truncation error between the FE Lagrangian solution and the constrained PGD methods. Left: Robin problem. Right: Neumann problem.



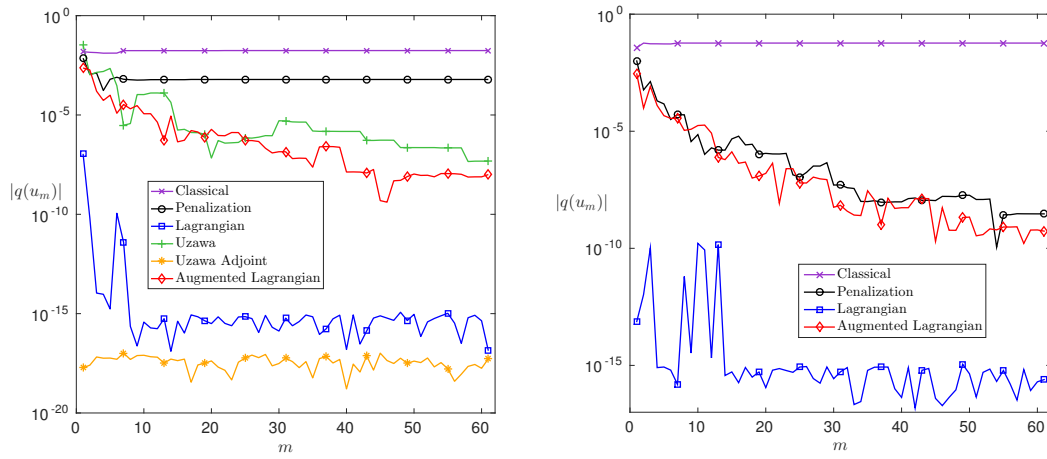


Figure 4: Absolute value of the mean-value. Left: Robin problem. Right: Neumann problem.

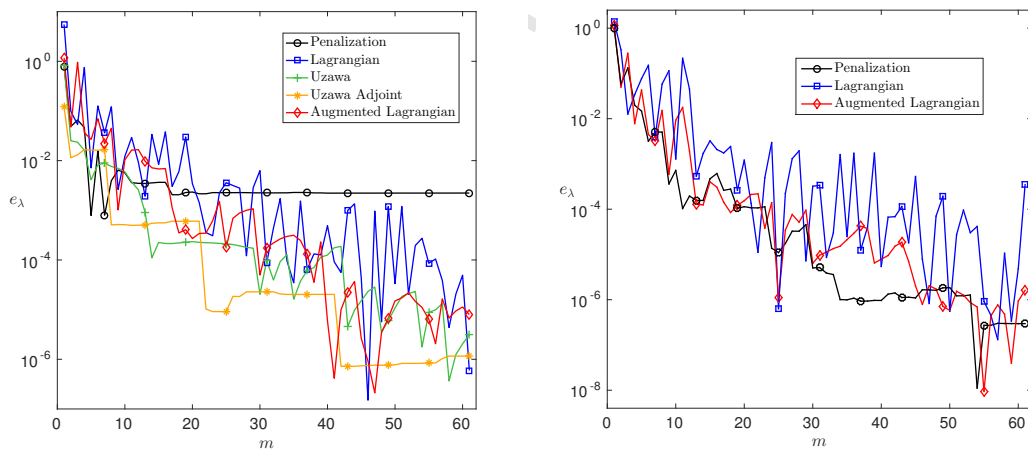


Figure 5: Error in the Lagrange multiplier. Left: Robin problem. Right: Neumann problem.

In terms of the semi-norm induced by  $b$ , all PGD solutions converge towards the FE solution of the Lagrangian problem, except for the unconstrained and the penalized approaches for the Robin case, as is to be expected. Concerning the mean-value, all constrained PGD solutions tend to satisfy the constraint as the number of modes increases, except for the penalized Robin case, because of the aforementioned trade-off between energy and constraint satisfaction. We note that for the Uzawa Adjoint method, the constraint is satisfied up to machine precision, but this is only a consequence of the way the Lagrange multiplier is computed for this approach, i.e. following (4.22). Finally, the Lagrange multiplier also converges with the number of modes except for the penalized Robin case.

To summarize, the PGD methods based on the Lagrangian formulation (including the Uzawa and Augmented Lagrangian approaches) converge towards the FE Lagrangian solution. The PGD method based on the penalization formulation converges towards its penalized FE solution counterpart (not directly shown in these figures).

We now investigate the influence of the step length  $\alpha$  and of the impedance coefficient  $\varepsilon$  on the performance of the constrained PGD solved by the Uzawa method, again applied to the Robin problem. The results are collected in Table 2, where we measure the number of modes required to achieve a truncation error in the energy norm between the constrained PGD solution and the FE solution of the full Lagrangian problem (3.3) smaller than  $10^{-2}$ . For several values of the impedance coefficient  $\varepsilon$  (and thus several values of the Schur coefficient  $S$ ) we used different constant values of  $\alpha$  as well as the step length computed solving the auxiliary problems resulting from (4.20)–(4.21), bottom line entitled  $\alpha_{\text{opt}}$  in the table.

$\alpha \backslash \varepsilon$	$10^{-8}$	$10^{-7}$	$10^{-6}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$	$10^{-1}$	1
1	×	×	×	×	×	×	×	×	7
$10^{-1}$	×	×	×	×	×	×	×	8	9
$10^{-2}$	×	×	×	×	×	×	8	9	42
$10^{-3}$	×	×	×	×	×	7	7	43	335
$\alpha_{\text{opt}}$	○	○	10	10	7	8	11	9	7

Table 2: Number of modes needed to achieve a truncation error in the energy norm smaller than  $10^{-2}$  as a function of the step length  $\alpha$  and impedance coefficient  $\varepsilon$ . The “×” notation is employed to mean there was divergence of the numerical solutions (unbounded energy norm). The “○” notation is employed to mean the numerical solution had bounded energy norm but did not converge to the FE solution of the full Lagrangian problem (3.3).

We observe that choosing a constant step length  $\alpha$  is effective as long as the impedance coefficient  $\varepsilon$  is neither too small, which may let the numerical solution have unbounded energy norm, nor too large, which may require more modes to observe convergence. This is in agreement with Saad’s analysis [24]. Conversely, opting for the step length  $\alpha_{\text{opt}}$  yielded by the auxiliary problems

is a much more robust choice. However we note that when the impedance coefficient  $\varepsilon$  is too close to zero, even this choice does not yield satisfactory results. The reason is that for such values of the impedance coefficient  $\varepsilon$ , the Robin problem becomes closer and closer to the pure Neumann problem, for which the Uzawa approach is not applicable. We mention that the Uzawa Adjoint approach was stable for values of the impedance coefficient  $\varepsilon$  larger than  $10^{-13}$ .

Finally, computing times for the constrained PGD approaches were recorded and compared to the unconstrained (classical) PGD. We found that the extra cost associated to the constraint was in the 20% range of the total time, except for the Lagrangian approach, in which case the extra time was about 75%. This difference is likely due to the “Jacobi” nature of the fixed-point algorithm for the Lagrangian approach, which is known to require more iterations to converge than its “Gauss-Seidel” counterpart.

## 6 Conclusion

In this paper, we have introduced and analyzed several methods to incorporate a constraint within the PGD framework. We have considered the Lagrangian formulation and some classical numerical strategies such as the Uzawa and Augmented Lagrangian approaches, and the penalization approach. Using two problems, namely a pure Neumann problem and a Robin problem, we were able to show from the numerical examples that the constrained PGD based on the Lagrangian formulation converges towards the FE solution of the Lagrangian problem (except for the Uzawa approach when the Schur complement was too large), while the penalized PGD solution converges towards the penalized FE solution.

As a conclusion of the study, we recommend the use of the Uzawa method, if the Schur complement is moderately small, and the Lagrangian or Augmented Lagrangian methods otherwise, which offer satisfactory results. As far as the penalization parameter  $\beta$  in the Augmented Lagrangian approach is concerned, it should be chosen in such a manner that the step length remain accurate while avoiding introducing round-off errors in the solution. The optimal value of  $\beta$  for a given problem actually depends on many parameters, including the spectrum of the Schur complement. The penalization approach is much simpler to implement but provides only an approximation of the constraint, except in the particular case of the pure Neumann problem (unicity recovered through the constraint).

Future developments will focus on when to update the Lagrange multiplier in the Uzawa and Augmented Lagrangian approaches, on a possible proof of convergence for the PGD solutions when using the Lagrangian formulation, on higher dimensional constraints, e.g. for the Stokes problem or quasi-incompressible solid mechanics (the methods proposed in this paper could be extended as alternative approaches to the method presented in [19]), and on the incorporation of inequality constraints using the KKT (Karush-Kuhn-Tucker) conditions [20, 21].

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## Highlights

- A review of classical approaches (Penalization, Lagrangian, and Lagrangian Methods) and numerical methods to enforce a constraint on boundary-value problems is presented.
- These methods are extended and adapted for the time to our best knowledge to the Proper Generalized Decomposition (PGD) setting, except penalization.
- Extensive numerical results on a pure Neumann and a constrained Robin problems illustrate the performance of each method.
- Conclusion of the study is that the Uzawa method with optimal step length, if the Schur complement is moderately small, is the method of choice while the Lagrangian or Augmented Lagrangian methods offer satisfactory results otherwise.