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Numerical Identification of Boundary Condition for Reaction-Advection-Diffusion Partial Differential Equation

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Abstract. In this study, we consider a reaction-advection-diffusion partial differential equations (PDEs) in a plane domain with missed boundary data. We applied both the KMF algorithm and the conjugate gradient method to reconstruct the missed data by using the spectral element method. Several numerical examples were given illustrating the convergence of the used algorithms.

1. Introduction

Reaction-advection-diffusion partial differential equations (PDEs) are are widely used to predict several engineering phenomena such as population dynamics, nuclear reactors, and chemical reaction processes. Introduced firstly in the twentieth century when modeling the dynamics of population , they have been applied in several other phenomena such as climate change and combustion by combining spreading, stirring, growth and decay. This work is a contribution to the study of an inverse problem of reconstruction of boundary data from overdetermined data on another part of the boundary of a domain, the underlying physical phenomenon being governed by the reaction-advection-diffusion partial differential equation. The intuitive definition of the inverse problem would consist of going back to the causes of a phenomenon based on its effects in a given situation. More precisely, the prediction of the future state of a physical system, knowing its current state, is the typical example of direct problem. There are a multitude of inverse problems: for example, reconstructing the state past of the system knowing its current state (if the corresponding physical phenomenon is irreversible), or the determination of parameters of the system, knowing (part of) his evolution. This last problem is that of the identification of parameters, frame in which enters our study. We consider a rectangular domain that it is filled

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by a fluid such that measurements are possible on the input boundary are possible, however, it is not possible on the output one. Therefore, we aim to reproduce the unknown data on the out boundary using the over data on the input boundary. Such process is called data completion. It is not possible to resolve such problem trough direct methods since it is ill-posed, however, different iterative methods were proposed to resolve this problem were proposed in the literature [1–5].

In this paper, we aim to reconstruct the missed data for reaction-advection-diffusion partial differential equations (PDEs) in a two-dimensional domain. In the first step, we apply the KMF (Kozlov, Maz'ya, Fomin) algorithm [3] that approximate the solution of our problem. In the second step, we apply the conjugate gradient method to reconstruct that solution. Both algorithms were illustrated using spectral element method and several numerical example were given.

2. Reaction-advection-diffusion partial differential equations

Consider an open bounded two-dimensional domain Ω such that $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$ with $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$, $\mathrm{mes}(\partial\Omega_1) \neq 0$ and $\mathrm{mes}(\partial\Omega_2) \neq 0$. Assume that Ω is a rectangular conduct of a fluid such that $\partial\Omega_1$ is a fixed wall (Figure 1).

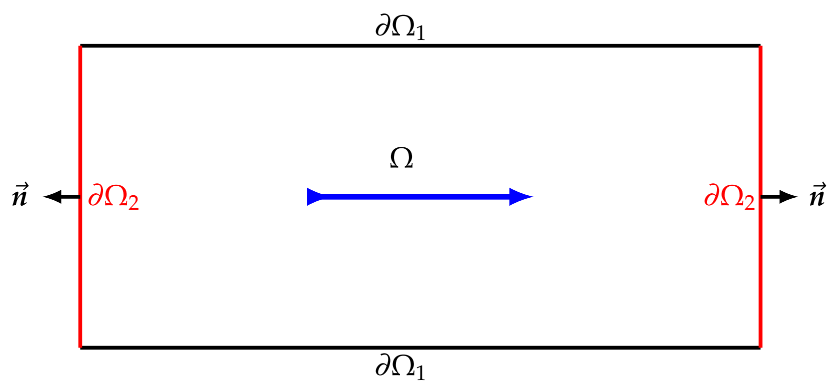

Figure 1. Ω is rectangular conduct of a fluid with a fiwed wall $\partial\Omega_1$ containing all vertices.

We aim to identify the solution, y, of the following partial differential equation:

$$\begin{cases} -\nabla \cdot (\mu_1 \nabla y) + \boldsymbol{v} \cdot \nabla y + \mu_2 y &= f \quad \text{in} \quad \Omega, \\ y &= g_1 \quad \text{on} \quad \partial\Omega_1, \\ \mu_1 \dfrac{\partial y}{\partial \boldsymbol{n}} &= \varphi \quad \text{on} \quad \partial\Omega_2. \end{cases} \tag{2.1}$$

$f \in L^2(\Omega)$ describes the source function, μ_1 describes the diffusion coefficient, μ_2 describes the reaction coefficient, and $\boldsymbol{v} = (v_1, v_2)^T$ represents a vector field in $L^\infty(\Omega)^2$ describing the advection coefficient. μ_1 and μ_2 assumed to be positive. Equation (2.1) is called reaction-advection-diffusion partial differential equation (PDE). For more simplicity, we suppose that: div $\boldsymbol{v} = 0$ and $\boldsymbol{v} \cdot n = 0$. There are several approaches to regularizing poorly posed problems. Some of them transform this ill-posed problem into a well-posed problem in adding a penalty term in order to avoid oscillating solutions. But generally effective regularization techniques consist of solving the poorly posed problem by iterative methods and by choosing a suitable stopping criterion which determines an optimal solution. The resolution of this problem relies on the duality technique; but to explain it we need to recall the essential properties of the equation (2.1) with a homogeneous Dirichlet data. This direct problem is well-posed, it has a unique solution and it can be solved by direct method. The weak formulation of the system (2.1) is: find y in Y satisfying:

$$a(y,v) = l(v), \qquad \forall v \in V \tag{2.2}$$

where Y and V are the spaces given as following

$$Y = \{y \in H^1(\Omega) : \ y = g_1 \ \text{ on } \ \partial\Omega_1\}, \quad V = \{\omega \in H^1(\Omega) : \ \omega = 0 \ \text{ on } \ \partial\Omega_1\}.$$

The bilinear form $a(\cdot,\cdot)$ is given by

$$a(y,\omega) \ = \int_\Omega \Big(\mu_1 \nabla y \cdot \nabla\omega \ + \boldsymbol{v} \cdot \nabla y\omega + \mu_2 y\omega\Big)\, dx,$$

and the linear form $l(\cdot)$ is given by

$$l(\omega) \ = \ \int_\Omega f\omega \, dx + \int_{\partial\Omega_2} \varphi\omega \, ds.$$

The aim of this section is to present the numerical resolution of system (2.1) by the spectral element method (SEM) of a coercive variational boundary problem on a plane Ω regular domain. The "exact" problem is only solvable between "natural" spaces for the data and the solutions: these spaces are Sobolev spaces on the domain Ω and are of infinite dimension. As it is rare that analytical solutions are accessible, to resolve a such a problem, we go through a discretization which will bring back the resolution of the continuous problem to the resolution of a linear system. Finite difference method, finite element method, spectral element method are all discretization methods admissible for the problem considered. The numerical analysis of a method consists of describing it, including its implementation, and also to evaluate to what extent the solution of the discretized problem approaches the true solution. The mathematical goal of such an analysis is to demonstrate the stability of the method and the convergence of the approximate solutions towards the solution when the size of the system discretized tends towards infinity. The numerical goal is to optimize the calculation time and the precision of the result. In the spectral element method that we used here, the problem is discretized by "collocation" in points obtained from the Gauss-Labatto points — which are the roots of polynomials derived from Legendre polynomials. This discretization is equivalent to a Galerkin problem with numerical integration for a function space of type polynomial in single domain or "piecewise polynomial" in multidomain. The parameter natural of the discretization is the degree M of these polynomials.

We aim to use the spectral element method for the numerical resolution of the problem (2.1). Let M to be the interpolation degree, x_1^i and x_2^i, $i = 1, \cdots, M+1$ to be the Gauss-Lobatto Legendre

points.
We define the weights for Legendre-Gauss-Lobatto numerical integration as:

$$w_i = \frac{2}{M(M+1)} \frac{1}{L_M^2(x_1^i)}, i = 1, \cdots, M+1$$

Denote by $y_{ij} = y(x_1^i, x_2^j)$, and $f_{ij} = f(x_1^i, x_2^j)$, for $i, j = 1, \cdots, M+1$. Then y is expanded in terms of the Lagrange interpolants based on the Legendre-Gauss-Lobatto points

$$y_M(x_1, x_2) = \sum_{i,j=1}^{M+1} y_{ij} \eta_i(x_1) \eta_j(x_2)$$

where η_i are the Lagrange interpolants.

The discrete weak formulation is as follows: Find $y_M \in \mathcal{Y}^M$ satisfying

$$a_M(y_M, \omega_M) := D_M(y_M, \omega_M) + A_M(y_M, \omega_M) + R_M(y_M, \omega_M) = l_M(\omega_M)$$

where the forms $D_M(y_M, \omega_M) = (\mu_1 \nabla y_M, \nabla \omega_M)_M$, $A_M(y_M, \omega_M) = (\boldsymbol{v} \cdot \nabla y_M, \omega_M)_M$, and $R_M(y_M, \omega_M) = (\mu_2\, y_M, \omega_M)_M$ describe the diffusion, the advection and the reaction terms. The discrete form of the inner product $(\cdot, \cdot)_M$ is given as

$$(u, v)_M = \sum_{i,j=1}^{M+1} w_i w_j u(x_1^i, x_2^j) v(x_1^i, x_2^j).$$

For simplicity, we consider for all the rest that $\mu_1 = \mu_2 = 1$.

3. Inverse problem

Assume that the boundary $\partial\Omega_2 = \partial\Omega_2^i \cup \partial\Omega_2^o$ where $\partial\Omega_2^i \cap \partial\Omega_2^o = \emptyset$, $\text{mes}(\partial\Omega_2)^i \neq 0$ and $\text{mes}(\partial\Omega_2^o) \neq 0$. Furthermore, assume that Ω is a channel where $\partial\Omega_1$ is a fixed wall, $\partial\Omega_2^i$ and $\partial\Omega_2^o$ are the input and output of Ω, respectively (Figure 2).

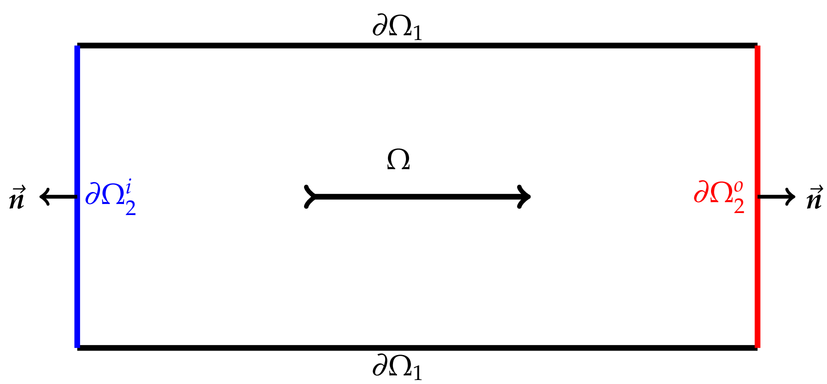

Figure 2. The domain Ω is rectangular such that $\partial\Omega_1$ is a fixed wall, $\partial\Omega_2^i$ is accessible for measurements however $\partial\Omega_2^o$ is not accessible. The outward unit normal vector is denoted by $\vec{n}$.

Assume that we can obtain some exact data described by a Dirichlet condition (g_2^i) and Neumann condition (φ^i) on a part of the boundary ($\partial\Omega_2^i$) and we aim to reconstruct the unknown data on the other part of the boundary ($\partial\Omega_2^o$).

Assume that for a given data $(f, g_1, \varphi^i, g_2^i) \in L^2(\Omega) \times H^{\frac{1}{2}}(\partial\Omega_1) \times (H^{\frac{1}{2}}(\partial\Omega_2^i))' \times H^{\frac{1}{2}}(\partial\Omega_2^i)$, we have the incomplete problem:

$$\begin{cases} -\Delta y + \boldsymbol{v}.\nabla y + y &= f \quad \text{in} \quad \Omega \\ y &= g_1 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial y}{\partial \boldsymbol{n}} = \varphi^i, \ y &= g_2^i \quad \text{on} \quad \partial\Omega_2^i \end{cases} \tag{3.1}$$

and assume that (φ^i, g_2^i) are the trace and the normal derivative of a same solution y of the inverse problem (3.1) (we say that (φ^i, g_2^i) are compatible) that can be extended to $\partial\Omega_2^o$ obtaining the reconstructed problem (3.1) defined as:

$$\begin{cases} -\Delta y + \boldsymbol{v}.\nabla y + y &= f \quad \text{in} \quad \Omega \\ y &= g_1 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial y}{\partial \boldsymbol{n}} = \varphi^i, \ y &= g_2^i \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial y}{\partial \boldsymbol{n}} = \varphi^o, \ y &= g_2^o \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.2}$$

3.1. **KMF algorithm.** Several numerical methods were proposed to resolve ill-posed problems similar to our problem (3.2). In our case, we reconsider in the first step the KMF (Kozlov, Maz'ya, Fomin) algorithm [3] as used in several previous works [6–9]). This method consider two problems and it resolve them by alternating them to approximate the unknown data on one part of the boundary. Consider an arbitrary Dirichlet boundary condition $\vartheta_0 \in H^{\frac{1}{2}}(\partial\Omega_2^o)$. Therefore, the KMF algorithm is formulated as given in Figure 3.

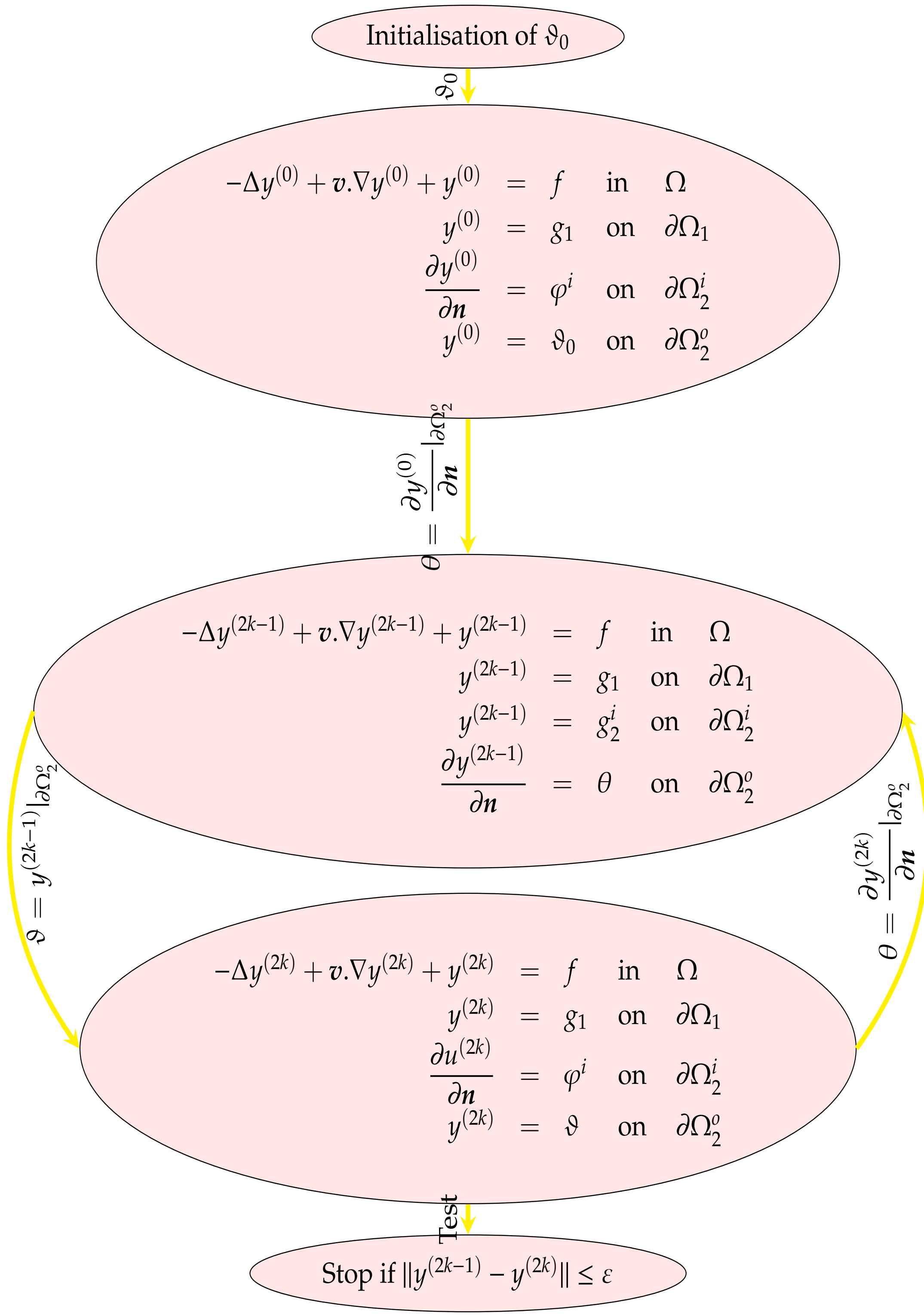

FIGURE 3. KMF algorithm design for reaction-advection-diffusion partial differential equations (PDEs) in a two-dimensional domain. Note that (φ^i, g_2^i) are compatible if $(\theta, \vartheta) = (\varphi^o, g_2^o)$. The controlling test is applied on the norm $\|y^{(2k-1)} - y^{(2k)}\|$ on the hole domain Ω.

3.2. **Minimisation approach and conjugate gradient method.** With the aim to resolve the system (3.2), (φ^o, g_2^o) can be approached by minimising an energy functional as studied for other partial differential equations in [1, 6, 8, 10]. Assume that we have a given data (θ, ϑ), let consider the following mixed problems given hereafter:

$$\begin{cases} -\Delta y_1 + \boldsymbol{v}.\nabla y_1 + y_1 &= f \quad \text{in} \quad \Omega \\ y_1 &= g_1 \quad \text{on} \quad \partial\Omega_1 \\ y_1 &= g_2^i \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial y_1}{\partial \boldsymbol{n}} &= \theta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \quad (3.3) \qquad \begin{cases} -\Delta y_2 + \boldsymbol{v}.\nabla y_2 + y_2 &= f \quad \text{in} \quad \Omega \\ y_2 &= g_1 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial y_2}{\partial \boldsymbol{n}} &= \varphi^i \quad \text{on} \quad \partial\Omega_2^i \\ y_2 &= \vartheta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \quad (3.4)$$

Note that the solution y_1 and y_2 coincide only if the data (θ, ϑ) coincide with the real data (φ^o, g_2^o) on the inaccessible boundary $\partial\Omega_2^o$. A good way to approach the real data is to solve this problem by minimising an energy functional as the following:

$$\begin{cases} (\varphi^o, g_2^o) = \arg\min\limits_{\theta,\vartheta} \ F(\theta, \vartheta) \\ F(\theta, \vartheta) := \|y_1 - y_2\|^2_{H^1(\Omega)} = \displaystyle\int_\Omega (\nabla y_1 - \nabla y_2)^2 + \int_\Omega (y_1 - y_2)^2 \\ \text{where } y_1 \text{ and } y_2 \text{ are the solutions of problems (3.3) and (3.4), respectively} \end{cases} \quad (3.5)$$

The functional $F(\theta, \vartheta)$ is a convex quadratic positive functional admitting an absolute minimum at $y_1 = y_2$.

For simplicity, we consider the case where $\boldsymbol{v} \equiv \boldsymbol{0}$ and we reproduce the calculus given in [1]. As y_1 and y_2 are solutions of systems (3.3) and (3.4), we can derive a simple expression of the functional F as follows:

$$\begin{aligned} F(\theta, \vartheta) &= -\int_\Omega \Delta(y_1 - y_2)(y_1 - y_2) + \int_{\partial\Omega_2^o} (\theta - \frac{\partial y_2}{\partial \boldsymbol{n}})(y_1 - \vartheta) \\ &\quad + \int_{\partial\Omega_2^i} (\frac{\partial y_1}{\partial \boldsymbol{n}} - \varphi^i)(g_2^i - y_2) + \int_\Omega (y_1 - y_2)^2 \\ &= \int_{\partial\Omega_2^o} (\theta - \frac{\partial y_2}{\partial \boldsymbol{n}})(y_1 - \vartheta) + \int_{\partial\Omega_2^i} (\frac{\partial y_1}{\partial \boldsymbol{n}} - \varphi^i)(g_2^i - y_2) \end{aligned}$$

For a given data (θ, ϑ), we obtain the partial derivatives of F as the following:

$$\begin{aligned} \frac{\partial F(\theta, \vartheta)}{\partial \theta}\psi &= \int_{\partial\Omega_2^o} [y_1 - \vartheta]\psi + \int_{\partial\Omega_2^i} \frac{\partial \xi_1}{\partial \boldsymbol{n}}[g_2^i - y_2] \\ \frac{\partial F(\theta, \vartheta)}{\partial \vartheta}h &= \int_{\partial\Omega_2^o} [\frac{\partial y_2}{\partial \boldsymbol{n}} - \theta]h + \int_{\partial\Omega_2^i} [\varphi^i - \frac{\partial y_1}{\partial \boldsymbol{n}}]\xi_2 \end{aligned} \quad (3.6)$$

for all $(h, \psi) \in H_{00}^{1/2}(\partial\Omega_2^o) \times H_{00}^{-1/2}(\partial\Omega_2^o)$ with ξ_1 and ξ_2 are the solution of the following systems that are depending on the directions ψ and h:

$$\left\{\begin{array}{rcll} -\Delta\xi_1+\xi_1 &=& 0 & \text{on} \quad \Omega \\ \xi_1 &=& 0 & \text{on} \quad \partial\Omega_1 \\ \xi_1 &=& 0 & \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial\xi_1}{\partial \boldsymbol{n}} &=& \psi & \text{on} \quad \partial\Omega_2^o \end{array}\right. \tag{3.7}$$

$$\left\{\begin{array}{rcll} -\Delta\xi_2+\xi_2 &=& 0 & \text{in} \quad \Omega \\ \xi_2 &=& 0 & \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial\xi_2}{\partial \boldsymbol{n}} &=& 0 & \text{on} \quad \partial\Omega_2^i \\ \xi_2 &=& h & \text{on} \quad \partial\Omega_2^o \end{array}\right. \tag{3.8}$$

The expressions (3.6) can be simplified by using adjoint states, denoted by ω_1 and ω_2 as in the following Proposition.

Proposition 3.1.

$$\frac{\partial F(\theta,\vartheta)}{\partial\theta}\psi = -2\int_{\partial\Omega_2^o}\omega_1\psi \quad \textit{and} \quad \frac{\partial F(\theta,\vartheta)}{\partial\vartheta}h = -2\int_{\partial\Omega_2^o}\frac{\partial\omega_2}{\partial\boldsymbol{n}}h,$$

where ω_1 and ω_2 are the solutions of the following systems:

$$\left\{\begin{array}{rcll} -\Delta\omega_1+\omega_1 &=& 0 & \textit{in} \quad \Omega \\ \omega_1 &=& 0 & \textit{on} \quad \partial\Omega_1 \\ \omega_1 &=& 0 & \textit{on} \quad \partial\Omega_2^i \\ \dfrac{\partial\omega_1}{\partial \boldsymbol{n}} &=& \dfrac{\partial y_2}{\partial \boldsymbol{n}}-\theta & \textit{on} \quad \partial\Omega_2^o \end{array}\right. \qquad \left\{\begin{array}{rcll} -\Delta\omega_2+\omega_2 &=& 0 & \textit{in} \quad \Omega \\ \omega_2 &=& 0 & \textit{on} \quad \partial\Omega_1 \\ \dfrac{\partial\omega_2}{\partial \boldsymbol{n}} &=& 0 & \textit{on} \quad \partial\Omega_2^i \\ \omega_2 &=& y_1-\vartheta & \textit{on} \quad \partial\Omega_2^o \end{array}\right.$$

Proof. A classical calculus conduct us to the following forms of the gradient components:

$$\begin{aligned} \frac{\partial F(\theta,\vartheta)}{\partial\theta}\psi &= 2\int_\Omega(\nabla y_1-\nabla y_2)\nabla\xi_1+2\int_\Omega(y_1-y_2)\xi_1 \\ &= -2\int_\Omega(\Delta y_1-\Delta y_2)\xi_1+2\int_{\partial\Omega_2^o}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})\xi_1+2\int_\Omega(y_1-y_2)\xi_1 \\ &= 2\int_{\partial\Omega_2^o}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})\xi_1 = 2\int_{\partial\Omega_2^o}(\theta-\frac{\partial y_2}{\partial\boldsymbol{n}})\xi_1 = -2\int_{\partial\Omega_2^o}\frac{\partial\omega_1}{\partial\boldsymbol{n}}\xi_1 \\ &= -2\int_\Omega\nabla\omega_1\nabla\xi_1-2\int_\Omega\Delta\omega_1\xi_1 = -2\int_\Omega\nabla\omega_1\nabla\xi_1-2\int_\Omega\omega_1\xi_1 \\ &= 2\int_\Omega\Delta\xi_1\omega_1-2\int_{\partial\Omega_2^o}\frac{\partial\xi_1}{\partial\boldsymbol{n}}\omega_1-2\int_\Omega\xi_1\omega_1 = -2\int_{\partial\Omega_2^o}\frac{\partial\xi_1}{\partial\boldsymbol{n}}\omega_1 \\ &= -2\int_{\partial\Omega_2^o}\omega_1\psi, \end{aligned}$$

and

$$\begin{aligned} \frac{\partial F(\theta,\vartheta)}{\partial\vartheta}h &= -2\int_\Omega(\nabla y_1-\nabla y_2)\nabla\xi_2-2\int_\Omega(y_1-y_2)\xi_2 \\ &= 2\int_\Omega\Delta\xi_2(y_1-y_2)-2\int_{\partial\Omega_2^o}\frac{\partial\xi_2}{\partial\boldsymbol{n}}(y_1-y_2)-2\int_\Omega(y_1-y_2)\xi_2 \\ &= -2\int_{\partial\Omega_2^o}\frac{\partial\xi_2}{\partial\boldsymbol{n}}(y_1-y_2) = -2\int_{\partial\Omega_2^o}\frac{\partial\xi_2}{\partial\boldsymbol{n}}(y_1-\vartheta) = -2\int_{\partial\Omega_2^o}\frac{\partial\xi_2}{\partial\boldsymbol{n}}\omega_2 \\ &= -2\int_\Omega\Delta\xi_2\omega_2-2\int_\Omega\nabla\xi_2\nabla\omega_2 = -2\int_\Omega\xi_2\omega_2+2\int_\Omega\xi_2\Delta\omega_2-2\int_{\partial\Omega_2^o}\frac{\partial\omega_2}{\partial\boldsymbol{n}}\xi_2 \\ &= -2\int_\Omega\xi_2\omega_2+2\int_\Omega\xi_2\omega_2-2\int_{\partial\Omega_2^o}\frac{\partial\omega_2}{\partial\boldsymbol{n}}\xi_2 = -2\int_{\partial\Omega_2^o}\frac{\partial\omega_2}{\partial\boldsymbol{n}}\xi_2 = -2\int_{\partial\Omega_2^o}\frac{\partial\omega_2}{\partial\boldsymbol{n}}h. \end{aligned}$$

□

The conjugate gradient method is an iterative method for solving an equation $Ax = b$, with A a positive definite symmetric matrix, or, equivalently, to find the minimum of the function $\Psi(x)$:

$$\Psi(x) = \frac{1}{2}x^t Ax - b^t x.$$

The minimisation of Ψ is successfully reached if the gradient of Ψ given by $\nabla\Psi(x) = Ax - b$ is zero.

The approach is based on subdivision of the state into compartments as follows:

$$y_1 = y_1^0 + y_1^*, \quad y_2 = y_2^0 + y_2^*$$

with y_1^*, y_2^*, y_1^0 and y_2^0 are solutions of the following partial differential equations

$$\begin{cases} -\Delta y_1^* + y_1^* &= 0 \quad \text{in} \quad \Omega \\ y_1^* &= 0 \quad \text{on} \quad \partial\Omega_1 \\ y_1^* &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial y_1^*}{\partial \boldsymbol{n}} &= \theta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.9}$$

$$\begin{cases} -\Delta y_2^* + y_2^* &= 0 \quad \text{in} \quad \Omega \\ y_2^* &= 0 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial y_2^*}{\partial \boldsymbol{n}} &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ y_2^* &= \vartheta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.10}$$

$$\begin{cases} -\Delta y_1^0 + y_1^0 &= f \quad \text{in} \quad \Omega \\ y_1^0 &= g \quad \text{on} \quad \partial\Omega_1 \\ y_1^0 &= g_2^i \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial y_1^0}{\partial \boldsymbol{n}} &= 0 \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.11}$$

$$\begin{cases} -\Delta y_2^0 + y_2^0 &= f \quad \text{in} \quad \Omega \\ y_2^0 &= g \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial y_2^0}{\partial \boldsymbol{n}} &= \varphi^i \quad \text{on} \quad \partial\Omega_2^i \\ y_2^0 &= 0 \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.12}$$

Similarly, we divide the adjoint states as followss:

$$\omega_1 = \omega_1^0 + \omega_1^*, \quad \omega_2 = \omega_2^0 + \omega_2^*$$

whith $\omega_1^*, \omega_2^*, \omega_1^0$ and ω_2^0 in $H^1(\Omega)$ are solutions of the following partial differential equations:

$$\begin{cases} -\Delta \omega_1^* + \omega_1^* &= 0 \quad \text{in} \quad \Omega \\ \omega_1^* &= 0 \quad \text{on} \quad \partial\Omega_1 \\ \omega_1^* &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial \omega_1^*}{\partial \boldsymbol{n}} &= \dfrac{\partial y_2^*}{\partial \boldsymbol{n}} - \theta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.13}$$

$$\begin{cases} -\Delta \omega_2^* + \omega_2^* &= 0 \quad \text{in} \quad \Omega \\ \omega_2^* &= 0 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial \omega_2^*}{\partial \boldsymbol{n}} &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ \omega_2^* &= y_1^* - \vartheta \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.14}$$

$$\begin{cases} -\Delta \omega_1^0 + \omega_1^0 &= 0 \quad \text{in} \quad \Omega \\ \omega_1^0 &= 0 \quad \text{on} \quad \partial\Omega_1 \\ \omega_1^0 &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ \dfrac{\partial \omega_1^0}{\partial \boldsymbol{n}} &= \dfrac{\partial y_2^0}{\partial \boldsymbol{n}} \quad \text{on} \quad \partial\Omega_2^o \end{cases} \tag{3.15}$$

$$\begin{cases} -\Delta \omega_2^0 + \omega_2^0 &= 0 \quad \text{in} \quad \Omega \\ \omega_2^0 &= 0 \quad \text{on} \quad \partial\Omega_1 \\ \dfrac{\partial \omega_2^0}{\partial \boldsymbol{n}} &= 0 \quad \text{on} \quad \partial\Omega_2^i \\ \omega_2^0 &= y_1^0 \quad \text{on} \quad \partial\Omega_2^o. \end{cases} \tag{3.16}$$

Let the linear operator A given by

$$\forall(\theta,\vartheta)\in H_{00}^{-\frac{1}{2}}(\partial\Omega_2^o)\times H_{00}^{\frac{1}{2}}(\partial\Omega_2^o),\quad A(\theta,\vartheta)^T=-\Big(\omega_1^*(\theta,\vartheta)|_{\partial\Omega_2^o},\ \frac{\partial\omega_2^*(\theta,\vartheta)}{\partial\boldsymbol{n}}|_{\partial\Omega_2^o}\Big)^T.$$

Proposition 3.2. (1) *The functional, F, is expressed as follows*

$$\forall(\theta,\vartheta)\in H_{00}^{-\frac{1}{2}}(\partial\Omega_2^o)\times H_{00}^{\frac{1}{2}}(\partial\Omega_2^o),\quad F(\theta,\vartheta)=(\theta,\vartheta)A(\theta,\vartheta)^T-2b(\theta,\vartheta)^T+c$$

with $b=\Big(\omega_1^0|_{\partial\Omega_2^o},\ \dfrac{\partial\omega_2^0}{\partial\boldsymbol{n}}|_{\partial\Omega_2^o}\Big)$ *, and c be a constant doesn't depend on (θ,ϑ).*

(2) *The operator A is symmetric, positive, and definite.*

Proof.

$$\begin{aligned}
F(\theta,\vartheta)= &\int_\Omega(\nabla y_1-\nabla y_2)^2+\int_\Omega(y_1-y_2)^2\\
= &-\int_\Omega(\Delta y_1-\Delta y_2)(y_1-y_2)+\int_{\partial\Omega_2^i\cup\partial\Omega_2^o}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-y_2)+\int_\Omega(y_1-y_2)^2\\
= &\int_{\partial\Omega_2^i}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-y_2)+\int_{\partial\Omega_2^o}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-y_2)\\
= &\int_{\partial\Omega_2^i}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\varphi^i)(g_2^i-y_2)+\int_{\partial\Omega_2^o}(\theta-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-\vartheta)\\
= &\int_{\partial\Omega_2^i}(\frac{\partial y_1}{\partial\boldsymbol{n}}g_2^i-\varphi^ig_2^i+\varphi^iy_2-\frac{\partial y_1}{\partial\boldsymbol{n}}y_2)+\int_{\partial\Omega_2^o}(\theta-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-\vartheta)
\end{aligned}$$

By using Green formula for the expression $\dfrac{\partial y_1}{\partial\boldsymbol{n}}y_2$, we deduce that

$$\begin{aligned}
\int_{\partial\Omega_2^i}\frac{\partial y_1}{\partial\boldsymbol{n}}y_2 = &\int_\Omega\Delta y_1y_2+\int_\Omega\nabla y_1\nabla y_2-\int_{\partial\Omega_2^o}\frac{\partial y_1}{\partial\boldsymbol{n}}y_2-\int_{\partial\Omega_1}\frac{\partial y_1}{\partial\boldsymbol{n}}y_2\\
= &\int_\Omega(y_1-f)y_2-\int_\Omega y_1\Delta y_2+\int_{\partial\Omega_2^i}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1+\int_{\partial\Omega_2^o}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1+\int_{\partial\Omega_1}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1\\
&-\int_{\partial\Omega_2^o}\theta\vartheta-\int_{\partial\Omega_1}\frac{\partial y_1}{\partial\boldsymbol{n}}g\\
= &\int_\Omega(y_1-f)y_2-\int_\Omega y_1(y_2-f)+\int_{\partial\Omega_2^i}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1+\int_{\partial\Omega_2^o}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1\\
&+\int_{\partial\Omega_1}\frac{\partial y_2}{\partial\boldsymbol{n}}y_1-\int_{\partial\Omega_2^o}\theta\vartheta-\int_{\partial\Omega_1}\frac{\partial y_1}{\partial\boldsymbol{n}}g\\
= &\int_\Omega f(y_1-y_2)+\int_{\partial\Omega_2^i}\varphi^ig_2^i+\int_{\partial\Omega_2^o}(\frac{\partial y_2}{\partial\boldsymbol{n}}y_1-\theta\vartheta)+\int_{\partial\Omega_1}(\frac{\partial y_2}{\partial\boldsymbol{n}}-\frac{\partial y_1}{\partial\boldsymbol{n}})g.
\end{aligned}$$

Therefore, the functional, F, becomes

$$\begin{aligned}
F(\theta,\vartheta) = &\int_{\partial\Omega_2^i}(\frac{\partial y_1}{\partial\boldsymbol{n}}g_2^i-\varphi^ig_2^i+\varphi^iy_2-\frac{\partial y_1}{\partial\boldsymbol{n}}y_2)+\int_{\partial\Omega_2^o}(\theta-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-\vartheta)\\
= &-\int_\Omega f(y_1-y_2)+\int_{\partial\Omega_1}(\frac{\partial y_1}{\partial\boldsymbol{n}}-\frac{\partial y_2}{\partial\boldsymbol{n}})g+\int_{\partial\Omega_2^i}(\frac{\partial y_1}{\partial\boldsymbol{n}}g_2^i-2\varphi^ig_2^i+\varphi^iy_2)\\
&+\int_{\partial\Omega_2^o}(\theta-\frac{\partial y_2}{\partial\boldsymbol{n}})(y_1-\vartheta)+\int_{\partial\Omega_2^o}(\theta\vartheta-\frac{\partial y_2}{\partial\boldsymbol{n}}y_1)
\end{aligned}$$

$$\begin{aligned} &= -\int_{\Omega} f(y_1-y_2) + \int_{\partial\Omega_1}(\frac{\partial y_1}{\partial \boldsymbol{n}} - \frac{\partial y_2}{\partial \boldsymbol{n}})g + \int_{\partial\Omega_2}(\frac{\partial y_1}{\partial \boldsymbol{n}} y_1^0 - 2\varphi^i g_2^i + \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_2) \\ &\quad + \int_{\partial\Omega_2^o}(\theta - \frac{\partial y_2}{\partial \boldsymbol{n}})(y_1-\vartheta) + \int_{\partial\Omega_2^o}(\theta\vartheta - \frac{\partial y_2}{\partial \boldsymbol{n}} y_1). \end{aligned}$$

Again, by using Green formula for the terms $\frac{\partial y_1}{\partial \boldsymbol{n}} y_1^0$ and $\frac{\partial y_2^0}{\partial \boldsymbol{n}} y_2$, we deduce that

$$\int_{\partial\Omega_2} \frac{\partial y_1}{\partial \boldsymbol{n}} y_1^0 = \int_{\Omega} f(y_1 - y_1^0) + \int_{\partial\Omega_2^i} \frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i + \int_{\partial\Omega_1}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_1}{\partial \boldsymbol{n}})g - \int_{\partial\Omega_2^o} \theta y_1^0,$$

and

$$\int_{\partial\Omega_2^i} \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_2 = \int_{\Omega} f(y_2^0 - y_2) + \int_{\partial\Omega_2^i} \varphi^i y_2^0 + \int_{\partial\Omega_1}(\frac{\partial y_2}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}})g_1 - \int_{\partial\Omega_2^o} \vartheta \frac{\partial y_2^0}{\partial \boldsymbol{n}}.$$

Therefore, the expression of the functional F can reduced as follows:

$$\begin{aligned} F(\theta,\vartheta) &= \int_{\Omega} f(y_2^0 - y_1^0) + \int_{\partial\Omega_2^i}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i - 2\varphi^i g_2^i + \varphi^i y_2^0) \\ &\quad + \int_{\partial\Omega_1}(\frac{\partial y_1}{\partial \boldsymbol{n}} - \frac{\partial y_2}{\partial \boldsymbol{n}} + \frac{\partial y_2}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}} + \frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_1}{\partial \boldsymbol{n}})g_1 \\ &\quad + \int_{\partial\Omega_2^o}\Big[(\theta - \frac{\partial y_2}{\partial \boldsymbol{n}})(y_1-\vartheta) + (\theta\vartheta - \frac{\partial y_2}{\partial \boldsymbol{n}} y_1) - \theta y_1^0 - \vartheta\frac{\partial y_2^0}{\partial \boldsymbol{n}}\Big] \\ &= \int_{\Omega} f(y_2^0 - y_1^0) + \int_{\partial\Omega_2^i}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i - 2\varphi^i g_2^i + \varphi^i y_2^0) + \int_{\partial\Omega_1}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}})g_1 \\ &\quad + \int_{\partial\Omega_2^o}\Big[\theta(y_1 - y_1^0) + \vartheta(\frac{\partial y_2}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}}) - 2\frac{\partial y_2}{\partial \boldsymbol{n}} y_1\Big] \end{aligned}$$

Let $c = \int_{\Omega} f(y_2^0 - y_1^0) + \int_{\partial\Omega_2^i}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i - 2\varphi^i g_2^i + \varphi^i y_2^0) + \int_{\partial\Omega_1}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}})g - 2\int_{\partial\Omega_2^o} \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_1^0$, and since $y_1 = y_1^* + y_1^0$ and $y_2 = y_2^* + y_2^0$, then we deduce the new form of the functional F as follows

$$\begin{aligned} F(\theta,\vartheta) &= \int_{\Omega} f(y_2^0 - y_1^0) + \int_{\partial\Omega_2^i}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i - 2\varphi^i g_2^i + \varphi^i y_2^0) + \int_{\partial\Omega_1}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}})g \\ &\quad + \int_{\partial\Omega_2^o}\Big[\theta y_1^* + \vartheta\frac{\partial y_2^*}{\partial \boldsymbol{n}} - 2(\frac{\partial y_2^*}{\partial \boldsymbol{n}} + \frac{\partial y_2^0}{\partial \boldsymbol{n}})(y_1^* + y_1^0)\Big] \\ &= \int_{\Omega} f(y_2^0 - y_1^0) + \int_{\partial\Omega_2^i}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} g_2^i - 2\varphi^i g_2^i + \varphi^i y_2^0) + \int_{\partial\Omega_1}(\frac{\partial y_1^0}{\partial \boldsymbol{n}} - \frac{\partial y_2^0}{\partial \boldsymbol{n}})g \\ &\quad -2\int_{\partial\Omega_2^o} \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_1^0 - 2\int_{\partial\Omega_2^o}(\frac{\partial y_2^*}{\partial \boldsymbol{n}} y_1^0 + \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_1^*) + \int_{\partial\Omega_2^o}\Big[\theta y_1^* + \vartheta\frac{\partial y_2^*}{\partial \boldsymbol{n}} - 2\frac{\partial y_2^*}{\partial \boldsymbol{n}} y_1^*\Big] \\ &= c - 2\int_{\partial\Omega_2^o}(\frac{\partial y_2^*}{\partial \boldsymbol{n}} y_1^0 + \frac{\partial y_2^0}{\partial \boldsymbol{n}} y_1^*) + \int_{\partial\Omega_2^o}\Big[\theta y_1^* + \vartheta\frac{\partial y_2^*}{\partial \boldsymbol{n}} - 2\frac{\partial y_2^*}{\partial \boldsymbol{n}} y_1^*\Big] \end{aligned}$$

$$\begin{aligned} &= c-2\int_{\partial\Omega_2^o}\Big(\frac{\partial y_2^*}{\partial \boldsymbol{n}}\omega_2^0+\frac{\partial \omega_1^0}{\partial \boldsymbol{n}}y_1^*\Big)+\int_{\partial\Omega_2^o}\Big[(\theta-\frac{\partial y_2^*}{\partial \boldsymbol{n}})y_1^*+(\vartheta-y_1^*)\frac{\partial y_2^*}{\partial \boldsymbol{n}}\Big] \\ &= c-2\int_{\partial\Omega_2^o}\Big(\frac{\partial y_2^*}{\partial \boldsymbol{n}}\omega_2^0+\frac{\partial \omega_1^0}{\partial \boldsymbol{n}}y_1^*\Big)-\int_{\partial\Omega_2^o}\Big[\frac{\partial \omega_1^*}{\partial \boldsymbol{n}}y_1^*+\omega_2^*\frac{\partial y_2^*}{\partial \boldsymbol{n}}\Big]. \end{aligned}$$

Again, by using Green formula for the expressions $\frac{\partial y_2^*}{\partial \boldsymbol{n}}\omega_2^0$, $\frac{\partial \omega_1^0}{\partial \boldsymbol{n}}y_1^*$, $\frac{\partial \omega_1^*}{\partial \boldsymbol{n}}y_1^*$ and $\omega_2^*\frac{\partial y_2^*}{\partial \boldsymbol{n}}$, we obtain

$$\int_{\partial\Omega_2^o}\frac{\partial y_2^*}{\partial \boldsymbol{n}}\omega_2^0=\int_\Omega \Delta y_2^*\omega_2^0+\int_\Omega \nabla y_2^*\nabla\omega_2^0=\int_\Omega y_2^*\omega_2^0-\int_\Omega y_2^*\Delta\omega_2^0+\int_{\partial\Omega_2^o}\frac{\partial \omega_2^0}{\partial \boldsymbol{n}}y_2^*=\int_{\partial\Omega_2^o}\frac{\partial \omega_2^0}{\partial \boldsymbol{n}}\vartheta,$$

$$\int_{\partial\Omega_2^o}\frac{\partial \omega_1^0}{\partial \boldsymbol{n}}y_1^*=\int_\Omega \Delta\omega_1^0 y_1^*+\int_\Omega \nabla\omega_1^0\nabla y_1^*=\int_\Omega \omega_1^0 y_1^*-\int_\Omega \omega_1^0\Delta y_1^*+\int_{\partial\Omega_2^o}\frac{\partial y_1^*}{\partial \boldsymbol{n}}\omega_1^0=\int_{\partial\Omega_2^o}\theta\omega_1^0,$$

$$\int_{\partial\Omega_2^o}\frac{\partial \omega_1^*}{\partial \boldsymbol{n}}y_1^*=\int_\Omega \Delta\omega_1^* y_1^*+\int_\Omega \nabla\omega_1^*\nabla y_1^*=\int_\Omega \omega_1^* y_1^*-\int_\Omega \omega_1^*\Delta y_1^*+\int_{\partial\Omega_2^o}\frac{\partial y_1^*}{\partial \boldsymbol{n}}\omega_1^*=\int_{\partial\Omega_2^o}\theta\omega_1^*,$$

and

$$\int_{\partial\Omega_2^o}\frac{\partial y_2^*}{\partial \boldsymbol{n}}\omega_2^*=\int_\Omega \Delta y_2^*\omega_2^*+\int_\Omega \nabla y_2^*\nabla\omega_2^*=\int_\Omega y_2^*\omega_2^*-\int_\Omega y_2^*\Delta\omega_2^*+\int_{\partial\Omega_2^o}\frac{\partial \omega_2^*}{\partial \boldsymbol{n}}y_2^*=\int_{\partial\Omega_2^o}\vartheta\frac{\partial \omega_2^*}{\partial \boldsymbol{n}}.$$

Therefore, the expression of the functional, F, reduces to

$$F(\theta,\vartheta)=c-2\int_{\partial\Omega_2^o}\Big(\theta\omega_1^0+\vartheta\frac{\partial \omega_2^0}{\partial \boldsymbol{n}}\Big)-\int_{\partial\Omega_2^o}\Big(\theta\omega_1^*+\vartheta\frac{\partial \omega_2^*}{\partial \boldsymbol{n}}\Big)=c-2b(\theta,\vartheta)^T+(\theta,\vartheta)A(\theta,\vartheta)^T.$$

In order to prove that A is symmetric, let $(\theta,\vartheta),(\psi,h)\in H_{00}^{-\frac{1}{2}}(\partial\Omega_2^o)\times H_{00}^{\frac{1}{2}}(\partial\Omega_2^o)$. Therefore,

$$\begin{aligned} \Big(A(\theta,\vartheta)^T,(\psi,h)^T\Big) &= \int_\Omega(\nabla y_1^*(\theta,\vartheta)-\nabla y_2^*(\theta,\vartheta))(\nabla y_1^*(\psi,h)-\nabla y_2^*(\psi,h)) \\ &\quad+\int_\Omega(y_1^*(\theta,\vartheta)-y_2^*(\theta,\vartheta))(y_1^*(\psi,h)-y_2^*(\psi,h)) \\ &= \int_\Omega(\nabla y_1^*(\psi,h)-\nabla y_2^*(\psi,h))(\nabla y_1^*(\theta,\vartheta)-\nabla y_2^*(\theta,\vartheta)) \\ &\quad+\int_\Omega(y_1^*(\psi,h)-y_2^*(\psi,h))(y_1^*(\theta,\vartheta)-y_2^*(\theta,\vartheta)) \\ &= \Big((\theta,\vartheta)^T,A(\psi,h)^T\Big). \end{aligned}$$

It remains to prove that the operator A is a positive and definite. Let $(\theta,\vartheta)\neq(0,0)$ thus

$$\Big(A(\theta,\vartheta)^T,(\theta,\vartheta)^T\Big) = \int_\Omega(\nabla y_1^*-\nabla y_2^*)^2+\int_\Omega(y_1^*-y_2^*)^2\geq 0.$$

Assume that $\Big(A(\theta,\vartheta)^T,(\theta,\vartheta)^T\Big)=0$ then $y_1^*=y_2^*$ thus $\Big(y_1^*(\theta,\vartheta)|_{\partial\Omega_2^i},\frac{\partial y_1^*(\theta,\vartheta)}{\partial \boldsymbol{n}}|_{\partial\Omega_2^i}\Big)=(0,0)$ therefore, by applying Holmgren's uniqueness theorem, we obtain $y_1^*=y_2^*=0$ which is impossible since $\Big(y_1^*(\theta,\vartheta)|_{\partial\Omega_2^o},\frac{\partial y_2^*(\theta,\vartheta)}{\partial \boldsymbol{n}}|_{\partial\Omega_2^o}\Big)\neq(0,0)$. Therefore, $\Big(A(\theta,\vartheta),(\theta,\vartheta)^T\Big)>0$. □

The Conjugate Gradient (CG) will be applied as follows:

(1) Solve dynamics (3.11)-(3.12)-(3.15)-(3.16).
(2) Choose an arbitrary initial data $z_0 = (\theta_0, \vartheta_0)$. Solve the dynamics (3.9)-(3.10)-(3.13)-(3.14) and calculate $p_0 = Az_0 - b$.
(3) Set $q_0 = -p_0$.
(4) For $i = 0, 1, 2, ...$, calculate

$$\begin{cases} \lambda_i &= \dfrac{p_i^T p_i}{q_i^T A q_i} \\ z_{i+1} &= z_i + \lambda_i q_i \\ p_{i+1} &= p_i + \lambda_i A q_i \\ \beta_{i+1} &= \dfrac{p_{i+1}^T p_{i+1}}{p_i^T p_i} \\ q_{i+1} &= -p_{i+1} + \beta_{i+1} q_i \end{cases}$$

(5) Solve the dynamics (3.9)-(3.10)-(3.13)-(3.14) and calculate Aq_{i+1}.
(6) Stop if $p_i \approx 0$.

4. Numerical simulations

Recall that our goal is to reconstruct the missed data on the boundary for reaction-advection-diffusion partial differential equations (PDEs). In this section, we aim to give several numerical examples that perform the numerical method discussed previously using the spectral element method (SEM) to resolve the direct problem and then the data completion problem. The algorithm is based on an energy error functional minimization by applying the conjugate gradient method. We shall resolve four systems (3.11)-(3.12)-(3.15)-(3.16) and then four other systems (3.9)-(3.10)-(3.13)-(3.14) for every iteration. Note that the KMF's algorithm resolve only two systems and thus it is not expensive compared to the energy error functional minimization. The necessary iteration's number of the KMF algorithm to converge will be smaller that the one used by the conjugate gradient method. The number of nodes(Polynomial degree) was fixed to $M = 18$ and the maximal number of iterations for both algorithms is fixed to $N_t = 3000$.

In the first example, we consider the exact solution given by $y(x_1, x_2) = (x_1^2 + 2x_1 - 8)(x_2^2 - 4)$ defined on a rectangular domain $\Omega = [-2, 3] \times [-4, 5]$ with $\mu_1 = 1$, $\mu_2 = 2$, $\boldsymbol{v}_1 = 2$ and $\boldsymbol{v}_2 = 2$. Therefore, the source function is given by $f(x_1, x_2) = -2\mu_1(x_1^2 + 2x_1 - 8) - 2\mu_1(x_2^2 - 4) + \mu_2(x_1^2 + 2x_1 - 8)(x_2^2 - 4) + 2\boldsymbol{v}_1(x_1 + 1)(x_2^2 - 4) + 2\boldsymbol{v}_2 x_2(x_1^2 + 2x_1 - 8)$ with the boundary conditions $g_2^i(x_2) = 7(x_2^2 - 4)$ and $\varphi^i(x_2) = 8(x_2^2 - 4)$.

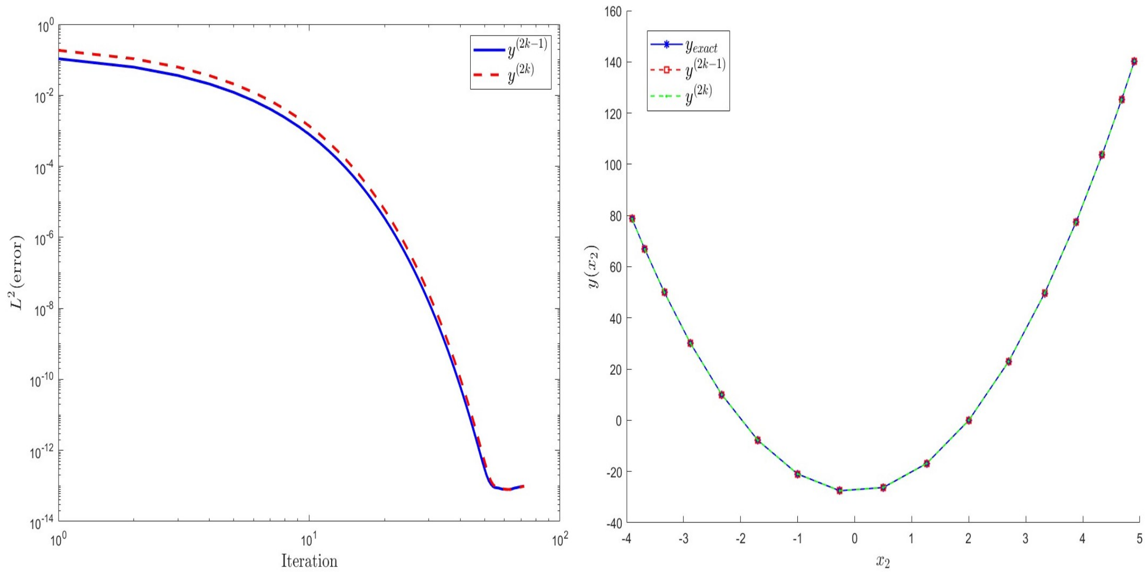

Figure 4. loglog plot of the L^2-relative errors on the missed boundary of the reconstructed solutions (left) using KMF algorithm. Solution on the missed boundary (right) for the first example where the exact solution is given by $y(x_1, x_2) = (x_1^2 + 2x_1 - 8)(x_2^2 - 4)$ on the rectangular domain $\Omega = [-2, 3] \times [-4, 5]$ with $\mu_1 = 1$, $\mu_2 = 2$, $v_1 = 2$ and $v_2 = 2$. Therefore, the source function is given by $f(x_1, x_2) = -2\mu_1(x_1^2 + 2x_1 - 8) - 2\mu_1(x_2^2 - 4) + \mu_2(x_1^2 + 2x_1 - 8)(x_2^2 - 4) + 2v_1(x_1 + 1)(x_2^2 - 4) + 2v_2 x_2(x_1^2 + 2x_1 - 8)$ with the boundary conditions $g_2^i(x_2) = 7(x_2^2 - 4)$ and $\varphi^i(x_2) = 8(x_2^2 - 4)$.

Figure 4 (left) presents the L^2-error between exact solution and the approximated one using the KMF algorithm. Figure 4 (right) presents the reconstructed data trough the KMF algorithm on the missed boundary, $\partial\Omega_2^o$. One can seen that the recovered data is close to the exact one. Figure 5 presents the gap between exact and recovered solution using the KMF algorithm. Figure 5 (left) presents the gap between the exact and the odd iterative solution. Figure 5 (right) presents the gap between the exact and the even iterative solution. In the second example, the domain is the square $\Omega = [0, 1]^2$ and we considered $v = (v_1, v_2)$, where $v_1 = -x_1(x_1 - 1)(2x_2 - 1)$ and $v_2 = x_2(x_2 - 1)(2x_1 - 1))$ and v verifies the assumptions div $v = 0$ in Ω and $v \cdot n = 0$ on $\partial\Omega$. One can easily verify that $y(x_1, x_2) := 4\pi e^{(x_1 + x_2)}$ is solution of system (2.1) where $f(x_1, x_2) = (\mu_1 + v_1 + v_2 + \mu_2) y(x_1, x_2)$ with $\mu_1 = 1$ and $\mu_2 = 2$. The boundary conditions are given by $g_2^i(x_2) = 4\pi e^{x_2}$ and $\varphi^i(x_2) = -4\pi e^{x_2}$.

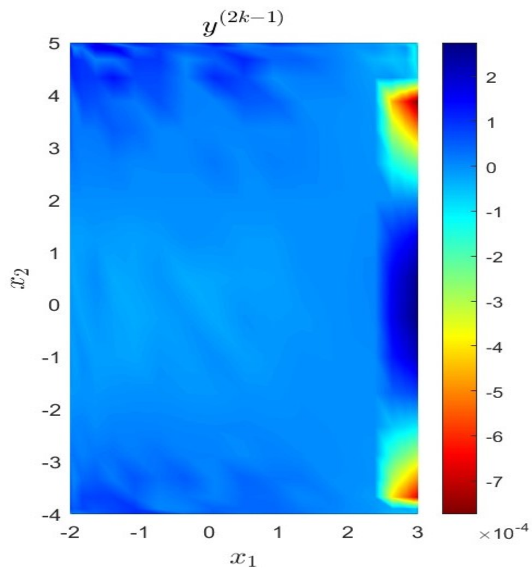

FIGURE 5. Gap between exact and recovered solution using KMF algorithm for the first example where the exact solution is given by $y(x_1, x_2) = (x_1^2 + 2x_1 - 8)(x_2^2 - 4)$ on the rectangular domain $\Omega = [-2, 3] \times [-4, 5]$ with $\mu_1 = 1$, $\mu_2 = 2$, $v_1 = 2$ and $v_2 = 2$. Therefore, the source function is given by $f(x_1, x_2) = -2\mu_1(x_1^2 + 2x_1 - 8) - 2\mu_1(x_2^2 - 4) + \mu_2(x_1^2 + 2x_1 - 8)(x_2^2 - 4) + 2v_1(x_1 + 1)(x_2^2 - 4) + 2v_2 x_2(x_1^2 + 2x_1 - 8)$ with the boundary conditions $g_2^i(x_2) = 7(x_2^2 - 4)$ and $\varphi^i(x_2) = 8(x_2^2 - 4)$.

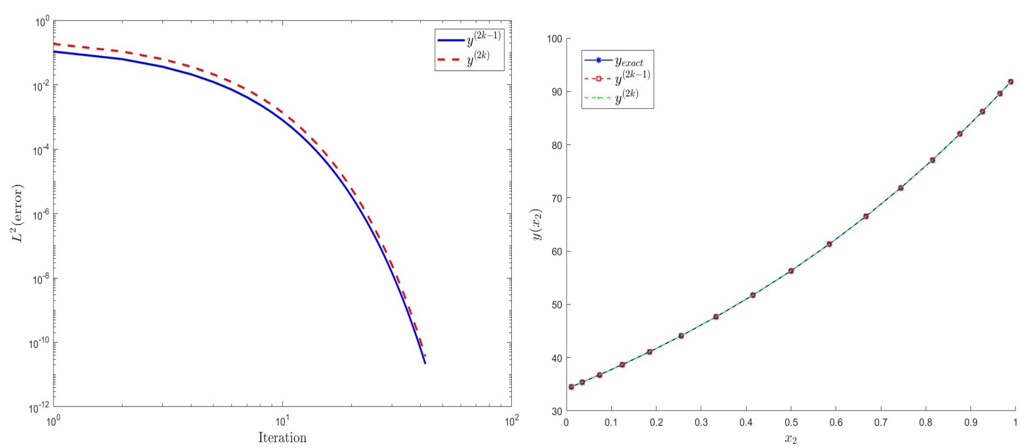

FIGURE 8. loglog plot of the L^2-relative errors on the missed boundary of the reconstructed solutions (left). Solution on the missed boundary (right) for the second example where the exact solution is given by $y(x_1, x_2) = 4\pi e^{(x_1+x_2)}$ on the rectangular domain $\Omega = [0, 1]^2$ with $v_1 = -x_1(x_1 - 1)(2x_2 - 1)$ and $v_2 = x_2(x_2 - 1)(2x_1 - 1)$). Therefore, the source function is given by $f(x_1, x_2) = (\mu_1 + v_1 + v_2 + \mu_2)y(x_1, x_2)$ with the boundary conditions given by $g_2^i(x_2) = 4\pi e^{x_2}$ and $\varphi^i(x_2) = -4\pi e^{x_2}$.

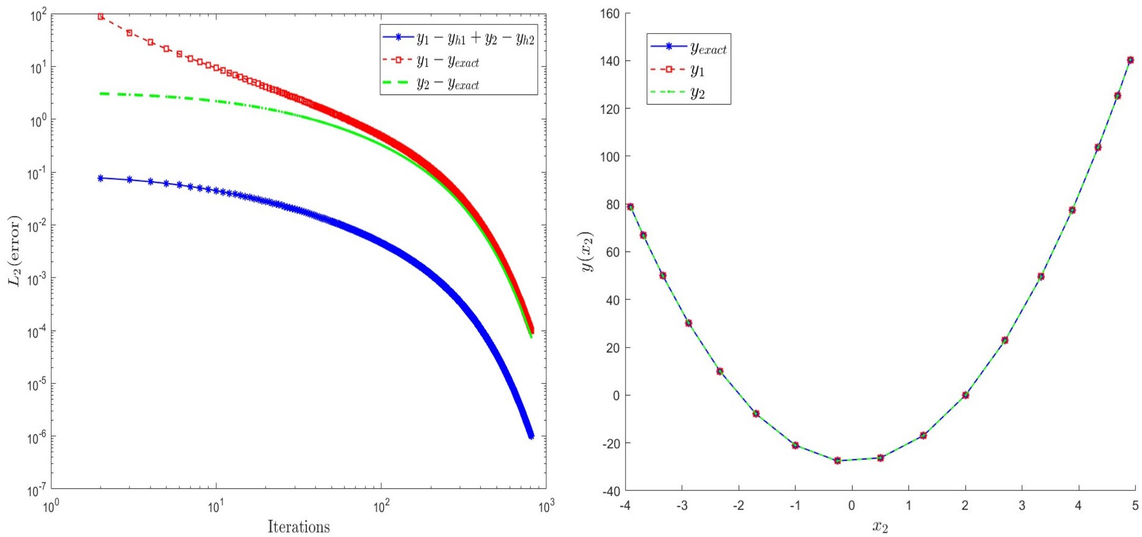

Figure 6. loglog plot of the L^2-relative errors on the missed boundary of the reconstructed solutions (left) using conjugate gradient method. Solution on the missed boundary (right) for the first example where the exact solution is given by $y(x_1, x_2) = (x_1^2 + 2x_1 - 8)(x_2^2 - 4)$ on the rectangular domain $\Omega = [-2, 3] \times [-4, 5]$ with $\mu_1 = 1$, $\mu_2 = 2$, $v_1 = 2$ and $v_2 = 2$. Therefore, the source function is given by $f(x_1, x_2) = -2\mu_1(x_1^2 + 2x_1 - 8) - 2\mu_1(x_2^2 - 4) + \mu_2(x_1^2 + 2x_1 - 8)(x_2^2 - 4) + 2v_1(x_1 + 1)(x_2^2 - 4) + 2v_2 x_2(x_1^2 + 2x_1 - 8)$ with the boundary conditions $g_2^i(x_2) = 7(x_2^2 - 4)$ and $\varphi^i(x_2) = 8(x_2^2 - 4)$.

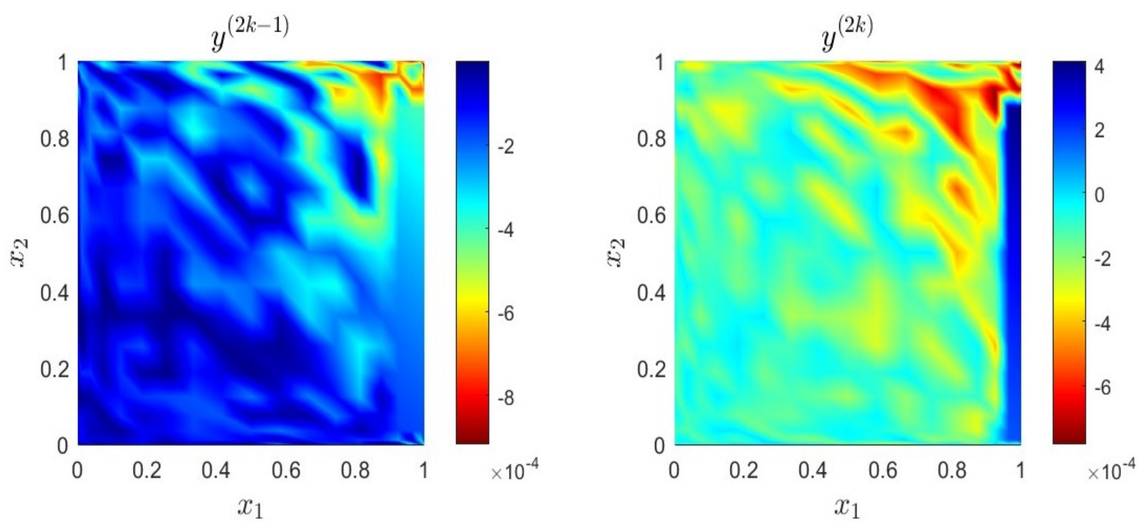

Figure 9. Gap between exact and recovered solution using KMF algorithm for the second example where the exact solution is given by $y(x_1, x_2) = 4\pi e^{(x_1+x_2)}$ on the rectangular domain $\Omega = [0, 1]^2$ with $v_1 = -x_1(x_1 - 1)(2x_2 - 1)$ and $v_2 = x_2(x_2 - 1)(2x_1 - 1))$. Therefore, the source function is given by $f(x_1, x_2) = (\mu_1 + v_1 + v_2 + \mu_2)y(x_1, x_2)$ with the boundary conditions given by $g_2^i(x_2) = 4\pi e^{x_2}$ and $\varphi^i(x_2) = -4\pi e^{x_2}$.

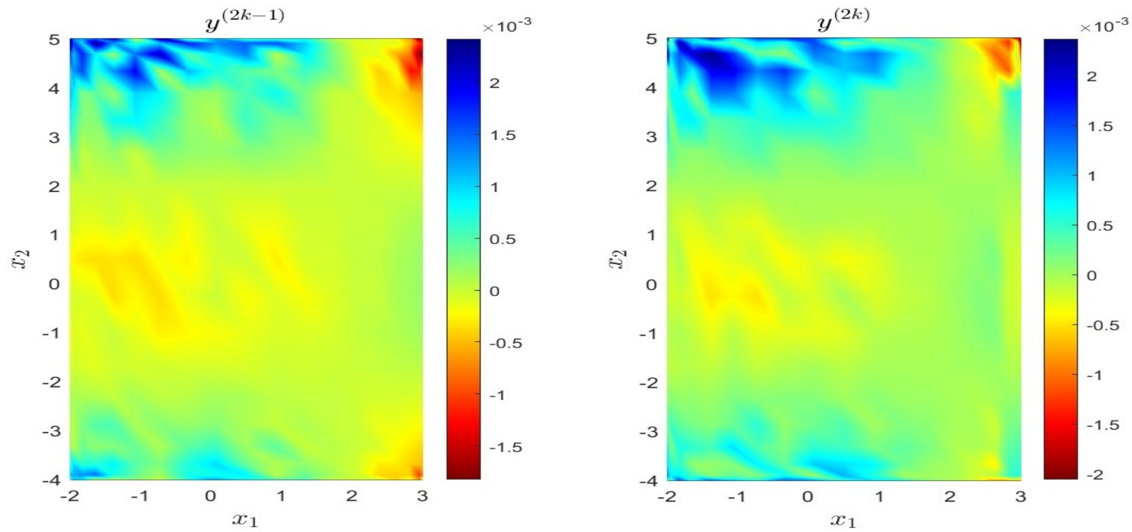

Figure 7. Gap between exact and recovered solution using conjugate gradient method for the first example where the exact solution is given by $y(x_1, x_2) = (x_1^2 + 2x_1 - 8)(x_2^2 - 4)$ on the rectangular domain $\Omega = [-2, 3] \times [-4, 5]$ with $\mu_1 = 1$, $\mu_2 = 2$, $v_1 = 2$ and $v_2 = 2$. Therefore, the source function is given by $f(x_1, x_2) = -2\mu_1(x_1^2 + 2x_1 - 8) - 2\mu_1(x_2^2 - 4) + \mu_2(x_1^2 + 2x_1 - 8)(x_2^2 - 4) + 2v_1(x_1 + 1)(x_2^2 - 4) + 2v_2 x_2(x_1^2 + 2x_1 - 8)$ with the boundary conditions $g_2^i(x_2) = 7(x_2^2 - 4)$ and $\varphi^i(x_2) = 8(x_2^2 - 4)$.

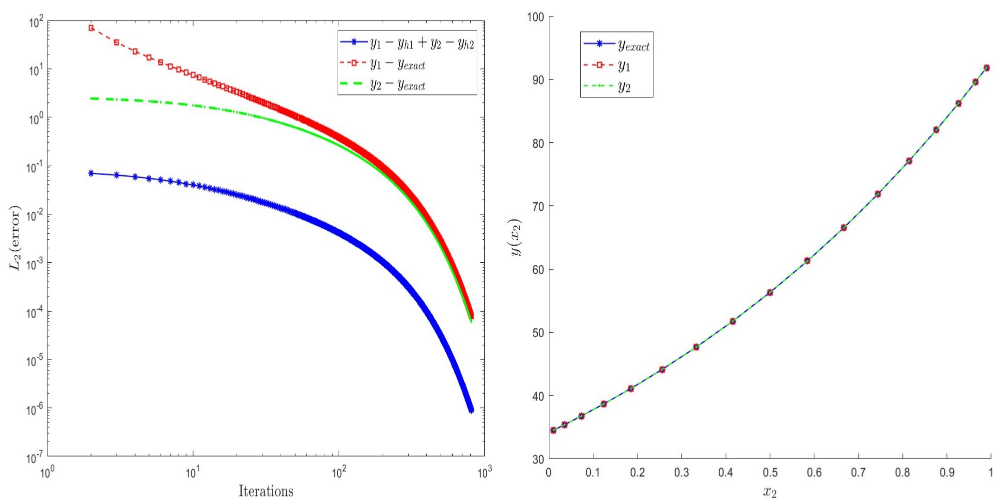

Figure 10. loglog plot of the L^2-relative errors on the missed boundary of the reconstructed solutions (left) using conjugate gradient method. Solution on the missed boundary (right) for the second example where the exact solution is given by $y(x_1, x_2) = 4\pi e^{(x_1 + x_2)}$ on the rectangular domain $\Omega = [0, 1]^2$ with $v_1 = -x_1(x_1 - 1)(2x_2 - 1)$ and $v_2 = x_2(x_2 - 1)(2x_1 - 1))$. Therefore, the source function is given by $f(x_1, x_2) = (\mu_1 + v_1 + v_2 + \mu_2)y(x_1, x_2)$ with the boundary conditions given by $g_2^i(x_2) = 4\pi e^{x_2}$ and $\varphi^i(x_2) = -4\pi e^{x_2}$.

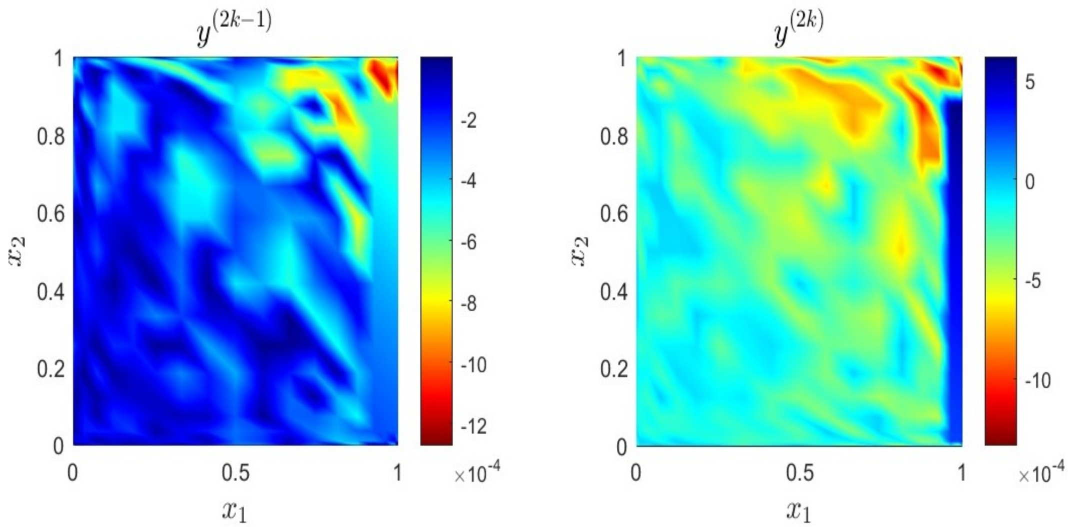

Figure 11. Gap between exact and recovered solution using conjugate gradient method for the second example where the exact solution is given by $y(x_1, x_2) = 4\pi e^{(x_1+x_2)}$ on the rectangular domain $\Omega = [0,1]^2$ with $v_1 = -x_1(x_1-1)(2x_2-1)$ and $v_2 = x_2(x_2-1)(2x_1-1))$. Therefore, the source function is given by $f(x_1, x_2) = (\mu_1 + v_1 + v_2 + \mu_2)y(x_1, x_2)$ with the boundary conditions given by $g_2^i(x_2) = 4\pi e^{x_2}$ and $\varphi^i(x_2) = -4\pi e^{x_2}$.

5. Conclusion

In this article, we considered a reaction-advection-diffusion partial differential equations (PDEs) in a two-dimensional domain with missed boundary data. We applied both the KMF algorithm and the conjugate gradient method trough the minimisation of an energy functional to reconstruct the missed data by using the spectral element method. We presented several numerical examples describing the convergence of both used algorithms by reconstructing both, traces and normal traces on the inaccessible boundary.

We aim in future works to resolve inverse problems applied to biological processes as described in [11–16].

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