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Identification of Initial Condition in Parabolic Convection Diffusion Equation Using Radial Basis Function Partition of Unity

Achraf Badahmane[1] and Youness El Yazidi[2]

ABSTRACT: The present paper deals with the identification problem of an unknown initial condition in convection diffusion equation. This inverse problem is transformed into a constrained optimization problem. We prove its solution existence. The radial basis function based partition of unity is considered as a discretization method. The obtained matrix system is solved via a robust approach based on preconditioning techniques. Using the quasi Newton algorithm we approach the solution of the optimization problem. At the end, we establish several numerical examples in order to illustrate our theoretical results and the validity of the constructed numerical scheme.

Key Words: Initial condition identification, RBF-PUM, preconditioning, Quasi Newton.

Contents

1. Introduction and motivation

The aim of this paper is to develop an efficient iterative scheme for solving the following ill-posed problem:

$$\begin{cases} \partial_t u - \kappa\Delta u - \vec{\nu}\cdot\nabla u = f & \text{in } \Omega\times]0,T[\\ u(x,t) = j_\delta & \text{on } \partial\Omega\times]0,T[\\ \kappa\nabla u(x,t)\cdot\vec{n} = g & \text{on } \Gamma_N\times]0,T[\\ u(x,T) = \vartheta & \text{on } \Omega \end{cases} \tag{1.1}$$

where Ω is a bounded open set of $\mathbb{R}^2$ with a Lipschitz boundary $\Gamma = \Gamma_D \cup \Gamma_N$, κ is the diffusion coefficient and $\vec{\nu}$ is a given velocity vector. The system (1.1) is overdetermined, the missing information in this problem is the initial condition $u(x,0)$. j_δ is assumed to be a noisy data of noise level $\delta > 0$, that holds

$$\|j_\delta - j\|_{L^2(\partial\Omega)} \leq \delta \tag{1.2}$$

with j being the exact data observation on $\partial\Omega\times]0,T[$.

In fact, a time-reversed advection-diffusion equation can model many phenomena in real life, such as reconstruction of the initial condition responsible for the final state at time T in pollution and chemical reaction [19,13]. Therefore the relevance of constructing efficient numerical scheme to reconstruct this missing initial condition.

Several numerical techniques were proposed for solving inverse problems [6,7,8]. Finite element method is one of the most useful discretization technique, it was used in [6] combined with Quasi Newton

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for the free boundary identification. In [7] FEM was enhanced with Finite volume method to reconstruct a nonsmooth diffusion coefficient. Nonlinear inverse problems have gained interest lately. It consists first to solve the nonlinear associated state equation, which can be challenging [10]. In [17] an inverse problem for nonlinear elastic wave equation was investigated. Recently, a radial basis functions technique was employed in the inverse identification of a unknown convection term in nonlinear partial differential equation [9].

Using meshless methods involves a challenging matrix form to solve directly with classical techniques. Projection methods are generally more efficient than direct methods for solving large, nonsymmetric linear systems. The GMRES algorithm [15], which is based on the Arnoldi process [1], is a widely used projection method for such problems. A significant drawback of GMRES is that its convergence can be prohibitively slow unless it is coupled with a suitable preconditioner. Consequently, the development of effective preconditioning techniques [3,4,5] has been a major focus of research for solving nonsymmetric systems.

Our main objective in this paper is to develop a numerical scheme based on a meshless technique to reconstruct the unknown initial condition and to approximate the solution of (1.1). First, we introduce a set of admissible initial conditions, then we reformulate the inverse problem into two well defined state equations. Let us first define the set of admissible initial conditions

$$\Xi = \left\{\eta \in H_D^1(\Omega) : \|\eta\| \leq M\right\} \tag{1.3}$$

with

$$H_D^1(\Omega) = \left\{u \in H_D^1(\Omega) : \ u = 0 \text{ on } \Gamma_D\right\}.$$

For some given $\eta \in \Xi$, we define two state equations, the first reads

$$\begin{cases} \partial_t u - \mathcal{L}u := \partial_t u - \kappa\Delta u - \vec{\nu}\cdot\nabla u = f & \text{in } \Omega\times]0,T[\\ u(x,t) = j_\delta & \text{on } \Gamma\times]0,T[\\ u(x,0) = \eta & \text{in } \Omega \end{cases} \tag{1.4}$$

The solution of this first state equation will be denoted by $z_\delta = \mathcal{D}(\eta)$. The second state equation reads

$$\begin{cases} \partial_t u - \mathcal{L}u = f & \text{in } \Omega\times]0,T[\\ u(x,t) = j & \text{on } \Gamma_D\times]0,T[\\ \kappa\nabla u(x,t)\cdot\vec{n} = g & \text{on } \Gamma_N\times]0,T[\\ u(x,0) = \eta & \text{in } \Omega \end{cases} \tag{1.5}$$

by considering the solution of this second state equation $u = \mathcal{S}(\eta)$, we introduce the cost functional

$$J_\delta(\eta) = \int_0^T \int_\Omega \Big((\mathcal{D}-\mathcal{S})(\eta)\Big)^2 dxdt + \int_\Omega (u(x,T)-\vartheta)^2 dx \tag{1.6}$$

Since the problem (1.1) is ill-posed in the sense of Hadamard, we manipulate the Tikhonov's regularization to ensure numerical stability especially with the given noisy observation. Thereafter, the cost functional will have the form

$$\mathcal{J}(\eta) = J_\delta(\eta) + \frac{\rho}{2}\|\nabla(\eta-\bar{\eta})\|^2_{L^2(\Omega)} \tag{1.7}$$

where $\bar{\eta}$ is an a prior knowledge of the missing initial condition of the problem (1.1).

To this end, the following constrained optimization problem will be considered numerically

$$\min_{\eta\in\Xi} \mathcal{J}(\eta) \quad \text{s.t.} \quad \mathcal{D}(\eta),\ \mathcal{S}(\eta) \text{ solutions of (1.4) and (1.5) respectively.} \tag{1.8}$$

2. Optimal solution existence

In this section we analyze the existence of an optimal solution of our constrained optimization problem. But first we recall some basic results concerning the existence of unique solution to the state equations.

We will concentrate only on the second state equation, since it has mixed boundary conditions. To address it, we manipulate the well known Galerkin method. It consists of considering a sequence of smooth functions $\varphi_k = \varphi_k(x)$ $(k = 1, \dots)$ satisfying

$$\{\varphi_k\}_{k=1}^{\infty} \text{ is an orthogonal basis of } H_D^1(\Omega) \text{ and } \{\varphi_k\}_{k=1}^{\infty} \text{ is an orthonormal basis of } L^2(\Omega). \tag{2.1}$$

A trivial choice of $\{\varphi_k\}_{k=1}^{\infty}$ is the complete set of normalized eigenfunctions for $\mathcal{L}$ in $H^1(\Omega)$.
The Galerkin method aims to find a function $\mathbf{u}_m : [0, T] \to H_D^1(U)$ of the following form

$$\mathbf{u}_m(t) := \sum_{k=1}^{m} c_m^k(t)\varphi_k, \tag{2.2}$$

such that, for $k = 1, \dots, m$ and $0 \le t \le T$ we have

$$d_m^k(0) = (\eta, \varphi_k) \quad \text{and} \quad (\mathbf{u}_m', \varphi_k) + B[\mathbf{u}_m, \varphi_k; t] = (f, \varphi_k) \tag{2.3}$$

where

$$B[\mathbf{u}_m, \varphi_k; t] = \sum_{l=1}^{m} e^{kl}(t) d_m^l(t), \tag{2.4}$$

for $e^{kl}(t) := B[\varphi_k, \varphi_k; t]$ for $k, l = 1, \dots, m$. Thereafter we have the following result [11]

Theorem 1 *For each integer $m = 1, 2, \dots$ there exists a unique function $\mathbf{u}_m$ of the form (2.2) satisfying (2.3), (2.4).*

Now, we can tend m to infinity in order to prove that the constructed solution's sequence $\{\mathbf{u}_m\}_m$ converges in term of subsequence. To guarantee this result we use the following uniform estimate.

Theorem 2 *There exists a constant C that depends on Ω, T and the coefficients of $\mathcal{L}$, such that*

$$\max_{0\le t\le T} \|\mathbf{u}_m(t)\|_{0,\Omega} + \|\mathbf{u}_m\|_{L^2(0,T;H_0^1(U))} + \|\mathbf{u}_m'\|_{L^2(0,T;H^{-1}(U))} \le C(\|f\|_{L^2(0,T;L^2(U))} + \|\eta\|_{0,\Omega}) \tag{2.5}$$

We have the following existence result

Theorem 3 *Consider $\eta \in \Xi$ and $f \in L^2(0, T; L^2(U))$. Suppose also $u \in L^2(0, T; H_D^1(\Omega))$, with $u' \in L^2(0, T; H^{-1}(\Omega))$, is the weak solution of (1.5). Then in fact*

$$u \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T; H_D^1(\Omega)), \quad u' \in L^2(0, T; L^2(\Omega)),$$

and we have the estimate

$$\operatorname*{ess\,sup}_{0\le t\le T} \|u(t)\|_{H_D^1(\Omega)} + \|u\|_{L^2(0,T;H^2(\Omega))} + \|u'\|_{L^2(0,T;L^2(\Omega))} \le C\left(\|f\|_{L^2(0,T;L^2(\Omega))} + \|\eta\|_{H_D^1(\Omega)}\right), \tag{2.6}$$

the constant C depending only on U, T and the coefficients of L.

Remark 2.1 *Same results holds for the first state equation (1.4).*

To this end, we have the existence of a unique solution of the state equations for each admissible initial condition η. Now, we need to ensure that the optimal control problem admits at least one solution.

Theorem 4 *the constrained optimization problem (1.8) admits at least one solution.*

Proof: Based on the direct technique in calculus of variations, the optimal solution exists when $\mathcal{J}$ is coercive and weakly lower semicontinuous.
Since that $J(\eta)$ is non negative then we have

$$\mathcal{J}(\eta) \ge \frac{\rho}{2}\|\nabla(\eta - \bar{\eta})\|_{L^2(\Omega)}^2$$

with the reverse triangle inequality

$$\mathcal{J}(\eta) \geq \frac{\rho}{2}\left(\|\nabla\eta\|_{L^2(\Omega)} - \|\nabla\bar{\eta}\|_{L^2(\Omega)}\right)^2$$

Thereafter, we send $\|\nabla\eta\|_{L^2(\Omega)}$ to infinity, we obtain that the right-hand side goes also to infinity. Hence, $\mathcal{J}(\eta)$ is coercive, and there exists a minimizing sequence $\{\eta_k\}_{k\in\mathbb{N}} \subset \Xi$ such that

$$\lim_{k\to\infty} \mathcal{J}(\eta_k) = \inf_{\eta\in\Xi} \mathcal{J}(\eta)$$

this implies that $\{\eta_k\}$ is bounded in $H_D^1(\Omega)$, with the continuous embedding in $L^2(\Omega)$, we can extract a subsequence that converges weakly to some limit $\eta^* \in H_D^1(\Omega)$.
Now, we proceed with the proof of the lower semicontinuity. We need to show that

$$\mathcal{J}(\eta^*) \leq \liminf_{k\to\infty} \mathcal{J}(\eta_k)$$

we must pass to the limit in the three terms of the functional $\mathcal{J}$. The simplest term is of the regularization, it is a squared norm which means that is a convex and continuous functional, therefore

$$\|\nabla(\eta^* - \bar{\eta})\|^2_{L^2(\Omega)} \leq \liminf_{k\to\infty} \|\nabla(\eta_k - \bar{\eta})\|^2_{L^2(\Omega)}.$$

The first two fidelity terms depend on the state solutions mapping D, $S : \eta \mapsto z_\delta(\eta)$, $u(\eta)$. We note that D and S are linear and continuous from $L^2(\Omega)$ to the solution space $L^2(0,T,H_D^1(\Omega))$. Thanks to the Aubin-Lions Lemma [2], the weak convergence of initial conditions implies the strong convergence of the corresponding state solutions in $L^2(]0,T[,L^2(\Omega))$, and the weak convergence in $L^2(]0,T[,H_D^1(\Omega))$.
From another side, since the both fidelity terms are square norms and the state solutions mapping D and S are compact, with same argument we have

$$J(\eta^*) \leq \liminf_{k\to\infty} J(\eta_k)$$

To this end, the cost functional $\mathcal{J}$ is weakly lower semicontinuous. □

3. Computation of the cost functional gradient

Now, we need to compute the adjoint state, as it will be needed for our numerical method. For that, we introduce the Lagrangian $\mathcal{K}(\eta,u,p,q)$:

$$\mathcal{K}(\eta,u,z_\delta,p,q) = \mathcal{J}(\eta,u) - \int_0^T\int_\Omega p(\partial_t u - \kappa\Delta u - \vec{v}\cdot\nabla u - f)\,dx\,dt - \int_0^T\int_\Omega q(\partial_t z_\delta - \kappa\Delta z_\delta - \vec{v}\cdot\nabla z_\delta - f)\,dx\,dt$$

The first optimality conditions are obtained via the Gâteaux derivative of $\mathcal{K}$ with respect to the state solutions u and z_δ in any directions λ and μ to zero. Again, we will perform the one associated to u, the other will be the same and more simple. We have

$$D_u\mathcal{K}[\lambda] = \int_0^T\int_\Omega (u - z_\delta)\lambda\,dx\,dt + \int_\Omega (u(T) - \vartheta)\lambda(T)\,dx - \int_0^T\int_\Omega p(\partial_t\lambda - \kappa\Delta\lambda - \vec{v}\cdot\nabla\lambda)\,dx\,dt = 0$$

We perform now some integration by parts on the last integral. Let us start by the time derivative. We apply an integration by parts with respect to time we obtain

$$\int_0^T\int_\Omega p(\partial_t\lambda)\,dx\,dt = \int_\Omega \left([p(t)\lambda(t)]_{t=0}^{t=T} - \int_0^T (\partial_t p)\lambda\,dt\right)dx$$

Distributing the integrals, it becomes:

$$I_t = -\int_0^T\int_\Omega (\partial_t p)\lambda\,dx\,dt + \int_\Omega p(T)\lambda(T)\,dx - \int_\Omega p(0)\lambda(0)\,dx$$

Now, we treat the Laplacian term, applying Green's identity twice, we have

$$\int_\Omega p(\Delta\lambda)\,dx = \int_\Omega (\Delta p)\lambda\,dx + \int_{\partial\Omega}\left(p\frac{\partial\lambda}{\partial n} - \lambda\frac{\partial p}{\partial n}\right)ds$$

it yields that

$$-\int_0^T\int_\Omega p(\kappa\Delta\lambda)\,dxdt = -\int_0^T\int_\Omega \kappa(\Delta p)\lambda\,dx\,dt - \int_0^T\int_{\partial\Omega}\kappa\left(p\frac{\partial\lambda}{\partial n} - \lambda\frac{\partial p}{\partial n}\right)ds\,dt$$

Still to handle the convection term, with the divergence theorem we obtain the following

$$\int_\Omega p(v\cdot\nabla\lambda)\,dx = \int_{\partial\Omega} p\lambda(v\cdot n)\,ds - \int_\Omega \lambda(\nabla\cdot(pv))\,dx$$

thereafter

$$\int_0^T\int_\Omega p(v\cdot\nabla\lambda)\,dxdt = -\int_0^T\int_\Omega \lambda(\nabla\cdot(pv))\,dx\,dt + \int_0^T\int_{\partial\Omega} p\lambda(v\cdot n)\,ds\,dt$$

Gathering all obtained equalities, we derive the adjoint state equation associated to the state solution u, it reads

$$\begin{cases} -\partial_t p - \kappa\Delta p + \nabla\cdot(\vec{v}p) = u - z_\delta & \text{in } \Omega\times]0,T[\\ p(x,t) = 0 & \text{on } \Gamma_D\times]0,T[\\ \kappa\nabla p(x,t)\cdot\vec{n} + (\vec{v}\cdot\vec{n})p = 0 & \text{on } \Gamma_N\times]0,T[\\ p(x,T) = u(x,T) - \vartheta & \text{in } \Omega \end{cases} \tag{3.1}$$

it is a backward convection diffusion equation. Similarly we obtain the other adjoint equation associated to z_δ

$$\begin{cases} \partial_t q + \kappa\Delta q - \nabla\cdot(q\vec{v}) = -(u - z_\delta) & \text{in } \Omega\times]0,T[\\ q(x,t) = 0 & \text{on } \Gamma\times]0,T[\\ q(x,0) = 0 & \text{in } \Omega \end{cases} \tag{3.2}$$

To this end, we can derive now the gradient of the cost functional $\mathcal{J}$ by differentiating the Lagrangian with respect to the control η. We have

$$\left\langle\frac{\partial\mathcal{J}}{\partial\eta},\xi\right\rangle - \int_0^T\int_\Omega p\frac{\partial}{\partial\eta}(\partial_t u - \kappa\Delta u - \vec{v}\cdot\nabla u - f)\,dx\,dt - \int_0^T\int_\Omega q\frac{\partial}{\partial\eta}(\partial_t z_\delta - \kappa\Delta z_\delta - \vec{v}\cdot\nabla z_\delta - f)\,dx\,dt = 0$$

manipulating the adjoint states, we obtain

$$\left\langle\frac{\partial\mathcal{J}}{\partial\eta},\xi\right\rangle = \int_\Omega \rho\nabla(\eta-\bar{\eta})\cdot\nabla\xi\,dx - \int_\Omega p(0)\xi\,dx$$

with an integration by part we derive the gradient of the cost functional as follows

$$\left\langle\frac{\partial\mathcal{J}}{\partial\eta},\xi\right\rangle = \int_\Omega \left(-\rho\Delta(\eta-\bar{\eta}) - p(0)\right)\xi\,dx$$

4. The Proposed numerical scheme

In this section we are concerned with the description of the discretization RBF-PUM technique as the first fold. Then we express the steps to minimize the optimization problem at hand.

4.1. Description of the RBF-PUM method

Consider a N points in $\mathbb{R}^s$, to compute the RBF interpolant we write

$$u(\mathbf{x}) = \sum_{j=1}^{N} \xi_j \phi_\varepsilon \left(\left\| \mathbf{x} - \mathbf{x}_j^c \right\|_2 \right), \tag{4.1}$$

where $\xi_1, \ldots, \xi_N$ are the freedom coefficients that we seek to compute, ϕ is a radial basis function, $\|\cdot\|_2$ is the Euclidean norm, and ε is the shape parameter. The freedom coefficients are computed by solving the following system

$$\begin{bmatrix} \phi_\varepsilon\left(\|\mathbf{x}_1 - \mathbf{x}_1^c\|\right) & \cdots & \phi_\varepsilon\left(\|\mathbf{x}_1 - \mathbf{x}_N^c\|\right) \\ \vdots & \ddots & \vdots \\ \phi_\varepsilon\left(\|\mathbf{x}_N - \mathbf{x}_1^c\|\right) & \cdots & \phi_\varepsilon\left(\|\mathbf{x}_N - \mathbf{x}_N^c\|\right) \end{bmatrix} \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_N \end{bmatrix} = \begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}. \tag{4.2}$$

We can also write the last interpolation as follows

$$u(x) = \sum_{j=1}^{N} \psi_j(x) u_j, \tag{4.3}$$

with $\{\psi_j\}_{j=1}^N$ is a cardinal basis function, defined by $\psi_j(x_k) = 1$ if $j = k$ and 0 otherwise.

The obtained RBF interpolant matrix is symmetric and generally nonsingular, this is depending on several factors such the choice of the RBF function and the shape parameter. This later is delicate to choose randomly, many authors proposed some techniques to overcame this issue. In [12] proposed to vary the shape parameter in a given range, then the optimal is the one with small approximating in error. In [16], the shape parameter is chosen with respect to the condition number variation's of the linear system.

Now let us consider a family $\{\Omega_k\}_{k=1}^M$ of open bounded sets covering Ω. We say that $\{\Omega_k\}_{k=1}^M$ satisfy a mild overlap condition if it the following holds

$$\forall x \in \Omega, \quad I(x) = \{k \,/\, x \in \Omega_k\}, \quad card(I(x)) \leq K$$

with K is a fixed constant independent of M.

Definition 1 *Consider Ω a bounded set in $\mathbb{R}^d$ and let $\{\Omega_k\}_{k=1}^M$ be an open bounded covering of Ω. We call a l-stable partition of unity with respect to $\{\Omega_k\}_{k=1}^M$ any family of non-negative functions $\{w_k\}_{k=1}^M$ with $w_k \in C^k\left(\mathbb{R}^d\right)$ that satisfies:*

1. $\operatorname{supp}(w_k) \subseteq \Omega_k$,
2. $\sum_{k=1}^M w_k(\boldsymbol{x}) = 1$ *with* $x \in \Omega$,
3. *for any multi-index $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq l$ there exists a constant $C_\alpha > 0$ such that*

$$\left\| D^\alpha w_k \right\|_{L_\infty(\Omega_j)} \leq \frac{C_\alpha}{\operatorname{diam}(\Omega_j)^{|\alpha|}}, \quad k = 1, \ldots, M$$

The construction of the weight functions w_j for each sub-domain Ω_j follows the Shepard's method, which reads

$$w_j(x) = \frac{\varphi_j(x)}{\sum_{k \in I(x)} \varphi_k(x)}, \quad j = 1, \ldots, M,$$

with $\varphi_j(\boldsymbol{x})$ being a compactly supported function with $supp(\varphi_j) \subset \Omega_j$ for every j. Several choices exists for this kind of functions, in our application we choose the Wendland functions [14] defined as follows

$$\varphi(r) = \begin{cases} (1-r)^4(4r+1) & \text{if } 0 \leq r \leq 1, \\ 0 & \text{if } r > 1. \end{cases}$$

To guarantee the non-negativity and compact support proprieties of φ_j, we define the center points $\{c_j\}_{j=1}^M$, and $\{r_j\}_{j=1}^M$ be radius of the hyper-spherical patches $\Omega_j, j = 1, \ldots, M$, then we construct φ_j as next

$$\varphi_j(x) = \varphi\left(\frac{\|x - c_j\|}{r_j}\right)$$

Now, the global approximation of u with RBF-PUM is obtained with

$$u(x) = \sum_{j=1}^{M} w_j(x) u_j(x), \tag{4.4}$$

where u_j is a local RBF approximation of $u(x)$ on the sub-domain Ω_j. From the definition of $w_j(x)$, it is seen that

$$\sum_{j \in I(x)} w_j(x) = 1 \quad \text{and} \quad w_j(x) = 0, \forall j \notin I(x) \tag{4.5}$$

with those information, the approximation (4.4) can be rewritten as

$$u(x) = \sum_{k \in I(x)} w_k(x) u_k(x).$$

Now, to approximate the solution of time-dependent problems (1.4) or (1.5) with RBF-PUM, we write

$$u(x,t) = \sum_{j \in I(x)} w_j(x) u_j(x,t), \tag{4.6}$$

with $u_j(x,t)$ is a local RBF approximation of u on the patch Ω_j, it means that

$$u_j(x,t) = \sum_{k \in I_j} \psi_k(x) u_k(t), \tag{4.7}$$

I_j is the set of indexes given as $I_j = \{k \mid x_k \in \Omega_j\}$, represents the indexes of nodes in Ω_j. Combining the last two equations, it yields to

$$u(x,t) = \sum_{j \in I(x)} \sum_{k \in I_j} \left(w_j(x)\psi_k(x)\right) u_k(t), \tag{4.8}$$

4.2. Discretization of the direct problem

Let us consider two multi-indices α and β. With the famous Leibniz rule, the derivative of order α of the global approximation is given by

$$\frac{\partial^{|\alpha|} u}{\partial x^\alpha}(x,t) = \sum_{j \in I(x)} \sum_{k \in J(\Omega_j)} \left(\sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \frac{\partial^{|\alpha-\beta|} w_j}{\partial x^{\alpha-\beta}}(x) \frac{\partial^{|\beta|} \psi_k}{\partial x^\beta}(x) \right) u_k(t), \tag{4.9}$$

setting $x = x_i$ in last equality generates the ik-coefficient in the differentiation matrix associated to the α-derivative. To obtain the global matrix of a composite linear differential operator, we sum up each matrix associated to each linear component and the resulting matrix is denoted A. To this end, the obtained discrete system reads

$$\begin{cases} u' = Au + Bf & \text{if } t > 0, \\ u(x,0) = \eta & \text{if } t = 0. \end{cases} \tag{4.10}$$

The computational cost of our discrete direct problem can be divided into two parts, the cost associated to differentiation matrices assembly, and the matrix vector products in time integration. This time-stepping cost has in somehow the same order of complexity across iterative solvers, explicit and direct implicit schemes.

The computational complexity of the proposed discretization technique can be analyzed from three folds. First, matrix assembly, which requires factorizing the local differentiation matrix for each patch, the cost to establish the global differentiation matrices is $\mathscr{O}(Mn_{\text{loc}}^3)$, where M is the number of patches and n_{loc} is the number of local nodes per patch.
The cost for matrix vector multiplication in time stepping is lower compared to the first cost, it is of $\mathscr{O}(Mn_{\text{loc}}^2)$. Now, if we consider a N unstructured nodes, firstly we associate each node with appropriate patch. This operation costs $\mathscr{O}(MN)$, which can be more ineffective for large values of N. Using alternative for spatial structured data such as $k-d$ tree, this cost is reduced to $\mathscr{O}(Mn_{\text{loc}} \log N)$.

4.3. Preconditioned Generalized minimal residual (GMRES) method for solving linear system (4.2)

Projection methods like GMRES method are well-suited for solving high-dimensional sparse linear systems such as (4.2). Convergence is typically rapid when the preconditioned matrix has a clustered spectrum (away from zero) and is close to normal. However, convergence becomes more difficult to predict for highly non-normal problems, as the eigenvalues alone may not determine the behavior of nonsymmetric matrix iterations like GMRES method. A key limitation of GMRES method is its potential inefficiency, as it may require a large number of iterations to reach a given tolerance for certain problems. Preconditioning technique based on incomplete Lower-Upper (ILU) factorization , is commonly used to mitigate this issue. The core idea is to apply a linear transformation using a preconditioner, $\mathcal{P}$, to the original system (4.2). This transformation yields a new system with a more favorable spectrum for the matrix $\mathcal{P}^{-1}\mathcal{A}$. The preconditioned system is expressed as:

$$\mathcal{P}^{-1}\mathcal{A}u = \mathcal{P}^{-1}b. \tag{4.11}$$

Different implementations of this preconditioned iterative approach are possible, depending on the specific choice of $\mathcal{P}$ and the structure of $\mathcal{A}$. When solving equation (4.2) with the preconditioned GMRES method, the iteration process terminates under either of two conditions:

1. The Euclidean norm of the relative residual falls below a specified tolerance $\tau = 1 \times 10^{-6}$:

$$\frac{\|\mathcal{P}^{-1}b - \mathcal{P}^{-1}\mathcal{A}u^{(k)}\|_2}{\|\mathcal{P}^{-1}b\|_2} < \tau, \tag{4.12}$$

   where $u^{(k)}$ is the solution at the k-th iteration.

2. The number of iterations reaches a maximum of 200.

4.4. BFGS for Minimization

In this part, we describe the basic steps of the well known quasi-Newton variant method, the Broyden, Fletcher, Goldfarb and Shanno method (BFGS) [18]. First, we start with an initial guess η_0, the idea consists on the iteration

$$\eta_{n+1} = \eta_n + \vartheta_n d_n, \tag{4.13}$$

with d_n represents the direction of descent and ϑ_n stands for the step size. The descent direction is updated iteratively as solution of the linear system:

$$H_n d_n = -\nabla \mathcal{J}(\eta_n), \tag{4.14}$$

and H is the approximation of the Hessian matrix with H_0 is the identity matrix. It is updated following to the formula

$$H_{n+1} = H_n + \frac{\Lambda_n(\Lambda_n)^T}{<\zeta_n, \Lambda_n>} - \frac{H_n[\zeta_n(\zeta_n)^T]H_n}{<H_n\zeta_n, \zeta_n>}, \tag{4.15}$$

where

$$\zeta_n = \nabla \mathcal{J}(\eta_{n+1}) - \nabla \mathcal{J}(\eta_n), \quad \text{and} \quad \Lambda_n = \eta_{n+1} - \eta_n. \tag{4.16}$$

All the steps of the proposed scheme are summarized in Algorithm 1.

Algorithm 1:

Input: Choose tol_1, tol_2 N_{max}, ς, υ, N and M. set $err = 1$ and $iter = 0$.

while $n < N_{max}$ *and* $err > tol$ **do**

- Compute z_δ and u state solutions
- Find p and q adjoint states
- Compute the cost functional gradient gradient $\nabla \mathcal{J}(\eta_n)$
- Compute d_n solution of $H_n d_n = -\nabla \mathcal{J}(\eta_n)$
- Use a line search to find ρ_n
- Update $\eta_{n+1} = \eta_n + \vartheta_n d_n$
- Evaluate ζ_n and Λ_n
- Update matrix H_{n+1}
- Set $n = n + 1$, and $err = \mathcal{J}(\eta_{n+1})$

5. Numerical simulation

Now, we perform some numerical experiments to show the validity of the proposed scheme for solving the considered inverse problem. All codes are written in MATLAB software version R2023b. The numerical tests are executed on a laptop with an Intel Core i7 13th processor with 1.70GHz, and 16 GB of RAM.

For the radial basis functions we manipulate the inverse multi-quadratic, evaluated on different grids of size 10×10, 20×20 and 30×30. Besides to the preconditioning technique, we control the condition number of the obtained linear system by controlling the shape parameter ε, for that we use the methodology manipulated in [9]. We set $\varepsilon = 0.815 D_m$, with D_m stands for the minimum distance between two collocation points.

5.1. Example 1

Taking our unsteady convection diffusion equation when the analytical solution is given by the following

$$u(x, y, t) = (x - t)(1 - x)(y - t)(1 - y)$$

the other datum are constructed from this analytical expression.

We run our experiments for different noise levels, the optimal initial conditions are illustrated in Figure 1.

For this first experiment, the obtained optimal initial coefficient is of good quality. When data are noisy, the approximated initial condition approaches the exact one perfectly for the cases of $\delta = 1\%$ and 5%. When we consider $\delta = 7.5\%$ and $\delta = 10\%$, it is observable that the optimal initial coefficients are quite deviated, although we can say that the obtained initial coefficients are acceptable.

To illustrate the cost's evolution with respect to different noise level and grid sizes, we have recorded Table 1. It is seen that when the noise level increases, the quality of cost decreases, which is normal.

Table 1: Example 1: Cost evolution with respect to grid size and noise level.

$N \times N$ \ δ	0%	1%	5%	7.5%	10%
10×10	0.00157	0.00650	0.00819	0.01577	0.04935
20×20	0.00371	0.00511	0.00959	0.00993	0.07125
30×30	0.00322	0.00651	0.00892	0.03315	0.08205

5.2. Example 2

This time we assume the exact initial coefficient can be constructed from the analytic state solution given as follows

$$u(x, y, t) = (2 - t)\cos(\pi x)\sin(\pi y)$$

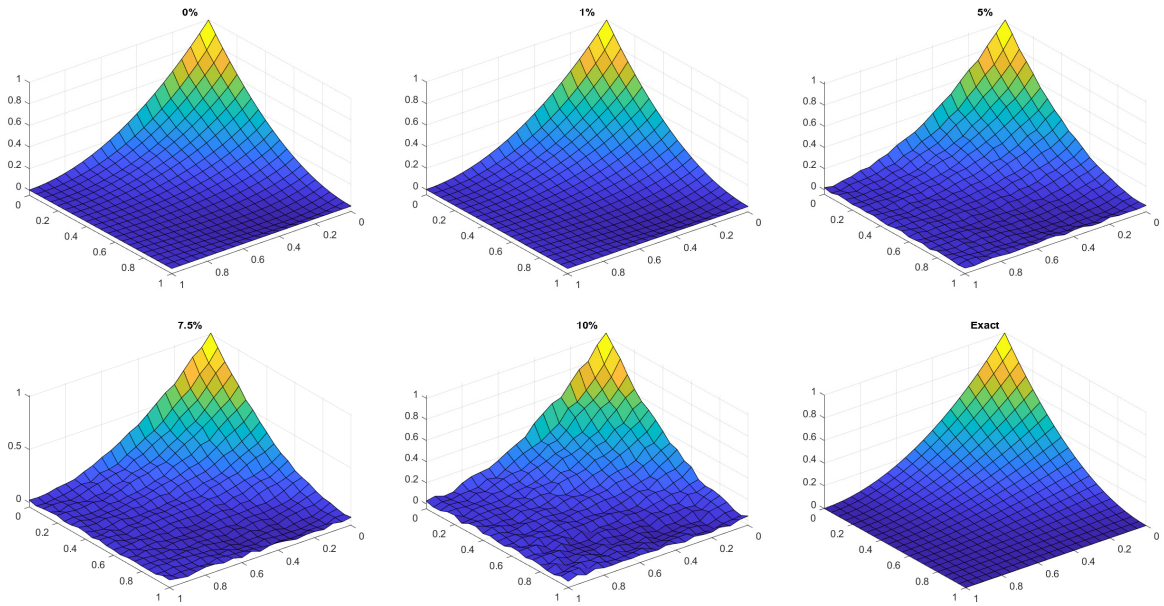

Figure 1: Example 1: comparison of identification of u_0 for different noise level.

We run our experiments for different noise level, the obtained results are illustrated in Figure 2. Another time, we illustrate in Table 2 the cost's evolution with respect to different noise level and grid sizes.

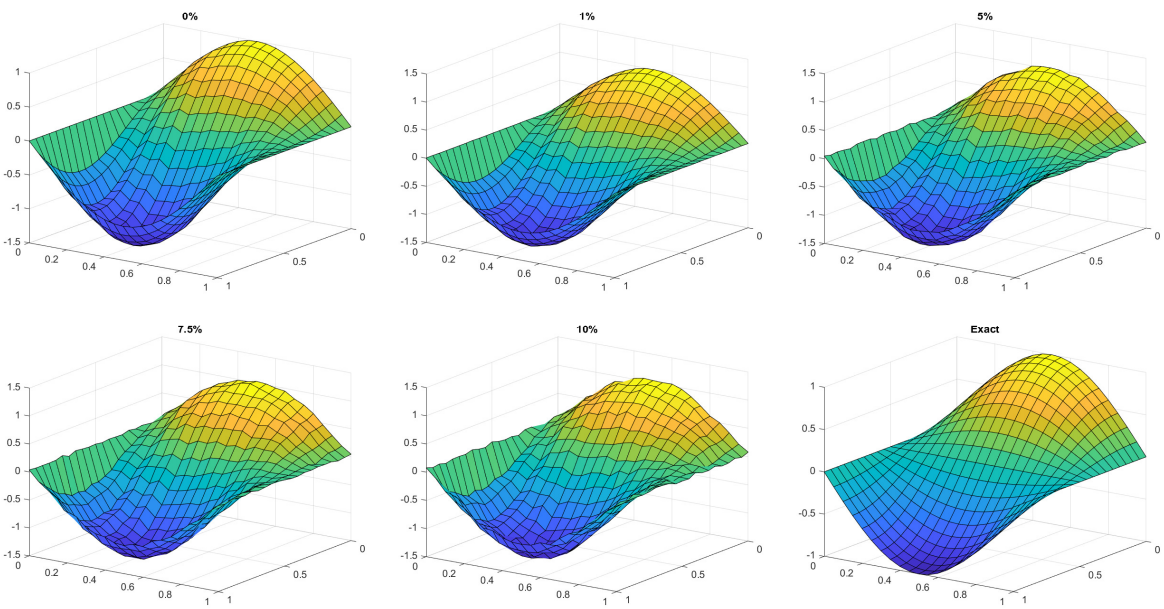

Figure 2: Example 2: comparison of identification of u_0 for different noise level.

Table 2: Example 2: Cost evolution with respect to grid size and noise level.

$N \times N$ \ δ	0%	1%	5%	7.5%	10%
10×10	0.00210	0.00310	0.00799	0.04018	0.06850
20×20	0.00243	0.00372	0.00858	0.05600	0.08037
30×30	0.00318	0.00705	0.01832	0.04322	0.08113

Again, the optimal initial coefficient, when considering exact observation, is of good quality. Considering noisy data, the optimal initial condition remains close enough to the exact one when $\delta = 1\%$ and 5%. For the noise level $\delta = 10\%$, the optimal is in somehow of acceptable quality.
At this stage, we conclude that the proposed numerical approach has succeed in identifying the unknown initial coefficient.

6. Conclusion

In this paper we constructed a numerical method for reconstructing the initial condition in convection diffusion equation. The meshless technique, radial basis function based partition of unity method is considered for discretizing the state equations. Using the quasi newton scheme we approach the solution of the optimization problem. The obtained results are illustrated with figures and tables, proving the validity of the proposed algorithm for recovering the missing initial coefficient. These first results are promising for developing advanced algorithm for the nonlinear case and when the initial coefficient is not smooth in some region of the computational domain.

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[1] *Universite Mohammed VI Polytechnique Faculte de Gouvernance Sciences Economiques et Sociales, Morocco*

[2] *Research Laboratory of Numerical Analysis, Nonlinear Analysis, and Applications (LaR2A),*

Faculty of Sciences, Abdelmalek Essaadi University, Tetouan,, Morocco.

E-mail address: badahmane.achraf@gmail.com, y.elyazidi@uae.ac.ma