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A PARAMETRIC OPTIMAL CONTROL PROBLEM INVOLVING A DIFFUSION COEFFICIENT

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Abstract. We investigate a parametric optimal control problem governed by a time dependent parabolic equation, where the control is a spatially varying diffusion coefficient. The objective is to minimize a tracking type cost functional under box constraints on the control. We establish the well posedness of the state equation, prove the existence of an optimal solution, and derive the first order optimality system consisting of the state equation, the adjoint equation, and a projection formula. A fully discrete numerical method combining finite element spatial discretization, implicit Euler time integration, and an adjoint based projected gradient algorithm is developed to solve the optimization problem efficiently. Numerical experiments demonstrate the accuracy, robustness, and effectiveness of the proposed approach.

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1. Motivation and introduction

Optimal control problems governed by parabolic partial differential equations arise in a wide range of applications: temperature regulation in thermal processes, diffusion of pollutants in the environment, energy management in distributed networks, optimization of chemical reactions in reactors, and so on. In all these contexts, the time evolution of the state is described by a dissipative diffusion–type dynamics, and one seeks to act on the system by means of a control distributed in space so as to force the state to follow a desired temporal trajectory, while keeping the control effort moderate. This naturally leads to state tracking cost functionals, complemented by a quadratic regularization term on the control and by box constraints that model the physical limitations of the actuation.[17][1][11]
In this work, we place ourselves within this general framework of time dependent parabolic control problems, while departing from it in a significant way. The problem we consider consists in optimizing a diffusion coefficient appearing in

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the parabolic operator $-\nabla \cdot (h\nabla u)$, in such a way that the state u is driven to follow a prescribed temporal trajectory, while penalizing at the same time the magnitude of the parametric control h, which is subject to box constraints. In contrast with classical formulations in which the control appears as a volume source or a boundary condition, the control acts here directly inside the differential operator, modifying the very structure of the diffusion and the effective properties of the medium. Interpreted as a finite set of parameters (conductivities of subdomains, equivalent rigidities, effective thicknesses, etc.), the coefficient h provides a parametric optimization framework well suited to the design and identification of heterogeneous materials or structures in an explicitly time–dependent setting.[18][21][8]
The aim of the study is twofold. On the analytical side, we seek to establish a rigorous functional framework ensuring the existence of an optimal solution for this tracking problem with box constraints on the diffusion coefficient, and to derive the associated first–order optimality system (state equation, adjoint equation, and projection formula onto the admissible set). On the numerical side, this optimality system serves as the basis for the construction of efficient algorithms of state–adjoint–projected–gradient type, obtained after temporal and spatial discretization by finite elements. To the best of our knowledge, the specific combination we propose spatial control of a diffusion coefficient in a time–dependent parabolic PDE, with box constraints on the control, rigorous analysis (existence and state–adjoint system), and numerical implementation via finite elements coupled with a projected adjoint–based gradient algorithm has not yet been investigated in a systematic way in the literature. This originality, together with the richness of the underlying mathematical questions and the relevance of the targeted applications, makes this problem a particularly attractive topic of study.[4][5][25]

2. Continuous setting and state equation

2.1. **Notation and functional setting.** Let $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, be a bounded open set with Lipschitz boundary $\partial\Omega$, and let $T > 0$ be a fixed final time. We denote

$$Q := \Omega \times (0,T), \qquad \Sigma := \partial\Omega \times (0,T).$$

We work with the standard Hilbert spaces

$$H := L^2(\Omega), \qquad V := H_0^1(\Omega),$$

where V is equipped with the norm $\|v\|_V := \|\nabla v\|_{L^2(\Omega)^d}$, which is equivalent to the usual H^1-norm on $H_0^1(\Omega)$ by the Poincaré inequality. We denote by V' the dual of V and use the duality pairing $\langle \cdot, \cdot \rangle_{V',V}$.

To describe the time evolution, we consider the Bochner spaces

$$L^2(0,T;V) \quad \text{and} \quad L^2(0,T;V'),$$

and define

$$W(0,T) := \big\{ u \in L^2(0,T;V) \ : \ \partial_t u \in L^2(0,T;V') \big\}.$$

Endowed with the norm

$$\|u\|_{W(0,T)}^2 := \int_0^T \|u(t)\|_V^2\,dt + \int_0^T \|\partial_t u(t)\|_{V'}^2\,dt,$$

the space $W(0,T)$ is a Hilbert space, and the continuous embedding $W(0,T) \hookrightarrow C([0,T];H)$ ensures that the initial value $u(0) \in H$ is well defined.

The data of the control problem are:

- an initial condition $u_0 \in H$,
- a source term $f \in L^2(0,T;V')$,
- a desired state $u_d \in L^2(Q)$.

The control variable is the diffusion coefficient h, assumed to be spatially dependent. We fix two constants

$$0 < h_{\min} < h_{\max} < \infty$$

and define the admissible set

$$U_{\mathrm{ad}} := \big\{h \in L^\infty(\Omega) \;:\; h_{\min} \le h(x) \le h_{\max} \text{ for a.e. } x \in \Omega\big\}. \tag{2.1}$$

The lower bound $h_{\min} > 0$ guarantees uniform ellipticity of the associated operator, while the upper bound $h_{\max}$ reflects physical limitations on the diffusion. The set U_{ad} is nonempty, closed, convex and bounded in $L^\infty(\Omega)$, which is a convenient framework for the analysis of the optimal control problem.

2.2. **State equation and weak formulation.** For a given control $h \in U_{\mathrm{ad}}$, the state $u : Q \to \mathbb{R}$ solves the time-dependent diffusion problem

$$\begin{cases} \partial_t u(x,t) - \nabla\cdot\big(h(x)\,\nabla u(x,t)\big) = f(x,t), & (x,t) \in Q,\\ u(x,t) = 0, & (x,t) \in \Sigma,\\ u(x,0) = u_0(x), & x \in \Omega. \end{cases} \tag{2.2}$$

For $h \in U_{\mathrm{ad}}$, we define the bilinear form

$$a_h(u,v) := \int_\Omega h(x)\,\nabla u(x)\cdot\nabla v(x)\,dx, \qquad u,v \in V. \tag{2.3}$$

Using $h_{\min} \le h(x) \le h_{\max}$ a.e. in Ω, we have

$$|a_h(u,v)| \le h_{\max}\,\|\nabla u\|_{L^2(\Omega)}\,\|\nabla v\|_{L^2(\Omega)} \le C\,\|u\|_V\|v\|_V, \tag{2.4}$$

$$a_h(v,v) = \int_\Omega h(x)\,|\nabla v(x)|^2\,dx \ge h_{\min}\,\|\nabla v\|_{L^2(\Omega)}^2 \ge c\,\|v\|_V^2. \tag{2.5}$$

To derive the weak formulation of (2.2), we multiply the PDE by a test function $v \in V$ and integrate over Ω:

$$\int_\Omega \partial_t u(x,t)\,v(x)\,dx - \int_\Omega \nabla\cdot\big(h(x)\,\nabla u(x,t)\big)\,v(x)\,dx = \int_\Omega f(x,t)\,v(x)\,dx.$$

Using integration by parts in space and the homogeneous Dirichlet boundary condition $v|_{\partial\Omega} = 0$, we obtain

$$-\int_\Omega \nabla\cdot\big(h\nabla u\big)\,v\,dx = \int_\Omega h(x)\,\nabla u(x,t)\cdot\nabla v(x)\,dx = a_h\big(u(t),v\big),$$

so that, for almost every $t \in (0,T)$,

$$\int_\Omega \partial_t u(x,t)\, v(x)\, dx + a_h\big(u(t),v\big) = \int_\Omega f(x,t)\, v(x)\, dx.$$

Interpreting the time derivative in the V'–V duality framework, this identity can be written as

$$\langle \partial_t u(t), v\rangle_{V',V} + a_h\big(u(t),v\big) = \langle f(t), v\rangle_{V',V}, \qquad \forall v \in V,$$

for almost every $t \in (0,T)$.

Equivalently, by integrating in time over $(0,T)$, the weak formulation can be expressed as

$$\int_0^T \langle \partial_t u(t), v\rangle_{V',V}\, dt + \int_0^T a_h\big(u(t),v\big)\, dt = \int_0^T \langle f(t), v\rangle_{V',V}\, dt, \qquad \forall v \in V,$$

with the initial condition $u(0) = u_0$ in H.

The weak formulation of (2.2) thus reads:

Problem 2.1. Find $u \in W(0,T)$ such that $u(0) = u_0$ in H and, for a.e. $t \in (0,T)$ and for all $v \in V$,

$$\langle \partial_t u(t), v\rangle_{V',V} + a_h\big(u(t),v\big) = \langle f(t), v\rangle_{V',V}. \tag{2.6}$$

2.3. Well-posedness of the state equation.

Theorem 2.2. *Let $h \in U_{\mathrm{ad}}$ be fixed, and assume that $u_0 \in H$ and $f \in L^2(0,T;V')$. Then there exists a unique solution $u(h) \in W(0,T)$ of Problem 2.1. Moreover, there exists a constant $C > 0$, independent of h, such that*

$$\|u(h)\|_{L^2(0,T;V)} + \|\partial_t u(h)\|_{L^2(0,T;V')} \le C\big(\|u_0\|_H + \|f\|_{L^2(0,T;V')}\big). \tag{2.7}$$

Proof. The proof follows the classical Galerkin approximation method for linear parabolic equations. Using the continuity and coercivity of the bilinear form $a_h(\cdot,\cdot)$, one constructs a sequence of finite-dimensional approximate solutions and derives uniform *a priori* estimates in $L^2(0,T;V)$ together with bounds for the time derivatives in $L^2(0,T;V')$. By weak compactness and the Aubin–Lions compactness theorem, one passes to the limit to obtain the existence of a weak solution. Uniqueness follows from a standard energy argument applied to the difference of two solutions. Finally, the stability estimate (2.7) is a direct consequence of the derived *a priori* estimates. The details are classical and are therefore omitted. □

3. Optimal control problem and existence of an optimal control

3.1. Admissible controls and cost functional. The control is the diffusion coefficient $h \in U_{\mathrm{ad}}$ defined in (2.1). The corresponding state is the unique solution $u(h) \in W(0,T)$ given by Theorem 2.2.

We define the cost functional

$$J(u,h) := \frac{1}{2}\int_0^T \int_\Omega |u(x,t) - u_d(x,t)|^2\, dx\, dt + \frac{\alpha}{2}\int_\Omega |h(x)|^2\, dx, \qquad \alpha > 0. \tag{3.1}$$

The reduced cost functional $j : U_{\mathrm{ad}} \to \mathbb{R}$ is defined by

$$j(h) := J\big(u(h), h\big). \tag{3.2}$$

The optimal control problem reads:

Problem 3.1. Find $h^* \in U_{\mathrm{ad}}$ such that

$$j(h^*) = \min_{h \in U_{\mathrm{ad}}} j(h), \tag{3.3}$$

where $u(h^*)$ is the solution of Problem 2.1 associated with h^*.

3.2. **Existence of an optimal control.**

Theorem 3.2. *Assume $u_0 \in H$, $f \in L^2(0,T;V')$ and $u_d \in L^2(Q)$. Then there exists at least one control $h^* \in U_{\mathrm{ad}}$ and an associated state $u^* = u(h^*) \in W(0,T)$ such that*

$$J(u^*, h^*) = \min_{h \in U_{\mathrm{ad}}} J\big(u(h), h\big).$$

Proof. We proceed by the direct method of the calculus of variations.

Since j is bounded from below (due to the nonnegativity of each term in J), there exists a minimizing sequence $(h_n)_{n\in\mathbb{N}} \subset U_{\mathrm{ad}}$, i.e.,

$$j(h_n) \to \inf_{h \in U_{\mathrm{ad}}} j(h) \quad \text{as } n \to \infty.$$

We denote by $u_n := u(h_n)$ the corresponding solutions of the state equation.

The set U_{ad} is bounded in $L^\infty(\Omega)$, hence there exists $h^* \in U_{\mathrm{ad}}$ and a (not relabeled) subsequence such that

$$h_n \rightharpoonup^* h^* \quad \text{in } L^\infty(\Omega).$$

From Theorem 2.2, the sequence (u_n) is bounded in $L^2(0,T;V) \cap H^1(0,T;V')$. Thus, there exists $u^* \in W(0,T)$ and a subsequence (again not relabeled) such that

$$u_n \rightharpoonup u^* \text{ in } L^2(0,T;V), \qquad \partial_t u_n \rightharpoonup \partial_t u^* \text{ in } L^2(0,T;V').$$

By the Aubin–Lions compactness lemma, we also have

$$u_n \to u^* \quad \text{strongly in } L^2(Q). \tag{3.4}$$

For each n and for all $v \in V$, the weak formulation reads

$$\langle \partial_t u_n(t), v\rangle_{V',V} + \int_\Omega h_n(x)\, \nabla u_n(t) \cdot \nabla v(x)\, dx = \langle f(t), v\rangle_{V',V} \quad \text{a.e. in } (0,T).$$

Using the convergences of u_n, $\partial_t u_n$ and h_n, one can show that (u^*, h^*) satisfies

$$\langle \partial_t u^*(t), v\rangle_{V',V} + \int_\Omega h^*(x)\, \nabla u^*(t) \cdot \nabla v(x)\, dx = \langle f(t), v\rangle_{V',V} \quad \text{a.e. in } (0,T),$$

i.e., u^* is the unique solution of Problem 2.1 associated with h^*.

From (3.4), we deduce

$$\frac{1}{2}\int_Q |u_n - u_d|^2\, dx\, dt \to \frac{1}{2}\int_Q |u^* - u_d|^2\, dx\, dt.$$

Moreover, since $h_n \rightharpoonup h^*$ in $L^2(\Omega)$ (boundedness in L^∞ implies boundedness in L^2), the term

$$\int_\Omega |h|^2\,dx$$

is weakly lower semicontinuous in $L^2(\Omega)$, hence

$$\int_\Omega |h^*|^2\,dx \le \liminf_{n\to\infty} \int_\Omega |h_n|^2\,dx.$$

Combining both facts yields

$$J(u^*, h^*) \le \liminf_{n\to\infty} J(u_n, h_n) = \inf_{h\in U_{\mathrm{ad}}} j(h).$$

Therefore (u^*, h^*) is an optimal pair, and h^* is an optimal control. □

4. First-order optimality system

4.1. **Lagrangian and adjoint equation.** To derive first-order optimality conditions, we introduce the Lagrangian functional

$$\mathcal{L}(u,h,p) := \frac{1}{2}\int_Q |u-u_d|^2\,dx\,dt + \frac{\alpha}{2}\int_\Omega |h|^2\,dx + \int_0^T\int_\Omega p(x,t)\,\big(\partial_t u - \nabla\cdot(h\nabla u) - f\big)(x,t)\,dx\,dt,$$

where $p : Q \to \mathbb{R}$ is the adjoint variable.

We consider variations w.r.t. u and h. For the state u, we assume that admissible variations δu satisfy $\delta u(\cdot,0) = 0$ (the initial condition is not controlled).
Derivative with respect to the state u. Let $\delta u \in W(0,T)$ with $\delta u(\cdot,0) = 0$. The derivative of $\mathcal{L}$ in the direction δu is

$$\mathcal{L}'_u(u,h,p)[\delta u] = \int_Q (u-u_d)\,\delta u\,dx\,dt + \int_0^T\int_\Omega p\,\partial_t(\delta u)\,dx\,dt - \int_0^T\int_\Omega p\,\nabla\cdot(h\nabla\delta u)\,dx\,dt.$$

Integrating by parts in time,

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

Since $\delta u(\cdot,0) = 0$, the term at $t = 0$ vanishes. To make the term at $t = T$ vanish for arbitrary $\delta u(\cdot,T)$, we impose the terminal condition

$$p(x,T) = 0 \quad \text{in } \Omega. \tag{4.1}$$

Under this condition, we obtain

$$\int_0^T\int_\Omega p\,\partial_t(\delta u)\,dx\,dt = -\int_0^T\int_\Omega (\partial_t p)\,\delta u\,dx\,dt.$$

Next, we integrate by parts in space the term involving $\nabla\cdot(h\nabla\delta u)$:

$$-\int_0^T\int_\Omega p\,\nabla\cdot(h\nabla\delta u)\,dx\,dt = \int_0^T\int_\Omega h\,\nabla p\cdot\nabla\delta u\,dx\,dt = -\int_0^T\int_\Omega \nabla\cdot(h\nabla p)\,\delta u\,dx\,dt,$$

where we used $u = 0$ and $\delta u = 0$ on $\partial\Omega$ so that boundary terms vanish.

Putting everything together, we obtain

$$\mathcal{L}'_u(u,h,p)[\delta u] = \int_Q \big(u - u_d - \partial_t p - \nabla\cdot(h\nabla p)\big)\,\delta u\,dx\,dt.$$

For an optimal triple (u^*, h^*, p^*), the stationarity condition $\mathcal{L}'_u(u^*,h^*,p^*)[\delta u] = 0$ for all admissible δu implies

$$-\,\partial_t p^*(x,t) - \nabla\cdot\big(h^*(x)\,\nabla p^*(x,t)\big) = u^*(x,t) - u_d(x,t) \quad \text{in } Q, \tag{4.2}$$

together with the boundary and final conditions

$$p^*(x,t) = 0 \quad \text{on } \Sigma, \qquad p^*(x,T) = 0 \quad \text{in } \Omega. \tag{4.3}$$

4.2. **Derivative with respect to the control h and gradient.** Let $\delta h \in L^\infty(\Omega)$ be an admissible variation such that $h + \varepsilon\delta h \in U_{\text{ad}}$ for small ε. We compute $\mathcal{L}'_h(u,h,p)[\delta h]$.

Only two terms in $\mathcal{L}$ depend on h:

$$\frac{\alpha}{2}\int_\Omega |h|^2\,dx \quad \text{and} \quad -\int_0^T\!\!\int_\Omega p\,\nabla\cdot(h\nabla u)\,dx\,dt.$$

The derivative of the first term gives

$$\frac{d}{d\varepsilon}\frac{\alpha}{2}\int_\Omega |h+\varepsilon\delta h|^2\,dx\Big|_{\varepsilon=0} = \alpha\int_\Omega h(x)\,\delta h(x)\,dx.$$

For the second term, we get

$$\frac{d}{d\varepsilon}\left[-\int_0^T\!\!\int_\Omega p\,\nabla\cdot\big((h+\varepsilon\delta h)\nabla u\big)\,dx\,dt\right]_{\varepsilon=0} = -\int_0^T\!\!\int_\Omega p\,\nabla\cdot(\delta h\,\nabla u)\,dx\,dt.$$

Integrating by parts in space as before,

$$-\int_\Omega p\,\nabla\cdot(\delta h\,\nabla u)\,dx = \int_\Omega \delta h(x)\,\nabla u\cdot\nabla p\,dx,$$

so that

$$-\int_0^T\!\!\int_\Omega p\,\nabla\cdot(\delta h\,\nabla u)\,dx\,dt = \int_0^T\!\!\int_\Omega \delta h(x)\,\nabla u(x,t)\cdot\nabla p(x,t)\,dx\,dt.$$

Hence

$$\begin{aligned}\mathcal{L}'_h(u,h,p)[\delta h] &= \alpha\int_\Omega h(x)\,\delta h(x)\,dx + \int_0^T\!\!\int_\Omega \delta h(x)\,\nabla u(x,t)\cdot\nabla p(x,t)\,dx\,dt\\ &= \int_\Omega\left(\alpha h(x) + \int_0^T \nabla u(x,t)\cdot\nabla p(x,t)\,dt\right)\delta h(x)\,dx.\end{aligned} \tag{4.4}$$

Using the chain rule, the derivative of the reduced cost j at h satisfies

$$j'(h)[\delta h] = \mathcal{L}'_h\big(u(h),h,p(h)\big)[\delta h],$$

where $u(h)$ is the state and $p(h)$ the corresponding adjoint. Comparing with (4.4), we identify the (Gâteaux) gradient of j:

$$\frac{\delta j}{\delta h}(x) = \alpha h(x) + \int_0^T \nabla u(x,t)\cdot\nabla p(x,t)\,dt, \quad \text{for a.e. } x\in\Omega. \tag{4.5}$$

4.3. **Variational inequality and projection formula.** Let $h^* \in U_{\mathrm{ad}}$ be an optimal control, and let u^*, p^* be the associated state and adjoint. Since U_{ad} is closed and convex in $L^2(\Omega)$, the first-order optimality condition for minimizing j on U_{ad} is the variational inequality

$$\int_\Omega \frac{\delta j}{\delta h}(x)\big(h(x) - h^*(x)\big)\,dx \;\geq\; 0 \quad \forall\, h \in U_{\mathrm{ad}}. \tag{4.6}$$

Using (4.5), this becomes

$$\int_\Omega \left(\alpha h^*(x) + \int_0^T \nabla u^*(x,t)\cdot\nabla p^*(x,t)\,dt\right)\big(h(x) - h^*(x)\big)\,dx \;\geq\; 0, \quad \forall h \in U_{\mathrm{ad}}. \tag{4.7}$$

Because U_{ad} is a box constraint

$$U_{\mathrm{ad}} = \{h \in L^\infty(\Omega) : h_{\min} \leq h(x) \leq h_{\max} \text{ a.e.}\},$$

(4.7) is equivalent to the pointwise projection formula

$$h^*(x) = \mathcal{P}_{[h_{\min},h_{\max}]}\left(-\frac{1}{\alpha}\int_0^T \nabla u^*(x,t)\cdot\nabla p^*(x,t)\,dt\right) \quad \text{for a.e. } x \in \Omega, \tag{4.8}$$

where $\mathcal{P}_{[a,b]}(z) := \min\{\max\{z,a\},b\}$ denotes the orthogonal projection of z onto the interval $[a,b]$.

Equations (2.2), (4.2)–(4.3) together with (4.8) form the first-order optimality system for the optimal control problem.

5. Finite element discretization and adjoint-based algorithm

5.1. **Spatial discretization.** Let $\mathcal{T}_h$ be a conforming mesh of Ω into simplices (triangles in 2D, tetrahedra in 3D). We define the finite element space

$$V_h := \big\{v_h \in C^0(\overline{\Omega}) : v_h|_K \text{ is affine for all } K \in \mathcal{T}_h, \quad v_h|_{\partial\Omega} = 0\big\},$$

and choose a nodal basis $\{\varphi_i\}_{i=1}^N$ of V_h.

We approximate the state and adjoint by

$$u_h(x,t) = \sum_{i=1}^N U_i(t)\,\varphi_i(x), \qquad p_h(x,t) = \sum_{i=1}^N P_i(t)\,\varphi_i(x),$$

and gather the coefficients into vectors

$$\mathbf{U}(t) := [U_1(t),\ldots,U_N(t)]^\top, \quad \mathbf{P}(t) := [P_1(t),\ldots,P_N(t)]^\top.$$

We define the mass matrix $M \in \mathbb{R}^{N\times N}$ by

$$M_{ij} = \int_\Omega \varphi_i(x)\,\varphi_j(x)\,dx, \qquad 1 \leq i,j \leq N. \tag{5.1}$$

The stiffness matrix associated with a coefficient $h(x)$ is given by

$$K(h)_{ij} = \int_\Omega h(x)\,\nabla\varphi_i(x)\cdot\nabla\varphi_j(x)\,dx. \tag{5.2}$$

In order to parametrize h, we may consider a partition of Ω into subdomains $(\Omega_k)_{k=1}^m$ and set

$$h(x) = \sum_{k=1}^{m} h_k\, \phi_k(x), \qquad \phi_k := \mathbf{1}_{\Omega_k}.$$

Then

$$K(h) = \sum_{k=1}^{m} h_k K^{(k)}, \qquad K_{ij}^{(k)} := \int_{\Omega_k} \nabla\varphi_i \cdot \nabla\varphi_j \, dx. \tag{5.3}$$

We also introduce the discrete right-hand side and desired state:

$$F_i(t) = \int_\Omega f(x,t)\, \varphi_i(x)\, dx, \qquad (U_d)_i(t) = \int_\Omega u_d(x,t)\, \varphi_i(x)\, dx, \tag{5.4}$$

and assemble the vectors $\mathbf{F}(t)$ and $\mathbf{U}_d(t)$.

5.2. **Time discretization of the state equation.** After spatial discretization by finite elements (see Section 5), the weak form of the state equation (2.6) leads to the following semidiscrete problem in time: find a function $\mathbf{U} : [0,T] \to \mathbb{R}^N$ such that

$$M\, \dot{\mathbf{U}}(t) + K(h)\, \mathbf{U}(t) = \mathbf{F}(t) \quad \text{for a.e. } t \in (0,T), \qquad \mathbf{U}(0) = \mathbf{U}^0, \tag{5.5}$$

where M is the mass matrix (5.1), $K(h)$ is the stiffness matrix (5.2) associated with the diffusion coefficient h, $\mathbf{F}(t)$ is the load vector defined in (5.4), and $\mathbf{U}^0$ is the finite element representation of the initial condition u_0 (for instance its L^2-projection or nodal interpolation onto V_h).

To approximate (5.5) in time, we introduce a uniform partition of the interval $[0,T]$ into N_t subintervals. We set

$$\Delta t := \frac{T}{N_t}, \qquad t^n := n\Delta t, \quad n = 0,\dots,N_t,$$

and denote by $\mathbf{U}^n \approx \mathbf{U}(t^n)$ and $\mathbf{F}^n \approx \mathbf{F}(t^n)$ the approximations of the state and the right-hand side at time level t^n.

We consider the backward (implicit) Euler scheme applied to (5.5). Between times t^n and t^{n+1}, the time derivative is approximated by the backward difference quotient

$$\dot{\mathbf{U}}(t^{n+1}) \approx \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t},$$

and the matrix $K(h)\mathbf{U}(t)$ and the load vector $\mathbf{F}(t)$ are evaluated at the new time level t^{n+1}. This yields, for $n = 0,\dots,N_t - 1$,

$$M\, \frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + K(h)\, \mathbf{U}^{n+1} = \mathbf{F}^{n+1},$$

which is precisely the discrete system

$$\frac{1}{\Delta t} M \big(\mathbf{U}^{n+1} - \mathbf{U}^n\big) + K(h)\, \mathbf{U}^{n+1} = \mathbf{F}^{n+1}, \quad n = 0,\dots,N_t - 1. \tag{5.6}$$

Rearranging terms, we obtain at each time step a linear system of the form

$$\big(M + \Delta t\, K(h)\big)\, \mathbf{U}^{n+1} = M\, \mathbf{U}^n + \Delta t\, \mathbf{F}^{n+1}, \quad n = 0,\dots,N_t - 1, \tag{5.7}$$

with initial condition $\mathbf{U}^0$ obtained by projecting u_0 onto V_h.

Since M is symmetric positive definite and $K(h)$ is symmetric positive semidefinite (and, in fact, positive definite on V_h under homogeneous Dirichlet boundary conditions), the matrix $M+\Delta t\, K(h)$ is symmetric positive definite for any $\Delta t > 0$. Therefore, for each time step n, system (5.7) admits a unique solution $\mathbf{U}^{n+1}$, and the implicit Euler scheme is unconditionally stable for this linear parabolic problem. In practice, the factorization of $M + \Delta t\, K(h)$ can be computed once and reused at all time steps, since h (and thus $K(h)$) is fixed when solving the state equation for a given control.

5.3. **Time discretization of the adjoint equation.** The continuous adjoint equation associated with the optimal control problem reads

$$-\partial_t p(x,t) - \nabla \cdot \big(h(x)\nabla p(x,t)\big) = u(x,t) - u_d(x,t) \quad \text{in } Q,$$

with homogeneous Dirichlet boundary condition

$$p(x,t) = 0 \quad \text{on } \Sigma,$$

and final-time condition

$$p(x,T) = 0 \quad \text{in } \Omega.$$

After spatial discretization by finite elements, this leads to the following semidiscrete problem in time: find $\mathbf{P} : [0,T] \to \mathbb{R}^N$ such that

$$-M\,\dot{\mathbf{P}}(t) - K(h)\,\mathbf{P}(t) = M\big(\mathbf{U}(t) - \mathbf{U}_d(t)\big) \quad \text{for a.e. } t \in (0,T), \qquad \mathbf{P}(T) = \mathbf{0},$$

where $\mathbf{U}(t)$ and $\mathbf{U}_d(t)$ denote the finite element coefficient vectors corresponding to $u(t)$ and $u_d(t)$, respectively.

We use the same uniform time grid as for the state equation: $\Delta t = T/N_t$, $t^n = n\Delta t$ for $n = 0, \ldots, N_t$. We denote

$$\mathbf{P}^n \approx \mathbf{P}(t^n), \qquad \mathbf{U}^n \approx \mathbf{U}(t^n), \qquad \mathbf{U}_d^n \approx \mathbf{U}_d(t^n),$$

and enforce the discrete final condition

$$\mathbf{P}^{N_t} = \mathbf{0}. \tag{5.8}$$

Since the adjoint equation is terminal-value (posed backward in time), we construct a time-stepping scheme that marches from t^{N_t} down to t^0. We apply a backward (implicit) Euler scheme to the semidiscrete equation. Evaluating the equation at time t^n and approximating the time derivative by

$$\dot{\mathbf{P}}(t^n) \approx \frac{\mathbf{P}^{n+1} - \mathbf{P}^n}{\Delta t}, \qquad n = N_t - 1, \ldots, 0,$$

we obtain

$$-M\,\frac{\mathbf{P}^{n+1} - \mathbf{P}^n}{\Delta t} - K(h)\,\mathbf{P}^n = M\big(\mathbf{U}^n - \mathbf{U}_d^n\big),$$

which is precisely

$$-\frac{1}{\Delta t} M(\mathbf{P}^{n+1} - \mathbf{P}^n) - K(h)\,\mathbf{P}^n = \mathbf{U}^n - \mathbf{U}_d^n, \tag{5.9}$$

for $n = N_t - 1, \ldots, 0$.

Rearranging the terms in (5.9), we isolate $\mathbf{P}^n$ on the left-hand side:

$$M\,\mathbf{P}^n + \Delta t\, K(h)\,\mathbf{P}^n = M\,\mathbf{P}^{n+1} + \Delta t\, M\big(\mathbf{U}^n - \mathbf{U}_d^n\big),$$

which yields the linear system

$$\big(M + \Delta t\, K(h)\big)\, \mathbf{P}^n = M\, \mathbf{P}^{n+1} + \Delta t\, M\big(\mathbf{U}^n - \mathbf{U}_d^n\big), \quad n = N_t - 1, \dots, 0. \tag{5.10}$$

Thus, starting from the terminal condition (5.8), the discrete adjoint solution is computed recursively in reverse time: for $n = N_t - 1, \dots, 0$, one solves (5.10) to obtain $\mathbf{P}^n$ from $\mathbf{P}^{n+1}$ and the known quantities $\mathbf{U}^n$ and $\mathbf{U}_d^n$.

We emphasize that the same matrix

$$A(h) := M + \Delta t\, K(h)$$

appears in the discrete state equation (5.7) and in the adjoint equation (5.10). This is particularly advantageous from a computational viewpoint: once a factorization of $A(h)$ (e.g., LU or Cholesky) has been computed, it can be reused for all time steps, both in the forward solve for the state and in the backward solve for the adjoint, thereby reducing the overall computational cost of each gradient evaluation.

5.4. **Discrete gradient with respect to the parameters.** In the parametrized case $h(x) = \sum_{k=1}^{m} h_k \phi_k(x)$, the continuous gradient formula (4.5) leads to the approximate discrete gradient

$$\frac{\partial J_h}{\partial h_k} \approx \alpha h_k + \sum_{n=0}^{N_t - 1} \Delta t \int_{\Omega_k} \nabla u_h^{n+1} \cdot \nabla p_h^{n+1}\, dx, \quad k = 1, \dots, m, \tag{5.11}$$

where $u_h^{n+1}(x) = \sum_i U_i^{n+1} \varphi_i(x)$ and $p_h^{n+1}(x) = \sum_i P_i^{n+1} \varphi_i(x)$.

Using the matrices $K^{(k)}$ from (5.3), we can write

$$\int_{\Omega_k} \nabla u_h^{n+1} \cdot \nabla p_h^{n+1}\, dx \approx (\mathbf{U}^{n+1})^\top K^{(k)} \mathbf{P}^{n+1}, \tag{5.12}$$

so that

$$\boxed{\frac{\partial J_h}{\partial h_k} \approx \alpha h_k + \sum_{n=0}^{N_t - 1} \Delta t\, (\mathbf{U}^{n+1})^\top K^{(k)} \mathbf{P}^{n+1}, \quad k = 1, \dots, m.} \tag{5.13}$$

5.5. **Adjoint-based gradient projection algorithm.** We briefly describe the adjoint-based algorithm to approximate an optimal parameter vector $h^* = (h_1^*, \dots, h_m^*)$.

Algorithm 1 Adjoint-based gradient projection method

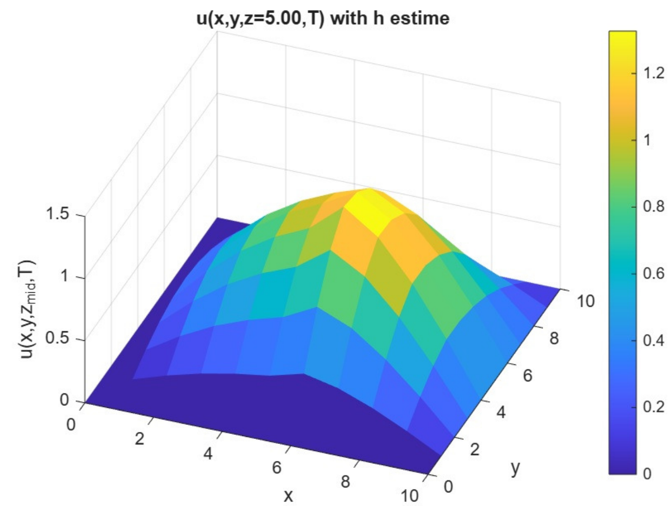
Require: initial guess $h^{(0)} = (h_1^{(0)}, \dots, h_m^{(0)}) \in U_{\mathrm{ad}}$; step size $\gamma > 0$; tolerances $\varepsilon_{\mathrm{grad}}, \varepsilon_{\mathrm{rel}} > 0$.

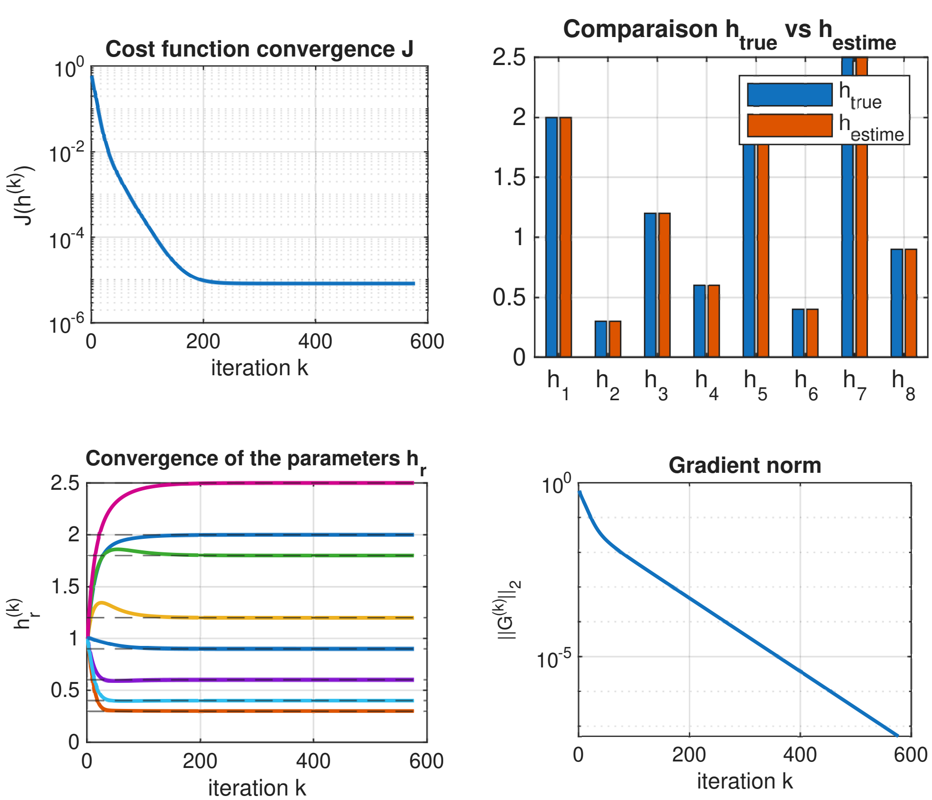
```
Set k = 0.
repeat
    Assemble K(h^(k)) = sum_{k=1}^{m} h_k^(k) K^(k).
    Factorize A^(k) := M + Δt K(h^(k)).
    State solve (forward in time):
    Set U^0 = U_0 (projection of u_0).
    for n = 0 to N_t − 1 do
        Solve A^(k) U^{n+1} = M U^n + Δt F^{n+1}.
    end for
    Adjoint solve (backward in time):
    Set P^{N_t} = 0.
    for n = N_t − 1 downto 0 do
        Compute right-hand side R^n = M P^{n+1} + Δt M(U^n − U_d^n).
        Solve A^(k) P^n = R^n.
    end for
    Gradient computation:
    for k_par = 1 to m do
        Initialize G_{k_par} ← α h_{k_par}^(k).
        for n = 0 to N_t − 1 do
            G_{k_par} ← G_{k_par} + Δt (U^{n+1})^⊤ K^(k_par) P^{n+1}.
        end for
    end for
    Denote G^(k) := (G_1, ..., G_m)^⊤.
    Stopping criterion:
    if ||G^(k)||_2 ≤ ε_grad and (relative change in J below ε_rel) then
        break
    end if
    Gradient step and projection:
    h̃^(k+1) = h^(k) − γ G^(k).
    for k_par = 1 to m do
        h_{k_par}^(k+1) = min{max{h̃_{k_par}^(k+1), h_min}, h_max}.
    end for
    k ← k + 1.
until convergence
```

The output of Algorithm 1 is an approximation $h^* \approx h^{(k)}$ of the optimal control and the corresponding state and adjoint sequences $\{\mathbf{U}^n\}_{n=0}^{N_t}$, $\{\mathbf{P}^n\}_{n=0}^{N_t}$.

5.6. **Matlab Algorithm for simulation.** The complete MATLAB implementation used for the numerical simulations has been made publicly available in a GitHub repository at:
https://github.com/danimohamed1/simulation-3D

FIGURE 1.





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