

Optimal Boundary Control of Reaction-Diffusion PDEs via Weak Variations

Scott J. Moura

UC President's Postdoctoral Fellow
Mechanical & Aerospace Engineering
University of California, San Diego
La Jolla, California 92093
Email: smoura@ucsd.edu

Hosam K. Fathy

Assistant Professor
Mechanical & Nuclear Engineering
Pennsylvania State University
University Park, PA 16802
Email: hkf2@psu.edu

This paper derives linear quadratic regulator (LQR) results for boundary controlled parabolic partial differential equations (PDEs) via weak-variations. Research on optimal control of PDEs has a rich 40-year history. This body of knowledge relies heavily on operator and semigroup theory. Our research distinguishes itself by deriving existing LQR results from a more accessible set of mathematics, namely weak-variational concepts. Ultimately, the LQR controller is computed from a Riccati PDE that must be derived for each PDE model under consideration. Nonetheless, a Riccati PDE is a significantly simpler object to solve than an operator Riccati equation, which characterizes most existing results. To this end, our research provides an elegant and accessible method for practicing engineers who study physical systems described by PDEs. Simulation examples, closed-loop stability analyses, comparisons to alternative control methods, and extensions to other models are also included.

1 Introduction

1.1 Problem Statement and Motivation

This paper derives finite-time linear quadratic regulator (LQR) results for boundary controlled parabolic partial differential equations (PDEs) via weak-variations. A broad spectrum of physical engineering systems exhibit dynamics described by parabolic PDEs. Examples include structural acoustics [1], fixed-bed reactors [2], multi-agent coordination control [3], stock investment models [4], and fluid mixing in channel flows [5]. A subset of these systems limit control to the boundaries, such as thermal/fluid flows [6], chemical reactors [7], and advanced batteries [8–10]. Optimal control of these PDE systems is particularly challenging

since actuation is limited to the boundary and the dynamics are notably more complex than ODE systems.

Although optimal boundary control of PDEs is a historically well-studied topic [2, 11–16], existing results are often difficult to apply in practice. Specifically, these results require users to have a notable background in semigroup theory and functional analysis. Moreover, one needs to ultimately solve operator Riccati equations - a conceptually difficult task. Motivated by these facts, this paper's overall goal is to develop optimal boundary control results for parabolic PDE systems that engineers with traditional mathematical backgrounds can easily derive and apply in practice. To begin, we focus on diffusion-reaction PDEs with Dirichlet actuation. We later extend the concepts to a general class of parabolic PDEs.

1.2 Brief Summary of Relevant Literature

Optimal control of PDE systems has a rich history [2, 11–16]. One can generally place this research into two categories. The first category projects the PDEs onto a finite-dimensional subspace to render the system into a series of ordinary differential equations (ODEs). This enables engineers to apply finite-dimensional optimal control results [17–21]. This method necessarily couples the control problem with the projection technique. The second category of research applies semigroup theory to represent PDE systems as ODE systems over Hilbert spaces. From here the classical optimal control results are extended to infinite-dimensional (Hilbert) spaces [11–14]. Ultimately, these techniques produce so-called operator Riccati equations (OREs), which have similarities to the results presented here. However OREs are a considerably more difficult object to solve [22] than the Ric-

cati PDEs derived in this article.

1.3 New Contributions

The main goal of this paper is to bridge the gap between the aforementioned two categories. Namely, we wish to separate the discretization techniques from the control design by maintaining the analysis in the infinite-dimensional domain. Secondly, we bypass semigroup theory and the associated issues with solving operator Riccati equations by applying the weak-variations concept directly to the PDEs. Consequently, this paper's most important new contribution is a method to derive Riccati PDEs for the LQR problem in boundary-controlled PDEs. This paper extends the authors' previous work [23] on diffusion-reaction systems by (i) supplying the proofs in full detail, (ii) computing the closed-loop spectrum, (iii) performing a stability robustness analysis, (iv) providing a comprehensive comparative analysis to existing results, and (v) deriving LQR results for a broad class of parabolic PDEs. Ultimately, this paper provides an optimal control result that is widely-accessible, constructive, and elegant for practicing engineers who develop control systems for physical systems described by PDEs.

1.4 Problem Statement

Consider the following class of linear parabolic diffusion-reaction partial differential equations:

$$\begin{aligned} u_t(x,t) &= u_{xx}(x,t) + cu(x,t) & (1) \\ u(0,t) &= 0 & (2) \\ u(1,t) &= U(t) & (3) \\ u(x,0) &= u_0(x) & (4) \end{aligned}$$

The first term in (1) represents diffusion and the second term models linear reaction phenomena. Non-unity diffusivity coefficients, lengths, input gains, etc. can be accounted for by non-dimensionalizing the system into the form given above. Suppose we can control the boundary value $u(1,t) = U(t)$ (Dirichlet control) and nothing else. Moreover, suppose we have noiseless measurements of the state available throughout the spatial domain. Our goal is to develop a state-feedback controller that optimally regulates the system to the origin. Specifically, we wish to minimize the following quadratic objective over a finite time-horizon:

$$\begin{aligned} J = \frac{1}{2} \int_0^T [\langle u(x,t), Q(u(x,t)) \rangle + RU^2(t)] dt + \\ \frac{1}{2} \langle u(x,T), P_f(u(x,T)) \rangle \end{aligned} \quad (5)$$

The symbols Q , R , and P_f are weighting kernels that respectively weight the state, control, and terminal state of the closed loop system. We assume that $Q \geq 0$, $R > 0$, $P_f \geq 0$, thus producing a convex cost functional. The condition on R is strictly positive to ensure bounded control signals. First, we derive the necessary conditions for optimality

of the open-loop finite-horizon control problem using weak variations. Instead of obtaining coupled *ordinary* differential equations with split initial conditions for finite-dimensional LQR, we obtain coupled *partial* differential equations with split initial conditions. Next, we postulate the open-loop control signal can be written in state-feedback form and derive the associated Riccati equation for the feedback linear operator. This Riccati equation is a 2-D spatial, 1-D temporal PDE. We then demonstrate the LQR result in simulation, analyze its properties, compare it to existing PDE control-theoretic results, and generalize the class of models under consideration.

1.5 Organization

The remainder of the paper is organized as follows: Section 2 presents linear quadratic regulator results for diffusion-reaction PDEs with Dirichlet boundary control. This includes the open loop control problem, state-feedback, and numerical examples. Section 3 computes the spectrum of the closed-loop system and analyzes stability robustness for the infinite-time LQR controller. Section 4 compares and contrasts the Riccati PDE results with operator Riccati equations and the backstepping method for PDEs. Section 5 provides the Riccati PDEs for various other plant boundary conditions and a more general reaction-advection-diffusion PDE model. Finally, Section 6 summarizes the key results of this paper.

2 Linear Quadratic Regulator Results

2.1 Open Loop Control

We start by deriving the first order necessary conditions for the open loop finite-time horizon problem.

Theorem 1. *Consider the linear diffusion-reaction PDE described by (1)-(4) defined on the finite-time horizon $t \in [0, T]$ with quadratic cost criterion (5). Let $u^*(x,t)$, $U^*(t)$, and $\lambda(x,t)$ respectively denote the optimal state, control, and co-state that minimize the quadratic cost. Then the first order necessary conditions for optimality are:*

$$u_t^*(x,t) = u_{xx}^*(x,t) + cu^*(x,t) \quad (6)$$

$$-\lambda_t(x,t) = \lambda_{xx} + c\lambda(x,t) + Q(u^*(x,t)) \quad (7)$$

with boundary conditions

$$u^*(0,t) = 0 \quad u^*(1,t) = U^*(t) \quad (8)$$

$$\lambda(0,t) = 0 \quad \lambda(1,t) = 0 \quad (9)$$

and split initial/final conditions

$$u^*(x,0) = u_0(x) \quad \lambda(x,T) = P_f(u^*(x,T)) \quad (10)$$

and the optimal control input is

$$U^*(t) = \frac{1}{R} \lambda_x(1,t) \quad (11)$$

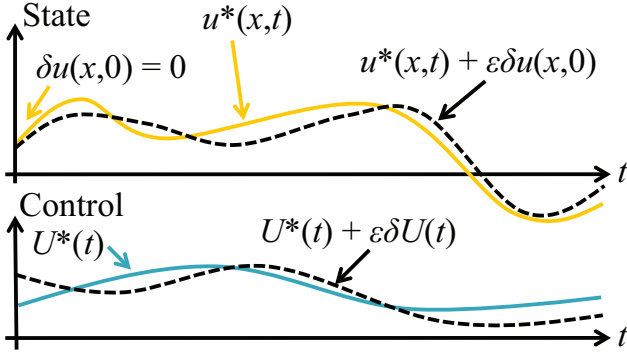


Fig. 1. A visualization of the weak variations concept for optimal state and control trajectories.

Proof. The necessary conditions are derived via weak variations [24]. Suppose $u^*(x,t)$ and $U^*(t)$ are the optimal state and control inputs. Let $u(x,t) = u^*(x,t) + \epsilon \delta u(x,t)$, $U(t) = U^*(t) + \epsilon \delta U(t)$ and $\delta u(x,0) = 0$ represent perturbations from the optimal solutions. See Fig. 1 for a visualization of the weak variations concept. Consequently, the cost is

$$J(u^* + \epsilon \delta u, U^* + \epsilon \delta U) = \frac{1}{2} \int_0^T [\langle u^* + \epsilon \delta u, Q(u^* + \epsilon \delta u) \rangle + R(U^* + \epsilon \delta U)^2] dt + \frac{1}{2} \langle u^*(T) + \epsilon \delta u(T), P_f(u^*(T) + \epsilon \delta u(T)) \rangle \quad (12)$$

Define $g(\epsilon)$ to be the cost functional above combined with the system dynamics constraint (1), using the method of Lagrange multipliers as follows:

$$g(\epsilon) := \frac{1}{2} \int_0^T [\langle u^* + \epsilon \delta u, Q(u^* + \epsilon \delta u) \rangle + R(U^* + \epsilon \delta U)^2] dt + \frac{1}{2} \langle u^*(T) + \epsilon \delta u(T), P_f(u^*(T) + \epsilon \delta u(T)) \rangle + \int_0^T \langle \lambda(x,t), u_{xx}^* + \epsilon \delta u_{xx} + c u^* + \epsilon c \delta u - \frac{\partial}{\partial t} (u^* + \epsilon \delta u) \rangle dt \quad (13)$$

where $\lambda(x,t)$ is the Lagrange multiplier (a.k.a. the co-state in the context of optimal control). Then the necessary condition for optimality is $dg(\epsilon)/d\epsilon|_{\epsilon=0} = 0$. Differentiating $g(\epsilon)$ gives:

$$\frac{dg}{d\epsilon}(\epsilon) = \int_0^T [\langle \delta u, Q(u^* + \epsilon \delta u) \rangle + R(U^* + \epsilon \delta U) \delta U] dt + \langle \delta u(T), P_f(u^*(T) + \epsilon \delta u(T)) \rangle + \int_0^T \langle \lambda(x), \delta u_{xx} + c \delta u - \frac{\partial}{\partial t} (\delta u) \rangle dt \quad (14)$$

We simplify the term $\langle \lambda(x), \delta u_{xx} \rangle$ in the third line of (14) by applying integration by parts twice. Specifically, one can

show that

$$\langle \lambda(x), \delta u_{xx}(x) \rangle = \lambda(1) \delta u_x(1) - \lambda(0) \delta u_x(0) - \lambda_x(1) \delta u(1) + \lambda_x(0) \delta u(0) + \langle \lambda_{xx}(x), \delta u(x) \rangle \quad (15)$$

The boundary conditions for $\delta u(x,t)$ are $\delta u(0,t) = 0$ and $\delta u(1,t) = \delta U(t)$, resulting in

$$\langle \lambda(x), \delta u_{xx}(x) \rangle = \lambda(1) \delta u_x(1) - \lambda(0) \delta u_x(0) - \lambda_x(1) \delta U(t) + \langle \lambda_{xx}(x), \delta u(x) \rangle \quad (16)$$

One can also use integration by parts to show that:

$$\int_0^T \langle \lambda(x), \frac{\partial}{\partial t} (\delta u) \rangle dt = \langle \lambda(T), \delta u(T) \rangle - \langle \lambda(0), \delta u(0) \rangle - \int_0^T \langle \lambda_t, \delta u \rangle dt \quad (17)$$

Note that $\delta u(x,0) = 0$ by definition. Therefore

$$\int_0^T \langle \lambda(x), \frac{\partial}{\partial t} (\delta u) \rangle dt = \langle \lambda(T), \delta u(T) \rangle - \int_0^T \langle \lambda_t, \delta u \rangle dt \quad (18)$$

At this point we plug (16) and (18) into (14) and collect like perturbation terms

$$\frac{dg}{d\epsilon}(\epsilon) = \int_0^T [\langle Q(u^* + \epsilon \delta u), \delta u \rangle + \langle \lambda_{xx} + c \lambda + \lambda_t, \delta u \rangle] dt + \int_0^T [R(U^* + \epsilon \delta U) - \lambda_x(1)] \delta U dt + \int_0^T [\lambda(1) \delta u_x(1) - \lambda(0) \delta u_x(0)] dt + \langle P_f(u^*(T) + \epsilon \delta u(T)) - \lambda(T), \delta u(T) \rangle \quad (19)$$

Now we evaluate the previous expression at $\epsilon = 0$ and set it equal to zero.

$$\frac{dg}{d\epsilon}(\epsilon)|_{\epsilon=0} = \int_0^T [\langle Q(u^*) + \lambda_{xx} + c \lambda + \lambda_t, \delta u \rangle] dt + \int_0^T [R U^* - \lambda_x(1)] \delta U dt + \int_0^T [\lambda(1) \delta u_x(1) - \lambda(0) \delta u_x(0)] dt + \langle P_f(u^*(T)) - \lambda(T), \delta u(T) \rangle = 0 \quad (20)$$

For the previous equation to hold true for all arbitrary $\delta u(x,t), \delta U(t), \delta u(x,T)$, the following conditions are suffi-

cient:

$$-\lambda_t(x,t) = \lambda_{xx}(x,t) + c\lambda(x,t) + Q(u^*(x,t)) \quad (21)$$

$$\lambda(0,t) = 0 \quad \lambda(1,t) = 0 \quad (22)$$

$$\lambda(x,T) = P_f(u^*(x,T)) \quad (23)$$

$$U^*(t) = \frac{1}{R}\lambda_x(1,t) \quad (24)$$

These conditions represent the co-state's PDE dynamics, boundary conditions, final condition, and the optimal boundary control, respectively. Coupled together with the plant model (1)-(4), these conditions verify the first order necessary conditions of optimality, which completes the proof.

Remark. In general weak-variations provide the necessary conditions for optimality and the Hamilton-Jacobi-Bellman equation provides the sufficient condition for optimality. However, both methods provide necessary and sufficient conditions when considering a strictly convex cost functional, as we do in this paper [13].

2.2 State-Feedback Control

Now let us consider the state-feedback problem. That is, let us postulate that the co-state λ is related to the states according to the time-varying linear transformation:

$$\lambda(x,t) = P^t(u(x,t)) = \int_0^1 P(x,y,t)u^*(y,t)dy \quad (25)$$

The superscript on P^t indicates the linear operator is time-dependent.

Theorem 2. *The optimal control in state-feedback form is:*

$$U^*(t) = \frac{1}{R} \int_0^1 P_x(1,y,t)u^*(y,t)dy \quad (26)$$

where the time-varying linear transformation P^t must satisfy the following Riccati-like PDE:

$$-P_t = P_{xx} + P_{yy} + 2cP + Q - \frac{1}{R}P_y(x,1)P_x(1,y) \quad (27)$$

with boundary conditions

$$P(0,y,t) = P(1,y,t) = P(x,0,t) = P(x,1,t) = 0 \quad (28)$$

and final condition

$$P(x,y,T) = P_f(x,y) \quad (29)$$

Proof. The proof consists of evaluating each λ term in (7), (9), and (10) using the postulated form in (25) and applying

integration by parts. Let us begin by evaluating each term in (7):

$$\begin{aligned} \lambda_t &= \int_0^1 [P_t(x,y,t)u^*(y,t) + P(x,y,t)u_t^*(y,t)]dy \\ &= \int_0^1 [P_t(x,y,t)u^*(y,t) + P(x,y,t)u_{yy}^*(y,t) \\ &\quad + cP(x,y,t)u^*(y,t)]dy \end{aligned} \quad (30)$$

$$\lambda_{xx} = \int_0^1 P_{xx}(x,y,t)u^*(y,t)dy \quad (31)$$

$$c\lambda = \int_0^1 cP(x,y,t)u^*(y,t)dy \quad (32)$$

$$Q(u(x,t)) = \int_0^1 Q(x,y)u^*(y,t)dy \quad (33)$$

Now we apply integration by parts to the second term in (30):

$$\begin{aligned} \int_0^1 P(x,y,t)u_{yy}^*(y,t)dy &= P(x,1)u_y^*(1) - P(x,0)u_y^*(0) \\ &\quad - P_y(x,1)u^*(1) + P_y(x,0)u^*(0) \\ &\quad + \int_0^1 P_{yy}(x,y,t)u^*(y,t)dy \end{aligned} \quad (34)$$

Now apply the boundary condition $u^*(0) = 0$ in (8) and boundary control $u^*(1) = U^*(t) = \frac{1}{R} \int_0^1 P_x(1,y)u^*(y,t)dy$ in (11), where the second equality comes from the postulated form in (25). Plug (30)-(34) into the PDE for the co-state, which will be verified under the following conditions:

$$-P_t = P_{xx} + P_{yy} + 2cP + Q - \frac{1}{R}P_y(x,1)P_x(1,y) \quad (35)$$

$$P(x,1,t) = 0 \quad (36)$$

$$P(x,0,t) = 0 \quad (37)$$

Next we apply the postulated form (25) to the boundary conditions of the co-state PDE in (9). These equations will be verified under the following conditions for $P(x,y,t)$:

$$P(0,y,t) = 0 \quad (38)$$

$$P(1,y,t) = 0 \quad (39)$$

Finally, we apply the postulates form (25) to the final time condition of the co-state PDE in (10) which gives

$$P(x,y,t) = P_f(x,y) \quad (40)$$

and completes the proof.

Remark. Proving the well-posedness of the Riccati PDE (27)-(29) remains an open question. The key difficulty is the nonlinear nature (specifically the quadratic term) of this PDE. For the cases used to generate simulation results in Section 2.3, the Riccati PDE is well-posed.

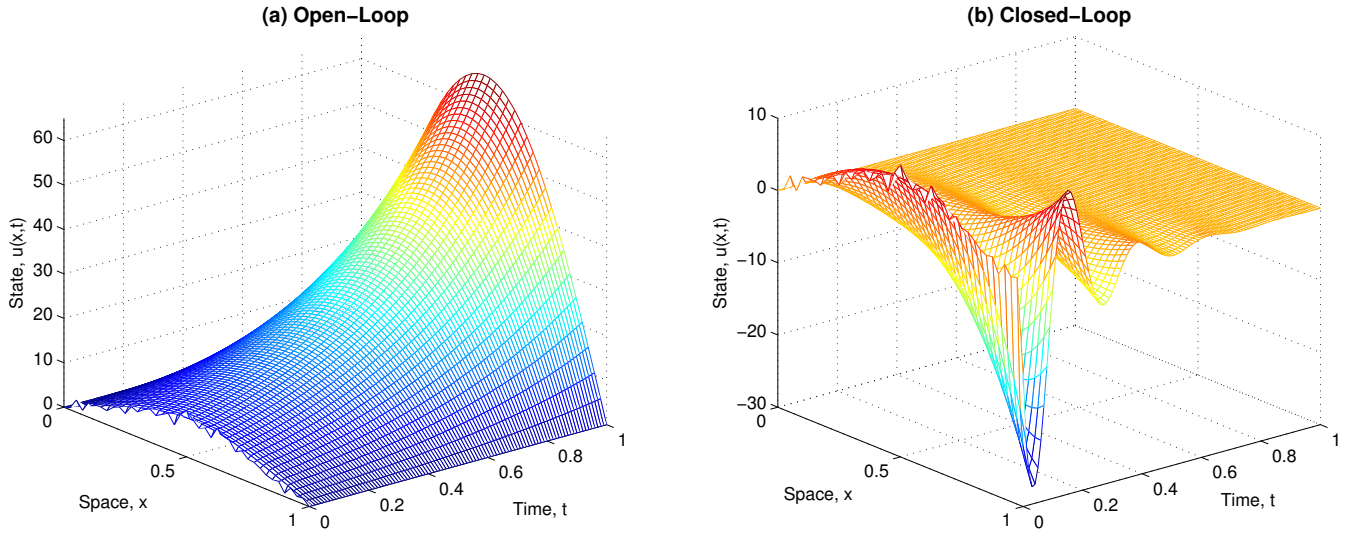


Fig. 2. Simulation example of state trajectories for the (a) open-loop and (b) closed-loop systems.

Remark. The infinite-time horizon LQR controller is given by the steady-state solution of the Riccati PDE. Namely,

$$P_{xx}^{\infty} + P_{yy}^{\infty} + 2cP^{\infty} + Q - \frac{1}{R}P_y^{\infty}(x,1)P_x^{\infty}(1,y) = 0 \quad (41)$$

with the homogenous boundary conditions (28). The solution of this algebraic Riccati PDE, denoted $P^{\infty}(x,y)$, produces the time-invariant state-feedback control law

$$U^*(t) = \frac{1}{R} \int_0^1 P_x^{\infty}(1,y) u^*(y,t) dy \quad (42)$$

2.3 Simulation Example

In this section we present simulation examples of the linear quadratic regulator. Until now the presented results are independent of the specific numerical scheme used to implement the controller. In this paper we use the central-difference method in space to solve PDEs. Throughout these

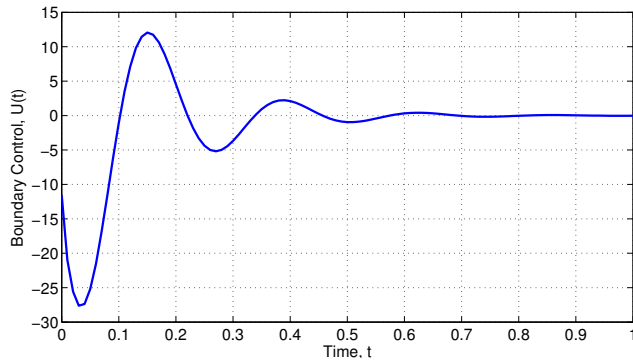


Fig. 3. Boundary control input for the LQR controller.

examples we consider the class of linear parabolic partial differential equation systems described by (1)-(4).

First, let us examine the plant in open-loop, i.e. when $U(t) = 0$. In open-loop one may use separation of variables to show the exact solution is given by

$$u(x,t) = 2 \sum_{n=1}^{\infty} e^{(c-\pi^2 n^2)t} \sin(\pi n x) \int_0^1 \sin(\pi n x) u_0(x) dx \quad (43)$$

The structure of this solution demonstrates that the eigenvalues are given by $c - \pi^2 n^2$ for $n = 1, 2, \dots$. Since the largest eigenvalue is given by $c - \pi^2$, we see that the plant is open-loop unstable for $c > \pi^2$.

Here we demonstrate the linear quadratic regulator results, where the optimal control is given by (26), and the time-varying linear operator $P(x,y,t)$ is the unique solution of the Riccati PDE (27)-(29). The parameters for this example are shown in Table 1. Note that the plant contains one unstable eigenvalue at $12 - \pi^2 \approx 2$.

The evolution of the state for the open and closed-loop systems are displayed in Fig. 2(a) and (b), respectively. Figure 2(a) visually demonstrates the unstable character of the

Table 1. Parameter Values for LQR Simulation Examples

Parameter	Value
Reaction coefficient	$c = 12$
State weight kernel	$Q(x,y) = 150 \sin(\pi x) \sin(\pi y)$
Control weight kernel	$R = 1$
Final state weight kernel	$P_f(x,y) = \sin(\pi x) \sin(\pi y)$
Time Horizon	$T = 1$

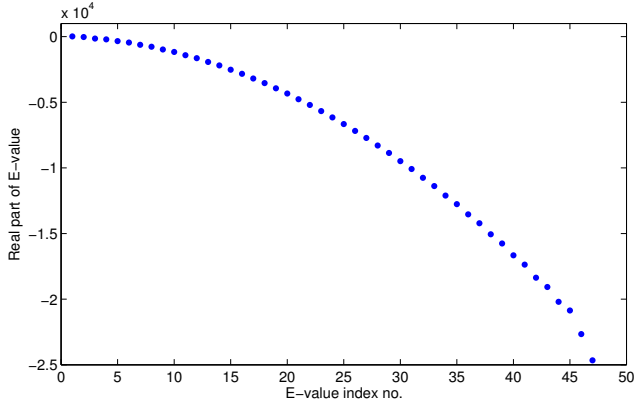


Fig. 4. Real part of eigenvalues for closed-loop spectrum of infinite-time LQR controlled system.

open-loop system. The state grows exponentially and takes the form of the eigenfunction corresponding to the unstable eigenvalue, namely $\sin(\pi x)$. In Fig. 2(b) the implemented LQR controller successfully regulates the state to the origin. Observe that the noisy initial condition is rapidly smoothed out in both cases, due to the diffusion operator. The optimal boundary control signal is shown in Fig. 3

3 Analysis of Infinite-Time LQR

3.1 Closed-loop Spectrum

Using separation of variables, one may show that the closed-loop spectrum for the infinite-time LQR controlled system is given by

$$\lambda_{lqr} = c - \beta^2 \quad (44)$$

where β is given by the solutions of

$$0 = \frac{1}{R} \int_0^1 P_x^\infty(1, y) \sin(\beta y) dy - \sin(\beta) \quad (45)$$

where $P^\infty(x, y)$ is the solution to the Riccati PDE (41) corresponding to the infinite-time LQR problem. Mathematically, one can see the eigenvalues have zero imaginary parts and negative real parts (for closed-loop stability). Moreover, the eigenvalues roughly increase toward $-\infty$ quadratically with index number, but need to be solved numerically. Figure 4 portrays this relationship graphically, for the infinite-time LQR controlled closed-loop system with parameters in Table 1.

3.2 Stability Robustness

Next we study if the LQR controller is robust to plant model uncertainty at the input. To this end, consider the open-loop transfer function from the plant's input $U(t)$ to the controller's output $\bar{U}(t)$, as shown in Fig. 5. To obtain the transfer function from $U(t)$ to $\bar{U}(t)$, we apply the Laplace

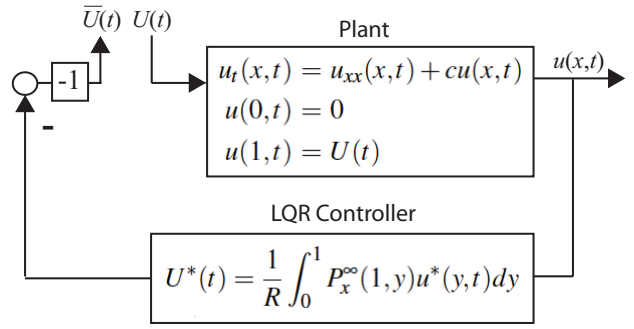


Fig. 5. Block Diagram for open-loop transfer function in negative feedback form to study stability robustness to uncertainty at the plant input.

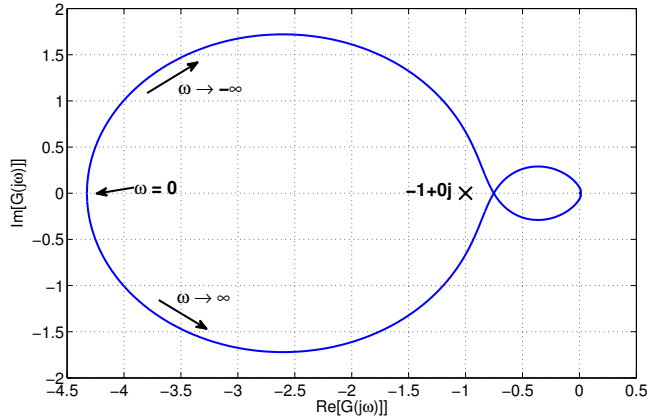


Fig. 6. Nyquist plot of $G(s)$, defined in (46).

transformation to the plant model PDE (1), solve the resulting second order ODE in x , and then apply the boundary conditions (2) and (42). The end result is

$$G(s) = \frac{\bar{U}(s)}{U(s)} = \frac{\int_0^1 P_x^\infty(1, y) \sin(\sqrt{c-s}y) dy}{R \sin(\sqrt{c-s})} \quad (46)$$

The Nyquist plot of $G(s)$, using parameters from Table 1, is provided in Fig. 6. Recall from Section 2.3 that the plant contains one unstable eigenvalue at $12 - \pi^2 \approx 2$. Therefore, according to the Nyquist Stability Criterion [25], the Nyquist plot of $G(s)$ must encircle the critical point $-1 + 0j$ once in the counter-clockwise direction for the closed-loop system to be stable. Indeed, this holds true in Fig. 6.

Gain and phase margins can be computed from the Nyquist plot. In the case of Fig. 6, the positive gain margin is 1.34 or 2.5 dB, the negative gain margin is 0.23 or -12.7 dB, and the phase margin is $\pm 25.2^\circ$. Note that the LQR controller for this diffusion-reaction PDE has smaller stability margins than the guaranteed stability margins (infinite positive gain margin and 60° phase margin) imposed by the return difference equality in finite-dimensional LQR controlled systems [26].

4 Relation to Existing Results

The LQR results derived in this paper have strong connections to existing results in PDE control. First, we discuss how the Riccati PDE (27)-(29) can be derived from the more general operator Riccati equation result. Secondly, we compare the proposed LQR results with PDE backstepping controller designs. Although these two control methods achieve similar results, the design paradigm is considerably different.

4.1 Operator Riccati Equations

A well-established result in optimal control for PDEs is the operator Riccati equation (ORE) [11–14]. This result begins by formulating the PDE model as a state-space system on an infinite-dimensional Hilbert space \mathcal{Z} in the following form:

$$\dot{z}(t) = \mathcal{A}z(t) + \mathcal{B}U(t) \quad (47)$$

$$z(0) = u(x, 0) \quad (48)$$

where the operator $\mathcal{A} : L^2(0, 1) \rightarrow \mathcal{Z}$ generates a C_0 -semigroup on \mathcal{Z} . The operator $\mathcal{B} : \mathbb{R} \rightarrow \mathcal{Z}$ maps the space of boundary control inputs into the Hilbert space \mathcal{Z} and is generally unbounded. The optimal state-feedback control w.r.t. the cost functional (5) is given by:

$$U^*(t) = -\mathcal{B}^*\Pi(t)z(t) \quad (49)$$

and $\Pi(t) = \Pi^*(t)$ is the solution to the ORE

$$-\frac{d}{dt}\Pi(t) = \mathcal{A}^*\Pi(t) + \Pi(t)\mathcal{A} + \Pi(t)\mathcal{B}R^{-1}\mathcal{B}^*\Pi(t) + Q \quad (50)$$

$$\Pi(T) = \mathcal{P}_f \quad (51)$$

where Q and \mathcal{P}_f are appropriately defined operators corresponding to Q and \mathcal{P}_f , respectively.

It is possible to show the Riccati operator $\Pi(t)$ has a representation of the form

$$[\Pi(t)u](x, t) = \int_0^1 P(x, y, t)u(y, t)dy \quad (52)$$

where the kernel $P(x, y, t)$ satisfies a Riccati PDE. Lions [11] shows this result using the Schwartz Kernel Theorem for several specific systems and cost functionals with distributed and Neuman boundary control. Hulsing [15] later extended this result to systems with Dirichlet and Robin boundary control by appropriately defining the operators \mathcal{A} and \mathcal{B} and substituting the functional representation (52) into the ORE (50).

Following the methods of Hulsing [15], one may derive the Riccati PDE (27)-(29) from the ORE (50). This process relies heavily upon concepts from functional analysis. In contrast, the weak-variational approach introduced in this paper derives Riccati PDEs directly from the PDE model and cost functional without requiring the abstract operator-theoretic notions associated with OREs.

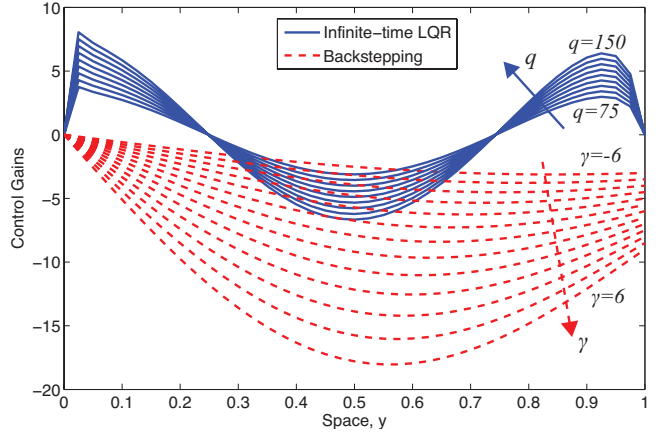


Fig. 7. Feedback control gains for the infinite-time LQR (solid lines) and backstepping (dashed) controllers. Parameter q corresponds to the state penalty: $Q(x, y) = q \sin(\pi x) \sin(\pi y)$. Parameter γ is the reaction coefficient in the backstepping target system (55).

4.2 Backstepping

In this section we compare the LQR results to a well-established boundary control technique - backstepping [16]. The heart of backstepping involves the design of a linear Volterra transformation that forces the closed-loop dynamics to an exponentially stable target system. The target system usually has a structure similar to the plant (e.g., the diffusion-reaction PDE for parabolic PDEs) with homogeneous boundary conditions. Like the methods presented here, backstepping ultimately involves the solution of a PDE related to the gain kernels. This so-called kernel PDE is usually linear, whereas the Riccati PDE is always quadratic. Explicit solutions to the backstepping kernel PDE can be found in some cases, whereas the Riccati PDE must always be solved numerically.

Consider the diffusion-reaction PDE model in (1)-(4). The backstepping method seeks to find the coordinate transformation

$$w(x, t) = u(x, t) - \int_0^1 k(x, y)u(y, t)dy \quad (53)$$

along with the feedback control

$$U(t) = \int_0^1 k(1, y)u(y, t)dy \quad (54)$$

which renders the model (1)-(4) into the target system

$$w_t(x, t) = w_{xx}(x, t) - \gamma w(x, t) \quad (55)$$

$$w(0, t) = 0 \quad (56)$$

$$w(1, t) = 0 \quad (57)$$

It has been shown in [16] that the backstepping control law

is

$$U(t) = - \int_0^1 (c + \gamma)y \frac{I_1(\sqrt{(c+\gamma)(1-y^2)})}{\sqrt{(c+\gamma)(1-y^2)}} u(y) dy \quad (58)$$

In Figure 7 the backstepping and infinite-time LQR control gains are shown for different values of γ and q , respectively. The two control gains have notably different characteristics. As γ and q increase, the magnitude of both control gains increases, since the state penalty in the optimization objective and stabilizing reaction term in the backstepping target system increase. Zero gain near $x = 0$ is logical due to the boundary condition $u(0) = 0$.

The critical difference between these two approaches lie in their design and computation. Namely, LQR design considers weighting kernels on the state and control, while backstepping designs a transformation that achieves a desirable target system. Computationally, LQR requires the solution of a quadratic PDE while backstepping requires the solution of a linear PDE.

5 Extensions to Other Plant Models

We now consider LQR designs for a broader class of PDE plant models. First, we consider diffusion-reaction systems with alternative boundary conditions. Table 2 summarizes the LQR results for these models. Next we consider the general reaction-advection-diffusion equation. Through an appropriate state transformation and scaling of time, we can render the reaction-advection-diffusion equation into the mathematical form we studied in Section 2. These extensions demonstrate how the LQR control design via weak-variations can be applied to a broad class of parabolic PDEs.

5.1 Alternative Boundary Conditions

To this point we have considered Dirichlet boundary conditions at the controlled and uncontrolled ends. In many physical problems Neumann boundary conditions are the appropriate modeling choice. Examples include thermal and chemical systems, where heat flux or ionic current densities are controlled. Combinations of Dirichlet and Neumann conditions are also physically meaningful, important plant models. LQR controllers for these systems can be derived using the same weak-variational approach in Section 2. The critical difference between each calculation is the evaluation of the appropriate boundary conditions when applying integration by parts. A summary of the Riccati PDEs corresponding to reaction-diffusion systems with various boundary conditions is provided in Table 2. For Dirichlet control or Neumann control the Riccati PDE remains the same, irrespective of the conditions at the uncontrolled end. The Riccati PDE's boundary conditions do change, however.

5.2 Reaction-Advection-Diffusion Equation

Next we demonstrate that it is possible to design an LQR controller for a general class of reaction-advection-diffusion

systems. Specifically, consider the following PDE, boundary conditions, and initial conditions:

$$u_t(x, t) = \epsilon u_{xx}(x, t) + bu_x(x, t) + cu(x, t) \quad (59)$$

$$u(0, t) = 0 \quad (60)$$

$$u(1, t) = U(t) \quad (61)$$

$$u(x, 0) = u_0(x) \quad (62)$$

We shall transform (59)-(62) into a form that is equivalent to the PDE (1)-(4) studied in Section 2. Specifically, we first eliminate the advection term by performing a state variable transformation found in the handbook by Polianin [27]. Then we scale time to eliminate the diffusion coefficient. The end result is a reaction-diffusion PDE, where the advection term and diffusion coefficient are absorbed into the reaction term coefficient.

Towards this goal, we first consider the following change of variables [27]:

$$v(x) = u(x)e^{\frac{b}{2\epsilon}x} \quad (63)$$

After taking temporal and spatial derivatives, it is easy to show that $v(x)$ must verify the following PDE:

$$v_t(x, t) = \epsilon v_{xx}(x, t) + \left(c - \frac{b^2}{4\epsilon}\right) v(x, t) \quad (64)$$

$$v(0, t) = 0 \quad (65)$$

$$v(1, t) = e^{\frac{b}{2\epsilon}} U(t) = V(t) = \text{control} \quad (66)$$

$$v(x, 0) = u_0(x)e^{\frac{b}{2\epsilon}x} \quad (67)$$

The second step is to scale time as follows:

$$\bar{t} = \epsilon t \quad (68)$$

which gives

$$v_{\bar{t}}(x, \bar{t}) = v_{xx}(x, \bar{t}) + \left(\frac{\epsilon c - b^2}{4\epsilon^2}\right) v(x, \bar{t}) \quad (69)$$

$$v(0, \bar{t}) = 0 \quad (70)$$

$$v(1, \bar{t}) = e^{\frac{b}{2\epsilon}} U(\bar{t}) = V(\bar{t}) = \text{control} \quad (71)$$

$$v(x, 0) = u_0(x)e^{\frac{b}{2\epsilon}x} \quad (72)$$

As a result, we arrive at a PDE whose form is identical to (1)-(4). As such, we can apply the exact same techniques to develop an infinite-dimensional LQR state feedback control for $V(\bar{t})$. Note that the cost functional (73) in the v -coordinate system retains its quadratic nature, but the weighting kernels take new definitions:

$$J = \frac{1}{2} \int_0^T [\langle v(x, \bar{t}), \bar{Q}(v(x, \bar{t})) \rangle + \bar{R}V^2(\bar{t})] d\bar{t} + \frac{1}{2} \langle v(x, T), \bar{P}_f(u(x, T)) \rangle \quad (73)$$

Table 2. Riccati PDEs for Reaction-Diffusion Plant with Dirichlet and Neumann Boudary Control

DIRICHLET CONTROL		NEUMANN CONTROL	
Plant PDE	Riccati PDE	Plant PDE	Riccati PDE
$u_t = u_{xx} + cu$	$-P_t = P_{xx} + P_{yy} + 2cP + Q - \frac{1}{\bar{R}}P_y(x,1)P_x(1,y)$	$u_t = u_{xx} + cu$	$-P_t = P_{xx} + P_{yy} + 2cP + Q - \frac{1}{\bar{R}}P(x,1)P(1,y)$
Plant B.C.'s	Riccati PDE B.C.'s	Plant B.C.'s	Riccati PDE B.C.'s
$u(0) = 0, u(1) = U(t)$	$P(0,y,t) = P(1,y,t) = P(x,0,t) = P(x,1,t) = 0$	$u(0) = 0, u_x(1) = U(t)$	$P(0,y,t) = P_x(1,y,t) = P(x,0,t) = P_y(x,1,t) = 0$
$u_x(0) = 0, u(1) = U(t)$	$P_x(0,y,t) = P(1,y,t) = P_y(x,0,t) = P(x,1,t) = 0$	$u_x(0) = 0, u_x(1) = U(t)$	$P_x(0,y,t) = P_x(1,y,t) = P_y(x,0,t) = P_x(x,1,t) = 0$
Final State Penalty	Riccati PDE Final Condition	Final State Penalty	Riccati PDE Final Condition
$P_f(x,y)$	$P(x,y,T) = P_f(x,y)$	$P_f(x,y)$	$P(x,y,T) = P_f(x,y)$

where

$$\bar{Q}(x,y) = e^{-\frac{b}{2\varepsilon}x}Q(x,y)e^{-\frac{b}{2\varepsilon}y} \quad (74)$$

$$\bar{R} = e^{-\frac{b}{\varepsilon}}R \quad (75)$$

$$\bar{P}_f(x,y) = e^{-\frac{b}{2\varepsilon}x}P_f(x,y)e^{-\frac{b}{2\varepsilon}y} \quad (76)$$

and satisfy the LQR assumptions $\bar{Q}(x,y) \geq 0$, $\bar{R} > 0$, $\bar{P}_f(x,y) \geq 0$. The final step is to apply the inverse transformations $U(t) = e^{-\frac{b}{2\varepsilon}V(\bar{t}/\varepsilon)}$. Consequently, we have shown that the optimal control methods developed in this article apply to a broad class of parabolic systems, including reaction-advection-diffusion PDEs with constant coefficients.

6 Conclusions

This paper presents a method for designing finite-time optimal controllers for boundary-controlled linear parabolic PDEs, oriented toward applied control engineers. The resulting Riccati PDEs are independent of the numerical implementation scheme and do not require semigroup theoretic notions. The critical conceptual tool we exploit to derive these results is a weak-variations principle. To begin, the paper focuses on diffusion-reaction systems with Dirichlet actuation. These results are demonstrated through simulation. We also analyzed the closed-loop characteristics of the infinite-time LQR controller and compared it to existing, well-established methods. Finally, we demonstrate how the Riccati PDE results are derived for a broad class of linear parabolic PDE systems. In this paper we restrict the presentation to LQR control of parabolic PDEs. However, the weak-variations derivation method is general to alternative PDE models, e.g. hyperbolic, wave, beam, etc. Future work may consider adaptive versions [28] of the controllers presented here. Ultimately, this paper provides fundamental optimal control methods that are accessible, constructive, elegant, computationally tractable, and intuitive to tune for practicing control engineers who study physical systems described by parabolic PDEs.

References

- [1] Avalos, G., and Lasiecka, I., 1996. "Differential Riccati equation for the active control of a problem in structural acoustics". *Journal of Optimization Theory and Applications*, **91**(3), pp. 695 – 728.
- [2] Aksikas, I., Fuxman, A., Forbes, J. F., and Winkin, J. J., 2009. "Lq control design of a class of hyperbolic pde systems: Application to fixed-bed reactor". *Automatica*, **45**(6), pp. 1542–1548.
- [3] Ferrari-Trecate, G., Buffa, A., and Gati, M., 2006. "Analysis of coordination in multi-agent systems through partial difference equations". *IEEE Transactions on Automatic Control*, **51**(6), pp. 1058 – 1063.
- [4] Zariphopoulou, T., 1999. "Optimal investment and consumption models with non-linear stock dynamics". *Mathematical Methods of Operations Research*, **50**(2), pp. 271 – 96.
- [5] Aamo, O. M., Krstic, M., and Bewley, T. R., 2003. "Control of mixing by boundary feedback in 2D channel flow". *Automatica*, **39**(9), pp. 1597 – 1606.
- [6] Vazquez, R., and Krstic, M., 2007. "Explicit output feedback stabilization of a thermal convection loop by continuous backstepping and singular perturbations". In 2007 American Control Conference, pp. 2177–2182.
- [7] Del Vecchio, D., and Petit, N., 2005. "Boundary control for an industrial under-actuated tubular chemical reactor". *Journal of Process Control*, **15**(7), pp. 771 – 784.
- [8] Doyle, M., Fuller, T., and Newman, J., 1993. "Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell". *Journal of the Electrochemical Society*, **140**(6), pp. 1526 – 33.
- [9] Fuller, T., Doyle, M., and Newman, J., 1994. "Simulation and optimization of the dual lithium ion insertion cell". *Journal of the Electrochemical Society*, **141**(1), pp. 1 – 10.
- [10] Forman, J., Bashash, S., Stein, J., and Fathy, H., 2011. "Reduction of an Electrochemistry-Based Li-Ion Battery Model via Quasi-Linearization and Padé Approx-

- imation”. *Journal of The Electrochemical Society*, **158**(2), pp. A93–A101.
- [11] Lions, J., and Mitter, S., 1971. *Optimal control of systems governed by partial differential equations*, Vol. 396. Springer Berlin.
- [12] Lasiecka, I., and Triggiani, R., 2000. *Control theory for partial differential equations: continuous and approximation theories*. Cambridge University Press.
- [13] Bensoussan, A., Da Prato, G., Delfour, M. C., and Mitter, S. K., 2007. *Representation and Control of Infinite Dimensional Systems*, 2nd ed. Birkhauser.
- [14] Curtain, R. F., and Zwart, H. J., 1995. *An introduction to infinite-dimensional linear systems theory*. Springer.
- [15] Hulsing, K., 1999. “Methods for Computing Functional Gains for LQR Control of Partial Differential Equations”. PhD thesis, Virginia Polytechnic Institute and State University.
- [16] Krstic, M., and Smyshlyaev, A., 2008. *Boundary control of PDEs: A Course on Backstepping Designs*. SIAM Advances in Design and Control series.
- [17] Di Domenico, D., Stefanopoulou, A., and Fiengo, G., 2010. “Lithium-ion battery state of charge and critical surface charge estimation using an electrochemical model-based extended Kalman filter”. *Journal of Dynamic Systems, Measurement and Control, Transactions of the ASME*, **132**(6).
- [18] Ravindran, S., 2000. “A reduced-order approach for optimal control of fluids using proper orthogonal decomposition”. *International Journal for Numerical Methods in Fluids*, **34**(5), pp. 425 – 48.
- [19] Xu, C., Ou, Y., and Schuster, E., 2011. “Sequential linear quadratic control of bilinear parabolic PDEs based on POD model reduction”. *Automatica*, **47**(2), pp. 418 – 426.
- [20] Park, H., and Kim, O., 2000. “Reduction method for the boundary control of the heat conduction equation”. *Journal of Dynamic Systems, Measurement and Control, Transactions of the ASME*, **122**(3), pp. 435 – 444.
- [21] Collinger, J., Wickert, J., and Corr, L., 2009. “Adaptive piezoelectric vibration control with synchronized switching”. *Journal of Dynamic Systems, Measurement and Control, Transactions of the ASME*, **131**(4), pp. 1 – 8.
- [22] Burns, J., and Hulsing, K., 2001. “Numerical methods for approximating functional gains in LQR boundary control problems”. *Mathematical and Computer Modelling*, **33**(1), pp. 89–100.
- [23] Moura, S., and Fathy, H., 2011. “Optimal Boundary Control & Estimation of Diffusion-Reaction PDEs”. In American Control Conference (ACC), 2011, pp. 921–928.
- [24] Bernstein, D. S., and Tsiotras, P., 2009. *A Course in Classical Optimal Control*. Pre-print.
- [25] Kuo, B., and Golnaraghi, F., 2003. *Automatic Control Systems*. No. v. 1 in Automatic Control Systems. John Wiley & Sons.
- [26] Freudenberg, J. S., 2008. *A First Graduate Course in Feedback Control*. University of Michigan, EECS 565.
- [27] Polianin, A. D., 2002. *Handbook of linear partial differential equations for engineers and scientists*. CRC Press LLC.
- [28] Smyshlyaev, A., and Krstic, M., 2007. “Adaptive boundary control for unstable parabolic PDEs-Part II: Estimation-based designs”. *Automatica*, **43**(9), pp. 1543–1556.