Low-Order Optimal Regulation of Parabolic PDEs with Time-Dependent Domain

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Observer and optimal boundary control design for the objective of output tracking of a linear distributed parameter system given by a two-dimensional (2-D) parabolic partial differential equation with time-varying domain is realized in this work. The transformation of boundary actuation to distributed control setting allows to represent the system's model in a standard evolutionary form. By exploring dynamical model evolution and generating data, a set of time-varying empirical eigenfunctions that capture the dominant dynamics of the distributed system is found. This basis is used in Galerkin's method to accurately represent the distributed system as a finite-dimensional plant in terms of a linear time-varying system. This reduced-order model enables synthesis of a linear optimal output tracking controller, as well as design of a state observer. Finally, numerical results are prepared for the optimal output tracking of a 2-D model of the temperature distribution in Czochralski crystal growth process which has nontrivial geometry. *AIChE J*, 61: 494–502, 2015
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Introduction

The synthesis and treatment procedures in many industrial plants including chemical, petrochemical, and pharmaceutical processes, lead to changes in the shape and material properties. This change in material can be characterized by transport phenomena associated with the material deformation, phase change mechanism, generation and consumption of chemical species through chemical reactions, heat and mass transfer. Mathematically, a broad collection of these processes is modeled by application of conservation laws and yield models in the form of moving boundary parabolic partial differential equations (PDEs). Methods for control of linear parabolic PDEs have been extensively studied in the past and have mainly focused on process systems with fixed spatial domains and boundary and/or distributed actuations. Specifically, the functional analytic formulation using semigroup theory and related concepts have proven to be a powerful tool for system analysis and control design.[1,2] Regarding process models with moving boundaries, it is established that parabolic PDE systems with time-varying domains are inherently nonautonomous.[3] In this context, there are several contributions which formulate the solutions to nonautonomous parabolic PDE systems with fixed spatial domain in terms of two-parameter semigroups which resemble the standard one-parameter semigroup generated by time-invariant parabolic operators.[4–6] However, in general an analytic expression for the two-parameter semigroup describing the nonautonomous system behavior can not be found, which prevents direct analysis and controller synthesis. In addition, only few contributions have reported the study of parabolic PDEs with time-varying domain, in which main results are focused on establishing existence and regularity properties of the solution. These include development of transformations to map the PDE onto a new time-invariant spatial domain[7–9] and evolution of continuously differentiable diffeomorphisms.[3,10] Among contributions along this line, a design of nonlinear distributed state observers for systems with moving boundaries using stochastic methods[11] is notable. In particular, Wang studied stabilization and optimal control problem of such systems[12] and later on synthesized the linear optimal controller for thermal gradient regulation of crystal growth processes.[13] Ng and Dubljevic presented a moving boundary PDE as an abstract evolution equation on an infinite-dimensional function space with nonautonomous parabolic operator which generates a two-parameter semigroup. With this formulation, they posed the time-varying optimal control[14] and optimal boundary control[15] problems for regulation of a parabolic PDE. However, the setting in[14,15] accounts only for a well-defined one-dimensional (1-D) or two-dimensional (2-D) time-varying trivial square domain while more practically motivated and physically relevant cases of irregular domain evolution are not addressed.

Another notable approach in the linear/semilinear PDE control area is the backstepping method emerging from nonlinear finite-dimensional control systems synthesis. In this methodology, a Volterra-type integral transformation is used to transform the PDE to a suitably selected stable target system. The

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kernel of transformation is defined by the solution of the kernel PDE that is of higher-order in space, leading to a state-feedback control law.[16] This technique provides a framework to handle a large class of distributed parameter systems controlled at the boundary, however, the complexity associated with finding the solution of the kernel PDE for distributed systems described in 2-D or three-dimensional (3-D) spaces prevents the use of this method for such problems.

Dissipative parabolic PDE systems have the property that the eigenspectrum of the spatial differential operator can be partitioned into a finite-dimensional slow subspace and the infinite-dimensional fast and stable complement, which implies that the dynamic behavior of such processes can be approximately described by finite-dimensional systems. Hence, if eigenfunctions of the parabolic operator can be expressed explicitly, one can use Galerkin's method to derive a reduced-order model (ROM) in terms of ordinary differential equations (ODEs) that accurately describe the dominant dynamics of the distributed parameter system and subsequently use it for the controller synthesis. Low-dimensional model identification of distributed parameter systems governed by parabolic PDEs attracted attention of a significant number of researchers in recent years. Among many, the most notable contributions came from Ray and coworkers,[17,18] Park and Cho,[19] Christofides and coworkers,[20,21] and Hoo and coworkers.[22,23] However, there is no analytic solution to the operator eigenvalue problem in general, the examples being the nonlinear spatial operator or problems with nontrivial geometric domain. In such cases, a well-known approach in the extraction of spatial characteristics (modes) of distributed parameter systems is the use of statistical tools, specifically the Karhunen–Loève (KL) decomposition on an ensemble of solutions of the system obtained by numerical resolution or experiments.[19] These modes, known as empirical eigenfunctions, can be adopted as the basis set of functions in the Galerkin's method to find a ROM. This approach is widely used in the derivation of accurate reduced-order approximations of many distributed parameter systems, for example, diffusion-reaction systems,[24–26] sheet-forming processes,[27] molten carbonate fuel cell model,[28] thermal microsystem models[29] and ground-water flow model.[30]

To obtain a ROM of parabolic PDE systems with a moving boundary domain, Armaou and Christofides used a mathematical transformation to represent the PDE on a time-invariant spatial domain and applied KL decomposition to find the set of eigenfunctions on the fixed domain.[31] In application, they used this approach in the nonlinear feedback[32] and robust[33] control of 1-D reaction-diffusion systems based on the use of Galerkin's method. However, this approach cannot be used in general, since the mathematical transformation does not always have an analytical form, for example, for nontrivial geometry. Recently, a more generalized approach to reduce the order of PDE systems with time-varying domain has been proposed,[34] in which the transformation that preserves the space-invariant properties of PDE solutions is found and the ensemble of the solution to the PDE is mapped to a selected fixed reference configuration. Subsequently, KL decomposition is applied on the mapped data to extract a low-dimensional set of eigenfunctions that contains most of the energy of the system on the fixed domain. These eigenfunctions are mapped on the time-varying domain using inverse transformation and as a result, a set of time-varying empirical eigenfunctions are obtained that can be used in Galerkin's method.

In this work, we develop a methodology to design an observer and to find an optimal control law for output tracking of linear parabolic distributed systems with nontrivial time-varying domain. As the boundary actuation of PDE systems rather than the distributed input is more realistic in applications, the boundary input control problem is formulated as finding the appropriate state-space representation of the PDE system. Then, the proposed method of model order reduction by empirical eigenfunctions on the time-varying domain is used. Although this approach can be used for general nonlinear parabolic PDE systems, we consider the order reduction of boundary actuated linear dissipative distributed parameter systems with subsequent realization of observer to synthesize a linear optimal output tracking controller. Finally, numerical results are prepared for a 2-D model of temperature distribution in the industrially relevant Czochralski (CZ) crystal growth process.

Mathematical Formulation

In this section, the mathematical aspects of the proposed method are reviewed. In particular, a general description of the parabolic PDE on the moving boundary domain and boundary actuation is presented. Then, the order reduction methodology is briefly reviewed followed by the optimal control formulation. Finally, the design of the state observer is considered.

Model description

We are interested in the model dynamics of an extensive property

$$G(t)=\int_{\Omega(t)} \rho(\xi,t)\sigma x(\xi,t)d\Omega$$

given by the scalar intensive property $x(\xi,t)$ at each point $\xi \in \Omega(t) \subset \mathbb{R}^n$ at time $t \in [0,t_f]$, where $\rho(\xi,t)$ is density and σ is a constant. The body $\Omega(t)$ under consideration has the velocity $v(\xi,t)$ and its boundary is denoted by $\Gamma(t)$. With the use of the Leibniz integral rule and divergence theorem, conservation of the property $G(t)$ for continuous media ($\nabla \cdot v=0$) is governed by the following parabolic PDE[14]

$$\rho\sigma\frac{\partial x}{\partial t}=\nabla\cdot(\kappa\nabla x)-\rho\sigma v\cdot\nabla x \tag{1}$$

where κ is diffusivity. This equation describes the differential form of a diffusion-convection process dynamics in terms of the property (state) $x(\xi,t)$ in the time-varying domain $\Omega(t)$. Initial conditions are given by $x(\xi,0)=x_0(\xi)$ and actuations $q_i(t)$ are applied to m portions of the domain boundary in the following form

$$\kappa n\cdot\nabla x=q_i \text{ on } \Gamma_i^{\mathrm{a}} \text{ for } i=1,2,\ldots,m \tag{2}$$

Other boundary conditions are given as Neumann or Dirichlet boundary conditions, respectively, as

$$\begin{aligned}\kappa n\cdot\nabla x=0 \text{ on } \Gamma^{\mathrm{n}}\\ x=0 \text{ on } \Gamma^{\mathrm{d}}\end{aligned} \tag{3}$$

In these equations n is the normal outward vector at each point on the $\Gamma(t)$.

It is assumed that the evolution of the domain $\Omega(t)$ is smooth and known *a priori*, as it can be easily measured in many chemical and material process systems. In the example of the model of industrial CZ semiconductor crystal growth, there are robust control practices in achieving a desired crystal shape by manipulating the pulling rate of the crystal from the melt and other control inputs (see the work of Abdollahi et al.[35] and series of studies by Gevelber et al.[36–39] for more details). Hence, the PDE domain evolution is considered independent of the thermal field and the mentioned assumption is valid in this case. Furthermore, we assume that the solution of the PDE (1) is unique and sufficiently smooth.

Boundary control formulation

In many relevant control applications, boundary actuation is more realistic than distributed control within spatial domain. The following formulation[19,40,41] converts the boundary control problem to a distributed control problem. In particular, the transformation

$$x(\xi,t)=p(\xi,t)+\sum_{i=1}^{m} b_i(\xi,t)q_i(t) \tag{4}$$

introduces the new state variable $p(\xi,t)$ along with m functions $b_i(\xi,t)$ that determine the spatial contribution of each actuation $q_i(t)$, where m is the number of actuators on the boundary, see (2). Rewriting (1–3) leads to the following PDE with initial and boundary conditions

$$\begin{aligned}
\rho\sigma\frac{\partial p}{\partial t}&=\nabla\cdot(\kappa\nabla p)-\rho\sigma v\cdot\nabla p-\rho\sigma\sum_{i=1}^{m} b_i\dot{q}_i\\
p(\xi,0)&=x_0(\xi)\\
\kappa n\cdot\nabla p&=0 \text{ on } \Gamma^{\mathrm{n}}\bigcup_{i=1}^{m}\Gamma_i^{\mathrm{a}}\\
p&=0 \text{ on } \Gamma^{\mathrm{d}}
\end{aligned} \tag{5}$$

providing that the function $b_i(\xi,t)$ satisfies

$$\begin{aligned}
\rho\sigma\frac{\partial b_i}{\partial t}&=\nabla\cdot(\kappa\nabla b_i)-\rho\sigma v\cdot\nabla b_i\\
b_i(\xi,0)&=0\\
\kappa n\cdot\nabla b_i&=1 \text{ on } \Gamma_i^{\mathrm{a}}\\
\kappa n\cdot\nabla b_i&=0 \text{ on } \Gamma^{\mathrm{n}}\\
b_i&=0 \text{ on } \Gamma^{\mathrm{d}}
\end{aligned} \tag{6}$$

for $i=1,2,\ldots,m$ with an over dot representing differentiation with respect to time. Note that (5) is a distributed parameter system actuated by distributed inputs $\dot{q}_i$ and functions $b_i(\xi,t)$ are the solutions to (6). Equations 5 can be written in the state-space form as

$$\begin{aligned}
\frac{\partial p}{\partial t}&=\mathscr{A}p-\bar{B}u\\
p(\xi,0)&=x_0(\xi)
\end{aligned} \tag{7}$$

where $\mathscr{A}$ is the spatial differential operator with given boundary conditions, $\bar{B}=[b_1 b_2 \cdots b_m]$ and

$$u=\dot{q}=[\dot{q}_1\dot{q}_2\cdots\dot{q}_m]^T \tag{8}$$

Order reduction of the infinite-dimensional system

In this section, the ROM of the infinite-dimensional system described by (7) is developed. To this end, we follow the methodology proposed by authors[34] for the PDE given by (5). This

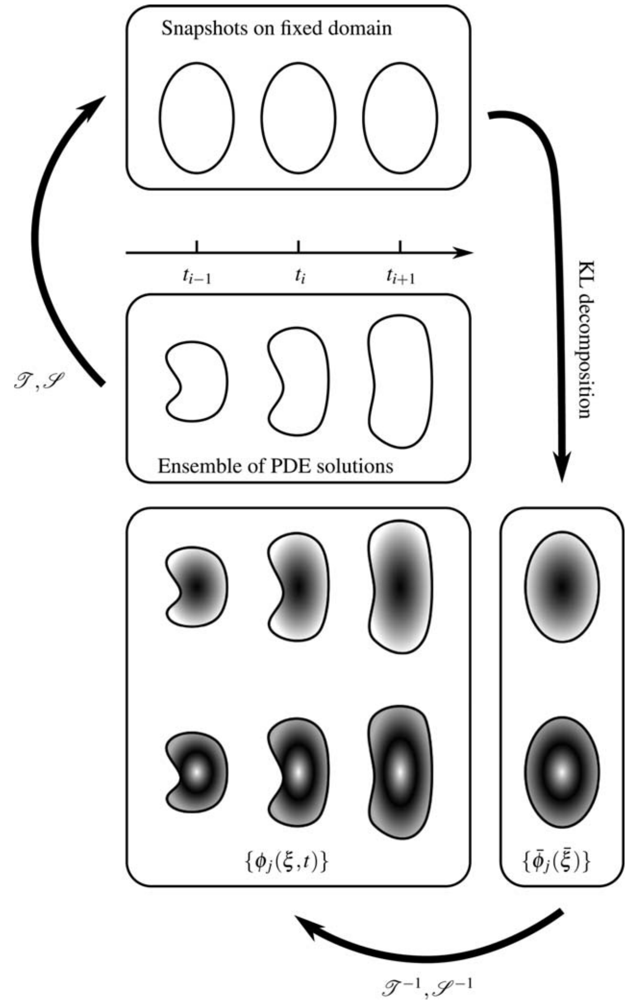

Figure 1. Schematics of the order-reduction approach: the transformations $\mathscr{T}(t)$ and $\mathscr{S}(t)$ map geometry and state of the PDE solution to a fixed domain.

Using KL decomposition, empirical eigenfunctions $\{\bar{\phi}_j(\bar{\xi})\}$ are extracted on the fixed domain and transformed to the time-varying domain by the application of $\mathscr{T}$ and $\mathscr{S}$ resulting in the time-varying basis $\{\phi_j(\xi,t)\}$.

approach, schematically depicted in Figure 1, yields to a set of time-varying empirical eigenfunctions $\{\phi_j(\xi,t)\}, j=1,2,\cdots,M$ that capture the most energy of the ensemble of solutions (snapshots) $\{p(\xi,t_i)\}, i=1,2,\cdots,N\gg M$. The fact that eigenfunctions are inherently time-varying is due to their moving boundary domain.

There exists the invertible smooth mapping $\mathscr{T}(t)$ that maps the domain $\Omega(t)$ to a fixed reference configuration $\bar{\Omega}$ as $\mathscr{T}(t):\xi\in\Omega(t)\mapsto\bar{\xi}\in\bar{\Omega}$ at each time t as shown in Figure 2, with the coordinate transformation $\bar{\xi}=\bar{\xi}(\xi,t)$ and the Jacobian matrix $[J(t)]=\frac{\partial\bar{\xi}}{\partial\xi}$.

Also, the transformation $\mathscr{S}(t_i)$ given by $\bar{p}_i(\bar{\xi})=p(\xi,t_i)J_i^{-1}$ maps the snapshot $p(\xi,t_i)$ on the moving boundary domain to $\bar{p}_i(\bar{\xi})$ on the fixed domain such that $\sigma p d\Omega=\sigma\bar{p}d\bar{\Omega}$, that is the space-invariant property $\sigma p d\Omega$ is preserved.[34] Given the ensemble $\{\bar{p}_i(\bar{\xi})\}$ on the reference configuration, KL decomposition can be applied to find the empirical eigenfunctions $\{\bar{\phi}_j(\bar{\xi})\}$ that can approximate each snapshot. KL decomposition is a procedure for representation of a stochastic field with a minimum number of degrees of freedom.[42,43]

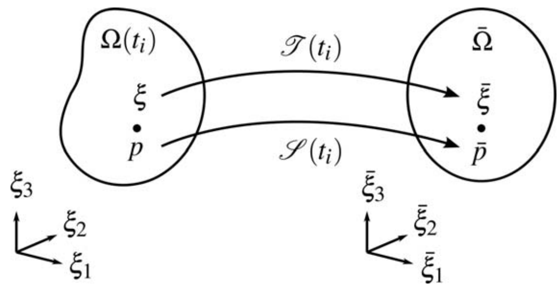

Figure 2. At each time instance t_i, $\mathscr{T}(t_i)$ maps moving boundary domain Ω to the fixed domain $\bar{\Omega}$ and the transformation $\mathscr{S}(t_i)$ maps the state $p(\xi, t_i)$ from time-varying domain to $\bar{p}_i(\xi)$ on the fixed domain.

Once the set of M eigenfunctions $\{\bar{\phi}_j(\bar{\xi})\}$ is found, they can be transformed to the time-varying domain $\Omega(t_i)$ at each time t_i using the inverse of $\mathscr{S}(t_i)$. Therefore, we have the basis of M time-varying eigenfunctions $\{\phi_j(\xi,t)\}$ which can be used to approximate the state p on the moving boundary domain $\Omega(t)$ as

$$p(\xi,t)=\sum_{i=1}^{M} a_i(t)\phi_i(\xi,t) \tag{9}$$

Finally, Galerkin's method is used to obtain the ROM by replacing (9) in (7) and projecting on the basis ϕ_j to get

$$\begin{aligned}\dot{a}(t)&=A(t)a(t)+B(t)u(t)\\ a(0)&=D^{-1}(0)y^0\end{aligned} \tag{10}$$

with terms defined as follows

$$\begin{aligned}a(t)&=[a_1(t)a_2(t)\cdots a_M(t)]^T\\ A(t)&=D^{-1}(t)H(t)\\ B(t)&=D^{-1}(t)F(t)\\ D_{ij}(t)&=<\phi_i,\phi_j>\\ H_{ij}(t)&=<\mathscr{A}\phi_i-\dot{\phi}_i,\phi_j>\\ F_{ij}(t)&=-<b_i,\phi_j>\\ y_i^0&=<x_0,\phi_i(\xi,0)>\end{aligned}$$

Equations 10 represent the reduced-order form of (7), which is a linear time-varying model of the process.

Optimal output tracking formulation

The control objective is to find a control law $u(t)$ based on the ROM (10), for which the PDE system state $x(\xi_i,t)=y_i$ at arbitrary points ξ_i, $i=1,2,\cdots,s$, tracks desired reference trajectories $y_i^r=x^r(\xi_i,t)$. Since the state $x(\xi,t)$ is described by $p(\xi,t)$ and boundary actuations $q_i(t)$ (see Eq. 4), the extended state is introduced as $a^e=[a^T q^T]^T$ and the boundary control problem is given by

$$\dot{a}^e(t)=A^e(t)a^e(t)+B^e(t)u(t) \tag{11}$$

$$a^e(0)=\left[a^T(0)q^T(0)\right]^T \tag{12}$$

where

$$A^e(t)=\begin{bmatrix}A(t) & 0\\ 0 & 0\end{bmatrix}, B^e(t)=\begin{bmatrix}B(t)\\ I\end{bmatrix}$$

and I is the identity matrix. Now, one may evaluate the state (4) at points ξ_j to get

$$y(t)=C(t)a^e(t) \tag{13}$$

which is considered as the system output equation, with

$$\begin{aligned}C(t)&=\left[\,\Phi(t)\bar{C}(t)\,\right]\\ \Phi_{ij}(t)&=\phi_i(\xi_j,t)\\ \bar{C}_{ij}(t)&=b_i(\xi_j,t)\end{aligned}$$

Equations 11 and 13 describe the extended system with an initial condition (12).

One can formulate the control problem as a classical linear optimal output tracking control problem for the process described by Eqs. (11–13) by minimizing the finite time linear quadratic cost functional

$$J=\frac{1}{2}\tilde{y}^T(t_f)P\tilde{y}(t_f)+\frac{1}{2}\int_0^{t_f}\left(\tilde{y}(t)^TQ\tilde{y}(t)+u(t)^TRu(t)\right)dt$$

where $\tilde{y}=y-y^r$. The optimal control is a time-varying linear state-feedback control law given by[44]

$$u(t)=-\kappa(t)a^e(t)+\omega(t) \tag{14}$$

where $\kappa(t)=R^{-1}B^{eT}(t)S(t), \omega(t)=R^{-1}B^{eT}(t)w(t)$, the real symmetric and positive-definite matrix S is the solution of the differential Riccati equation

$$\begin{aligned}-\dot{S}(t)&=A^{eT}(t)S(t)+S(t)A^e(t)-S(t)B^e(t)R^{-1}B^{eT}(t)S(t)+C^T(t)QC(t),\\ S(t_f)&=C^T(t_f)PC(t_f)\end{aligned}$$

and the vector $w(t)$ is the solution of the linear vector differential equation

$$\begin{aligned}-\dot{w}(t)&=\left[A^e(t)-B^e(t)R^{-1}B^{eT}(t)S(t)\right]^Tw(t)+C^T(t)Qy^r(t)\\ w(t_f)&=C^T(t_f)Py^r(t_f)\end{aligned}$$

Replacing (14) into (11) yields the following

$$\dot{a}^e(t)=(A^e(t)-B^e(t)\kappa(t))a^e(t)+B^e(t)\omega(t)$$

Let $\bar{A}(t)=A^e(t)-B^e(t)\kappa(t)$, the controllability of the process results in exponential stability of $\dot{a}^e(t)=\bar{A}(t)a^e(t)$ which guarantees the existence of a continuously differentiable symmetric bounded positive definite matrix $\Pi_1(t)$ that satisfies the differential Lyapunov equation

$$-\dot{\Pi}_1(t)=\Pi_1(t)\bar{A}(t)+\bar{A}^T(t)\Pi_1(t)+\chi_1(t) \tag{15}$$

where $\chi_1(t)$ is a continuous, symmetric, and positive definite. Hence, the candidate $V_1(a^e,t)=a^{eT}\Pi_1a^e$ is the Lyapunov function with time-derivative $\dot{V}_1=-a^{eT}\chi_1a^e$.

Observer design

In practice, state variables may not be accessible for the application of state-feedback control (14), specifically, the ROM state $a(t)$ cannot be measured or physically interpreted. However, the finite-dimensional representation (10) provides tools for state estimation where the measurements of physical properties are usually available at domain boundaries in applications. In this section, a state observer is designed to be used in the closed-loop setup depicted in Figure 3. This controller-observer configuration is chosen due to the fact that the PDE deriving signal $q(t)$ can be determined by integration of an input signal $u(t)$ from (8), hence, there is no

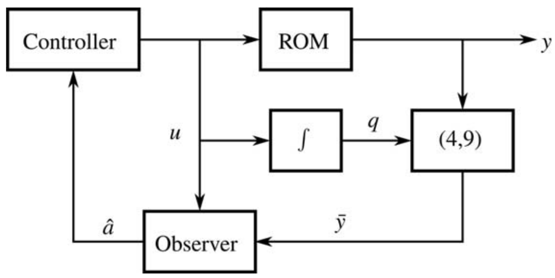

Figure 3. Block diagram representation of the controller-observer setup.

need to estimate $q(t)$ in the extended state $a^e(t)$. Also, having the measurement $y(t)$ and the knowledge of $q(t)$, one can determine the new output variable $\bar{y}(t)=\Phi(t)a(t)$ from (4,9).

Now the open-loop Luenberger-type observer with time-varying gain $\lambda(t)$ is introduced as

$$\dot{\hat{a}}(t)=A(t)\hat{a}(t)+B(t)u(t)+\lambda(t)(\bar{y}(t)-\Phi(t)\hat{a}(t))$$

with the estimation error $e(t)=a(t)-\hat{a}(t)$. It can be readily shown that the error dynamics is given by

$$\dot{e}(t)=(A(t)-\lambda(t)\Phi(t))e(t) \tag{16}$$

Although the matrices A and Φ are time-dependent, the continuous observer gain $\lambda(t)$ can be evaluated at each time instance t such that $A(t)-\lambda(t)\Phi(t)$ becomes time-independent with (stable) eigenvalues placed at desired pre-specified values. Therefore, there exists symmetric positive definite time-independent matrices Π_2 and χ_2 that satisfy the Lyapunov equation

$$\Pi_2(A(t)-\lambda(t)\Phi(t))+(A(t)-\lambda(t)\Phi(t))^T\Pi_2+\chi_2=0 \tag{17}$$

and the Lyapunov function $V_2(a)=a^T\Pi_2 a$ with time-derivative $\dot{V}_1=-a^T\chi_2 a$ implies the exponential stability of (16).

Now, the state-feedback gain $\kappa(t)$ is partitioned as

$$u(t)=-\begin{bmatrix}\kappa_1(t) & \kappa_2(t)\end{bmatrix}\begin{bmatrix}\hat{a}(t)\\ q(t)\end{bmatrix}+\omega(t)$$

which develops the following state-equation for the overall system shown in Figure 3:

$$\begin{bmatrix}\dot{a}\\ \dot{q}\\ \dot{e}\end{bmatrix}=\begin{bmatrix}A-B\kappa_1 & -B\kappa_2 & B\kappa_1\\ \kappa_1 & -\kappa_2 & \kappa_1\\ 0 & 0 & A-\lambda\Phi\end{bmatrix}\begin{bmatrix}a\\ q\\ e\end{bmatrix}+\begin{bmatrix}B\\ I\\ 0\end{bmatrix}\omega \tag{18}$$

Consider the continuously differentiable function

$$V(a,q,e,t)=\begin{bmatrix}a^T & q^T & e^T\end{bmatrix}\begin{bmatrix}\Pi_1 & 0\\ 0 & \Pi_2\end{bmatrix}\begin{bmatrix}a\\ q\\ e\end{bmatrix}$$

which is a valid Lyapunov function candidate. It can be shown that its time derivative is given by

$$\dot{V}=-\begin{bmatrix}a^T & q^T & e^T\end{bmatrix}\chi\begin{bmatrix}a\\ q\\ e\end{bmatrix}$$

where

$$\chi=\begin{bmatrix}\chi_1 & -2\Pi_1\begin{bmatrix}B\kappa_1\\ \kappa_1\end{bmatrix}\\ 0 & \chi_2\end{bmatrix}$$

All matrices defining χ are continuous and bounded. Moreover, at each time instance the eigenvalues of χ are the union of eigenvalues of positive definite matrices χ_1 and χ_2. So χ is positive definite and V is indeed a Lyapunov function that implies the exponential stability of the dynamics of (18). Thus inserting the observer does not affect the original state-feedback law and it can be designed separately.

Numerical Simulation

In this section, the results from previous section are applied to the boundary control of a 2-D representation of CZ crystal depicted in Figure 4. The CZ process is one of the main methods in the manufacturing of semiconductor materials on a large-scale for the use in modern photovoltaic and high performance electronic devices, such as microprocessors and microcontrollers. In this process, a mechanical arm simultaneously rotates and vertically drags out the crystal rod from the surface ($z=0$) of a heated pool of melt contained in a crucible. One can observe that the shape of the gradually grown crystal is nontrivial.

Temperature distribution in the grown crystalline material is modeled by the form of the PDE given in (1) with the heaters located around the surface of the solid crystal as boundary actuators. We consider the axisymmetric diffusive system described by the following nondimensionalized parabolic PDE[14,45]

$$\frac{\partial x}{\partial t}=k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x}{\partial r}\right)+\frac{\partial^2 x}{\partial z^2}\right]-\dot{L}\frac{\partial x}{\partial z} \tag{19}$$

for $x(r,z,t)$ being the temperature in the time-varying domain $\Omega(t)$ subject to boundary actuations $q_i(t)$ on two portions of

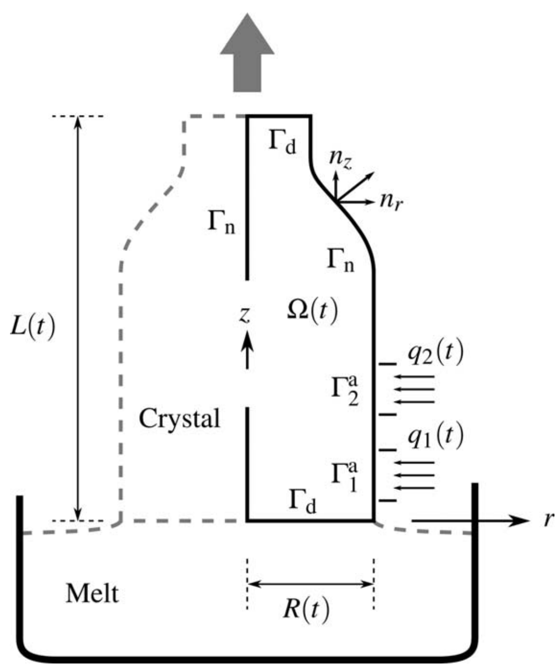

Figure 4. Schematic representation of axisymmetric crystal domain in CZ growth process where *L*(*t*) and *R*(*t*) are the height and radius of crystal at time *t*, respectively.

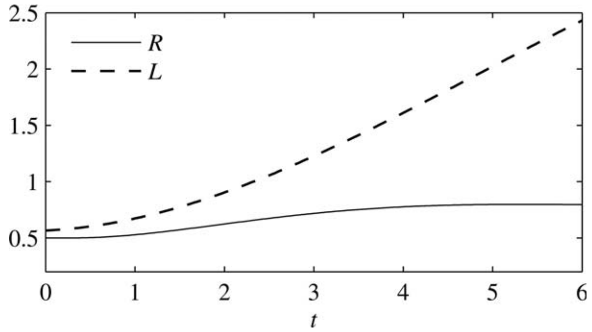

Figure 5. Domain evolution result from radius control strategy.

the domain boundary Γ_i^a, $i=1$, 2 and Neumann and Dirichlet boundary conditions. In (19), $k=6.25$ is the dimensionless process parameter and $\dot{L}(t)$ represents the domain velocity which is the derivative of the height function $L(t)$ with respect to time. A simplified radius control strategy arising from geometric model provides the domain evolution in terms of $L(t)$ and $R(t)$ as shown in Figure 5, see the work of Abdollahi et al.[35] for more details.

We developed a finite element model (FEM) that is used to find the solutions to the aforementioned PDE, as well as using as a process plant to apply the synthesized control. As the geometry of the domain is time-varying and the evolution is known, the Arbitrary Lagrangian Eulerian mesh moving scheme is used in formulating FEM.[46] The domain of interest is spatially discretized by 11 × 29 2-D linear four-node elements into 297 degrees of freedom. The evolution of the time-dependent set of ODEs obtained from the finite element discretization is realized by first-order implicit time integration with the time step $dt=0.0333$. Figure 6 shows the schematics of moving elements and functions $b_1(r,z,t)$ and $b_2(r,z,t)$ obtained from the solutions to corresponding PDEs by FEM.

The reference configuration $\bar{\Omega}$ on which the solutions of (19) are mapped for the order reduction purpose is considered to be a rectangular with dimensions $\bar{R}=0.7$ and $\bar{L}=1.25$. The mapping $\mathscr{T}(t_i)$ can be numerically constructed by introducing sets of computational grid points on the moving boundary domain and reference configuration at time instance t_i. Associating each grid point of the time-varying domain to a grid point on the fixed-domain defines the one-to-one and onto (and hence invertible) mapping. Note that the Jacobian matrix of transformation in this case is space-dependent.

To apply KL decomposition on the ensemble of snapshots mapped on the fixed domain, we used Schmidt–Hilbert technique which assumes that each eigenfunction is a linear combination of all snapshots. This will result in solving the eigenvalue problem of the snapshots correlation matrix with a size as large as the number of snapshots. We used Arnoldi algorithm to solve the large matrix eigenvalue problem to reduce computational costs.[34] We chose three empirical

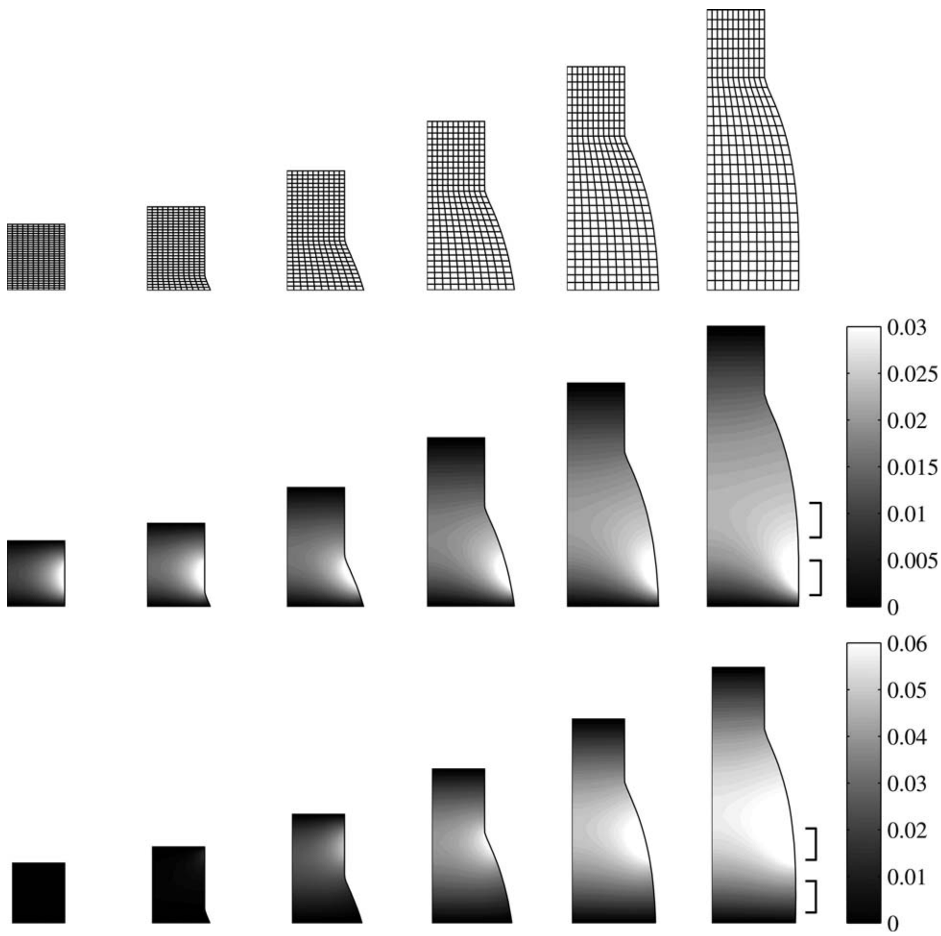

Figure 6. Finite element moving mesh (top) and functions b_1 (*r*, *z*, *t*) (middle) and b_2 (*r*, *z*, *t*) (bottom) at $t=0.1$, 1.27, 2.43, 3.63, 4.8, and 6.

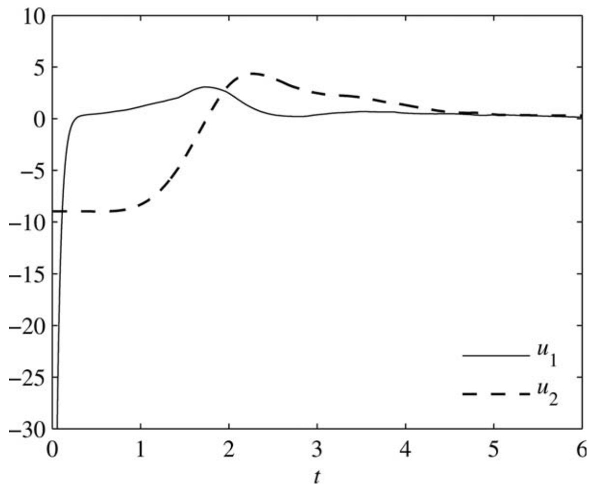

Figure 7. Optimal boundary inputs applied to the crystal.

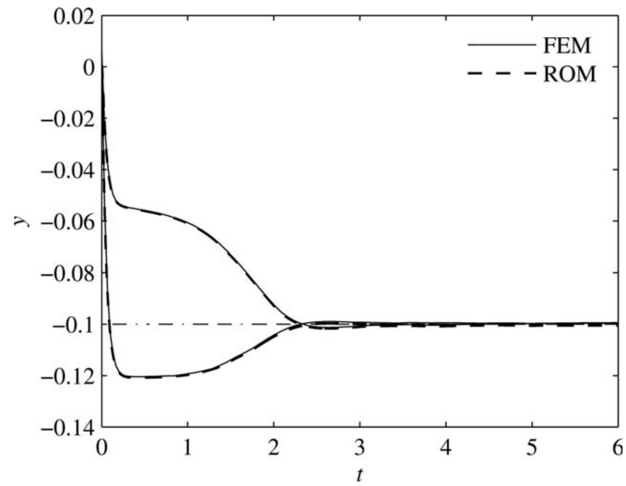

Figure 9. Outputs of the ROM and finite element plant.

eigenfunctions which contains more than 99.9% of the energy of snapshots, to construct the ROM.

The temperature field in the grown crystal cannot be measured directly, however, boundary measurements are available by the use of sensing devices. To reconstruct the state of the ROM of the CZ process, the temperature of a point on the outer surface of the crystal close (at the distance of 0.1) to the pulling arm (top of the crystal) is measured, this point can be considered on the crystal seed that was initially used to grow crystal on.

Thermal gradients near the melt interface in the grown crystal play a key role in the properties of the product. Structural defects in the form of dislocations can be generated by thermal stress, which is related to the thermal gradients near the interface.[47] Also, thermally induced stress can cause slip in the crystal structure. Stress analysis results have shown that thermal stress is largest at the crystal surface.[38]

We have chosen two target points close to the interface and crystal surface, namely at $z=0.2$ and at distances 0.05 and 0.25 from the crystal surface. The objective is to keep the dimensionless temperature at these target points $y(t)$ to track reference value of $y^r=[-0.1 -0.1]^T$ which complies with the requirements for the thermal gradients. Hence, the optimal control problem is to find the control law to track the reference temperature at the target points. The input profiles $u(t)$ generated as the time-varying linear state-feedback control using the estimated state for the reduced-order system is shown in Figure 7. Figure 8 shows the convergence of the estimated states to ROM states when state-feedback control is applied to the system.

Figure 9 shows the closed-loop response of the ROM as well as the response of the finite element. As it can be seen, the response of the system converges to the reference value. Also, there is a perfect match between the profiles of the two models showing the capability of the ROM to be used for controller design. Finally, the overall temperature profile of the crystal and target points are captured in Figure 10 showing the evolution of the state $x(r,z,t)$ of the finite element plant.

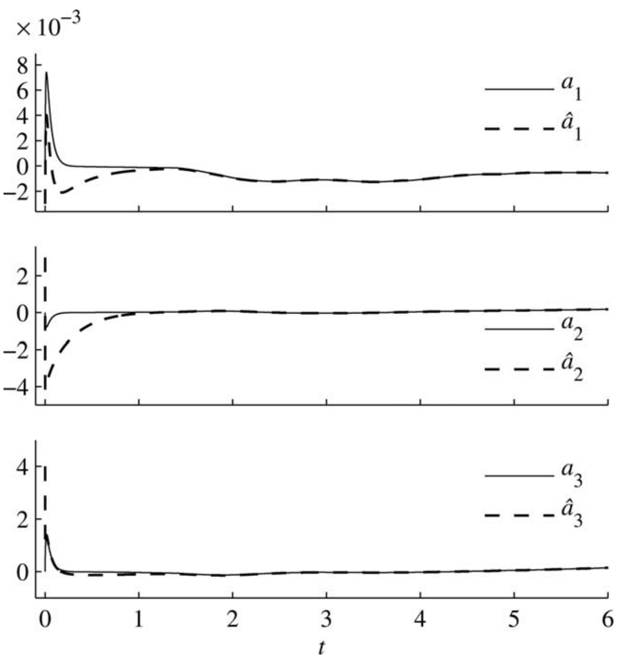

Figure 8. Evolution of the states of ROM and corresponding estimates.

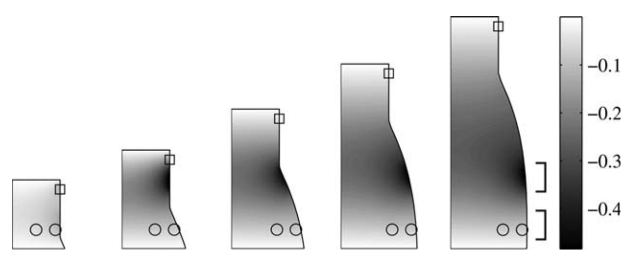

Figure 10. Dimensionless crystal temperature distribution from the FOM at $t = 1.27$, 2.43, 3.63, 4.8, and 6.

Temperature measurement is taken at the point indicated by square on the boundary and target points are shown by circles (supplemental video is available online).

Conclusion

This article considers the state estimation and optimal control problem with boundary actuation for linear parabolic PDEs defined on time-dependent spatial domains. The formulation of the time-varying parabolic system as a boundary control problem enabled order reduction of the system by extracting the set of time-varying empirical eigenfunctions that capture the most energy of PDE snapshots and the utilization of Galerkin's method. The ROM which is in the form of a linear time-varying system facilitated the Luenberger-type observer design and synthesis of a time-varying linear feedback controller based on a quadratic cost minimization. As an illustrative example, the CZ crystal growth process with the 2-D crystal temperature distribution was considered and the proposed controller formulation was applied. The numerical results of the simulated system demonstrated the output tracking of the system in the time-dependent crystal by the optimal feedback controller through boundary actuation.

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