Multiscale dynamics optimal control of parabolic PDE with time varying spatial domain (crystal growth process)

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Abstract—This paper considers the multi-scale optimal control of the Czochralski crystal growth process. The temperature distribution of the crystal is realized by heat input at the boundary and by the force applied to the mechanical subsystem drawing the crystal from a melt. A parabolic partial differential equation (PDE) model describing the temperature distribution of the crystal is developed from first-principles continuum mechanics to preserve the time-varying spatial domain dynamical features. The evolution of the temperature distribution is coupled to the pulling actuator finite-dimensional subsystem with dynamics modelled as a second order ordinary differential equation (ODE) for rigid body mechanics. The PDE timevarying spatial operator with natural boundary conditions is characterized as a Riesz-spectral operator in the $\mathbb{L}_2(0, l(t))$ functional space setting. The finite and infinite-time horizon optimal control law for the infinite-dimensional system is obtained as a solution to a time-dependent and time-invariant differential Riccati equation.

I. INTRODUCTION

The optimal control of transport-reaction processes has many industrial applications such as tubular reactors with axial dispersion, metal casting and crystal growth where it is of interest to maintain the temperature or concentration profile of a material within the specified processing requirements. The treatment of the material during its processing regime causes a change in shape, state or other material property as a part of the desired manufacturing result, [1]. The validity of the process model as the basis for controller formulation must account for the transport phenomena arising from the domain time-evolution. In this paper, the importance of these phenomena is clearly demonstrated and provides an enriched theory complementing the existing works on control of distributed parameter systems, see [2] and [3].

The Czochralski crystal growth process depicted in Fig.1 that is used for the production of semiconductor material is a prime example of a transport-reaction process with time-varying domain evolution, see [4]. During the process a mechanically actuated pulling arm draws a crystal seed from a melt in a heated furnace resulting in the formation of a large single ingot as the melt solidifies at the crystal-melt interface, see [5], [6], [7], [4]. The control objective is the production of high-purity crystals with specified shape which depend on the temperature distribution throughout the crystal domain and the rate at which the ingot is formed by adjusting

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James Ng, Ilyasse Aksikas and Stevan Dubljevic are with the Department of Chemical & Materials Engineering, University of Alberta, T6G 2V4, Canada jcng, aksikas, stevan.dubljevic@ualberta.ca the force applied to the pulling arm and the heat applied at the boundary of the crystal. Several works consider control of Czochralski crystal growth and control of time-varying domain parabolic PDEs in which the domain evolution is pre-specified, see [8], [9]. In similar works, the optimal control realization of the process is considered using multiscale models given by parabolic PDEs with time varying boundaries coupled to finite-dimensional subsystems, see [10] and [11].

This paper is organized to provide a concise formulation of a complete control problem starting from Section 2 where the transport-reaction process model is derived from principles of continuum mechanics to include the boundary domain time evolution. In Section 3, the analysis of the time dependent-spatial operator of the derived PDE is studied in the functional space context of infinite-dimensional statespace linear system theory to demonstrate that the timevarying spatial operator is a Riesz-spectral operator. Finally, utilization of the Riesz-spectral operator properties leads to the optimal control synthesis for the coupled problem of finite dimensional optimal regulation of the domain's boundary evolution and optimal infinite dimensional temperature regulation problem.



Fig. 1. A simple process diagram of a crystal slab being drawn from a melt (shaded area) in the direction ξ_1 . The boundary l(t) is moving with velocity w(t) in respect to the scalar property $f(\xi)$ represents the temperature of the slab at a given point. At the $\xi_1 = 0$ boundary, there is zero flux boundary condition across the slab and pulling mechanism. At the $\xi = l(t)$ boundary, there is zero flux boundary condition across the interface (dashed lines), between the slab and the melt.

II. PRELIMINARIES

A. Configuration space setting

Let us consider the following configuration space setting in the development of the parabolic PDE for the timedependent spatial domain. Consider the manifold \mathbb{R}^3 where the physical space region is defined as the open set $\Omega \subset$ \mathbb{R}^3 with material points, $\hat{\xi} = (\hat{\xi}_1, \hat{\xi}_2, \hat{\xi}_3)$, containing an arbitrary time dependent, moving subregion that is the open set $\mathcal{U}(t_0, t_f) \subset \Omega$ with volume element dv and spatial points $\xi = (\xi_1, \xi_2, \xi_3)$. The surface of $\mathcal{U}(t_0, t_f)$ is the piecewise C^1 boundary $\partial \mathcal{U}(t_0, t_f)$ and consists of the element ds.

The spatial velocity field $w(\xi, t)$ describes the *regular* motion of the boundary $\partial \mathcal{U}(t_0, t_f)$ where w is the continuous and invertible mapping $w : \Psi_t(\Omega) \to \mathbb{R}^3$, such that $\mathcal{U}(t_0, t_f) = \Psi_t(\mathcal{U}_0)$ is the region at time t in the interval $[t_0, t_f]$ relative to its initial configuration at t_0 . Then the set $\mathcal{U}(t_0, t_f)$ preserves the one-to-one mapping $\Psi_t : \mathcal{U} \to \mathcal{U} \subset \mathbb{R}^3$. The motion is presumed to be regular, that is the boundary $\partial \mathcal{U}(t_0, t_f)$ remains intact such that $\mathcal{U}(t_0, t_f)$ is not divided or penetrated. The relationship between the spatial points $\xi \in \mathcal{U}(t_0, t_f)$ and material points $\hat{\xi} \in \Omega$ is the mapping $\xi = \Psi_t(\hat{\xi})$.

B. Model formulation

Considering the physical region in the configuration space settings facilitates the use of the *Reynolds Transport Theorem*, see [12], [13]. In particular one can consider the *scalar physical quantity* of temperature defined $f = f(\xi, t)$ as a C^1 function on $\partial \mathcal{U}(t_0, t_f)$ and also bounded on $\mathcal{U}(t_0, t_f)$. By the *Transport theorem*, the rate of change of f with respect to time in $\mathcal{U}(t_0, t_f)$ is expressed as:

$$\rho C_p \frac{d}{dt} \int_{\mathcal{U}(t_0, t_f)} f dv = \rho C_p \int_{\mathcal{U}(t_0, t_f)} \left(\frac{\partial f}{\partial t} + \nabla \cdot (fw) \right) dv$$
⁽¹⁾

where ρ and C_p respectively denote the physical parameters of mass density and specific heat capacity that are assumed to be invariant throughout $\mathcal{U}(t_0, t_f)$ for all $t \in [t_0, t_f]$. The integration and differentiation operators on f over $\mathcal{U}(t_0, t_f) = \Psi_t(\mathcal{U}_0)$ may be interchanged since the continuity of $\Psi_t(\cdot)$ preserves the structure of the domain for all $\xi \in \mathcal{U}(t_0, t_f)$ and $t \in [t_0, t_f]$, see [12].

Internal reactionary sources of the $\mathcal{U}(t_0, t_f)$ are denoted $\hat{h}f(\xi, t)$ and heat flux across ds in the direction opposite to the outward normal component n of ds is given as $g(\xi, t) = -\kappa \nabla f(\xi, t)$, where κ is the *thermal conductivity* constant. The *integral form* of the *Conservation Law* provides the total heat balance in the control volume $\mathcal{U}(t_0, t_f)$ as,

$$\rho C_p \frac{d}{dt} \int_{\mathcal{U}(t_0, t_f)} f dv = \int_{\mathcal{U}(t_0, t_f)} \hat{h} f dv - \int_{\partial \mathcal{U}(t_0, t_f)} g \cdot n \, ds \tag{2}$$

Substitution by Eq.1 for the time rate of change in f and invoking the *divergence theorem* relates the heat flux across $\partial \mathcal{U}(t_0, t_f)$ to the integral of f over $\mathcal{U}(t_0, t_f)$. The assumption of continuity throughout $\mathcal{U}(t_0, t_f)$ for all $t \in [t_0, t_f]$ allows for the *material form* of the heat balance in $U(t_0, t_f)$ to be determined from Eq.2 as, see [12]:

$$\rho C_p \frac{\partial f}{\partial t} = \nabla \cdot (\kappa \nabla f) - \rho C_p \nabla \cdot (fw) + \hat{h}f \qquad (3)$$

The contribution of the transport term term $\rho C_p \nabla \cdot (fw)$ distinguishes Eq.3 from the conventional material derivative expression for the transport of a scalar property, see [13]. Expansion of this transport term gives:

$$\nabla \cdot (fw) = f\nabla \cdot w + w \cdot \nabla f \tag{4}$$

One notices this transport phenomenon arises from the motion of the boundary, $\partial \mathcal{U}(t_0, t_f)$, along the spatial velocity field, w, which determines the configurations of $\mathcal{U}(t_0, t_f)$ and subsequently vanishes when $\partial \mathcal{U}(t_0, t_f)$ is the constant. The assumption of density invariance implies incompressibility of $\mathcal{U}(t_0, t_f)$ such that the divergence of the velocity field vanishes, i.e. $\nabla \cdot w = 0$. The velocity field $w(\xi, t) = \partial \Psi_t(\hat{\xi}, t)/\partial t = d\xi/dt$ provides the relation among the spatial and material coordinates $\hat{\xi} \in \Omega$ to $\xi \in \mathcal{U}(t_0, t_f)$ so that contribution of the moving boundary to the scalar quantity, f, is obtained as:

$$w \cdot \nabla f = \frac{d\xi_i}{dt} \frac{\partial f}{\partial \xi_i}, \qquad i = \{1, 2, 3\}$$
(5)

The term in Eq.5 can be viewed as the type of convective transport due to the motion of $\mathcal{U}(t_0, t_f)$. From Eqs.3-4-5, we obtain the expression for the heat equation for the region $\mathcal{U}(t_0, t_f)$ with moving boundary, $\partial \mathcal{U}(t_0, t_f)$, as follows:

$$c\rho\frac{\partial f}{\partial t} = \nabla \cdot (\kappa \nabla f) - c\rho(w \cdot \nabla f) + \hat{h}f \tag{6}$$

In the case when the domain becomes constant, Eq.6 leads to the well known expression of the reaction diffusion parabolic PDE with time invariant domain. The general form of the boundary conditions imposed upon Eq.6 for prescribed functions α , β and u on $\partial \mathcal{U}(t_0, t_f)$ is expressed as:

$$\left. \alpha f + \beta \frac{\partial f}{\partial n} \right|_{\partial \mathcal{U}(t_0, t)} = u \tag{7}$$

where $\partial f/\partial n$ is the outward normal component to $\partial \mathcal{U}(t_0, t_f)$. The boundary conditions of Eq.7 relate to the temperature, f, on the boundary of the region and the flux of f through $\partial \mathcal{U}(t_0, t_f)$.

Consider the process depicted in Fig.1 in the $\xi = \xi_1$ direction. The manifold in Euclidean space is the open set $\Omega \subset \mathbb{R}$ such that Ω is a topological space with mapping $\Psi_t : \mathbb{R} \to \mathbb{R}$ with material points $\xi \in (0, l(t))$, see [14]. The dynamics of the transport process are given by the 1D-PDE:

$$\frac{\partial f}{\partial t} = k \frac{\partial^2 f}{d\xi^2} - w(t) \frac{\partial f}{d\xi} + hf + F(\xi, t) \tag{8}$$

where $k = \frac{\kappa}{C_p \rho}$ is the diffusivity constant, $w(t) = \frac{d l(t)}{dt}$ is the boundary velocity, $h = \frac{\hat{h}}{C_p \rho}$ and $F(\xi, t)$ is the heating source term applied over the domain. The boundary conditions for this process model are given as, see [2]:

$$\frac{df}{d\xi}(0,t) = 0 = \frac{df}{d\xi}(l,t) \tag{9}$$

III. PROPERTIES OF TIME-VARYING SPATIAL OPERATOR

A. Functional space setting

The discussion of Riesz-spectral and infinite-dimensional linear system theory requires the following basic results from the functional analysis. Consider the set of measurable, square integrable functions $x \in \mathcal{H}$, i.e. for $[a, b] \subset \mathbb{R}$, we have $\int_a^b |x|^2 d\xi < \infty$, with x belonging to the equivalence class [x] where [x] = x almost everywhere, i.e. which differ only on a set of measure zero in [a, b]. \mathcal{H} is a normed linear space with norm given by ||x|| as one can show that [x] forms a linear vector space satisfying $||[x]|| := ||\hat{x}||$ for any $\hat{x} \in [x]$. Further, \mathcal{H} is a Hilbert space denoted as $\mathbb{L}^2(a, b)$ for any given two square integrable functions, $x, y \in \mathcal{H}$, each belonging to their respective equivalence classes, with inner product space $\langle \cdot, \cdot \rangle$ and assuming that the metric d(x,y) = ||x - y|| is complete, see [14]. The time-varying nature of model dynamics Eqs.8-9, requires satisfaction of the aforementioned topological properties on space \mathcal{H} at each time instance. i.e, given two functions $\{x(\xi,t), y(\xi,t)\} \in \mathbb{L}^2(0, l(t))$ the inner product is given as $\langle x, y \rangle_{\mathbb{L}^2(0,l)}$, for $t \in [t_0, t_f]$. Therefore, for the timevarying operator, one must consider a family of Hilbert spaces equipped with a family of inner products.

The analysis of the PDE system in Eqs.8-9 is carried out in $\mathbb{L}^2(0, l)$ where l = l(t) > 0 is the length of the domain at each time $t \in [t_0, t_f]$. The associated time-varying spatial operator is given in the following definition and considered with respect to the subsequent proposition.

Definition 1: Consider the operator \mathcal{L} defined on the domain: $\mathcal{D}(\mathcal{L}) := \{f \in \mathbb{L}^2(0, l) : f, \frac{df}{d\xi} \text{ absolutely continuous,} \\ \frac{d^2f}{d\xi^2} \in \mathbb{L}^2(0, l), \text{ and } \frac{df}{d\xi}(0) = 0, \frac{df}{d\xi}(l) = 0\}, \text{ where } 0 < l < \infty. \text{ For } f \in \mathcal{D}(\mathcal{L}), \text{ we define } \mathcal{L} \text{ as the operator:} \end{cases}$

$$\mathcal{L}f = k\frac{d^2f}{d\xi^2} - w\frac{df}{d\xi} + hf \tag{10}$$

where $w := \{\xi = l | w(t) : (l, t_0) \mapsto (l, t_f), 0 \le t_0 < t_f < \infty\}$, is the velocity of the domain's boundary for all $t \in [t_0, t_f]$, and $k \in \mathbb{R}$ is constant.

The adjoint operator \mathcal{L}^* and associated boundary conditions are obtained heuristically from $\langle \mathcal{L}\phi,\psi\rangle = \langle \phi,\mathcal{L}^*\psi\rangle$ as,

$$\mathcal{L}^* f = k \frac{d^2 f}{d\xi^2} + w \frac{df}{d\xi} + hf \tag{11}$$

Proposition 1: Consider the operator \mathcal{L} defined in Definition 1. If $f \in \mathbb{L}^2(0, l)$ is admissible in $\mathcal{D}(\mathcal{L})$ then the operator \mathcal{L} has adjoint \mathcal{L}^* with domain $\mathcal{D}(\mathcal{L}^*) := \{f \in \mathbb{L}^2(0, l) : f, \frac{df}{d\xi} \text{ absolutely continuous, } \frac{d^2f}{d\xi^2} \in \mathbb{L}^2(0, l) \text{ and } k \frac{df}{d\xi}(l) + wf(l) = 0, k \frac{df}{d\xi}(0) + wf(0) = 0\}$

Proof 1: For functions $\phi, \psi \in \mathbb{L}^2(0, l)$, application of the natural boundary conditions to $\langle \mathcal{L}\phi, \psi \rangle$ gives:

$$\langle \mathcal{L}\phi,\psi\rangle = -\phi(l)[k\psi'(l) + w\psi(l)]$$

$$+ \phi(0)[k\psi'(0) + w\psi(0)] + \langle\phi,\mathcal{L}^*\psi\rangle$$
(13)

The required adjoint boundary conditions for $\psi \in \mathcal{D}(\mathcal{L}^*)$ easily follow.

B. Riesz-spectral representation

One can consider the operator \mathcal{L} and its adjoint \mathcal{L}^* in association with the *Sturm-Liouville* operator \mathcal{S} such that for $f \in \mathcal{D}(\mathcal{S})$,

$$Sf = \frac{1}{\rho(\xi)} \frac{d}{d\xi} \left(-p(\xi) \frac{df}{d\xi} \right) + q(\xi)f \tag{14}$$

where $p(\xi) > 0, \rho(\xi) > 0$ and $q(\xi)$ are analytic real valued functions for $\xi \in (0, l)$. In particular, demonstrating the operator \mathcal{L} is the negative of a *Sturm-Liouville* operator in Eq.14 defined on $\mathcal{D}(S)$ gives that \mathcal{L} is a Riesz-spectral operator and infinitesimal generator of a C_0 -semigroup of bounded linear operators on $\mathbb{L}^2(0, l)$, see [15], [16], [17]. The features of \mathcal{L} with its *Sturm-Liouville* form, S, are related in the construction of a normed $\mathbb{L}^2(0, l)$ space with weight function $\rho(\xi)$ and inner product,

$$\langle \phi_m, \psi_n \rangle_\rho = \int_0^{l(t)} \rho \, \phi_m \, \psi_n d\xi = \delta_{mn} \tag{15}$$

where $\{\phi_m, \psi_n, n \in \mathbb{N}\}$ are eigenvectors forming a Rieszspectral basis of $\mathbb{L}^2(0, l)$ and S is Hermitian, i.e. $\langle S\phi, \psi \rangle_{\rho} = \langle \phi, S\psi \rangle_{\rho}$. By comparing Eq.10 with Eq.14 one easily obtains that $\rho = e^{-\frac{w}{k}\xi}$, $p = -ke^{-\frac{w}{k}\xi}$, q = h such that \mathcal{L} is a *Sturm-Liouville* operator of the form in Eq.14. Letting $f = e^{\frac{w}{2k}\xi}v(\xi)$, the eigenvalue problem $\mathcal{L}f = \lambda f$ is represented as,

$$k e^{\frac{w}{k}\xi} \frac{d}{d\xi} \left(e^{-\frac{w}{k}\xi} \frac{d e^{\frac{w}{2k}\xi} v}{d\xi} \right) + h e^{\frac{w}{2k}\xi} v = \lambda e^{\frac{w}{2k}\xi} v \qquad (16)$$

Application of the boundary condition in Definition 1 yields the countably infinite set of eigenvalues,

$$\lambda_0 = -\frac{1}{2k}\frac{w^2}{2} + h, \quad n = 0$$
(17)

$$\lambda_n = -k \left(\frac{n\pi}{l(t)}\right)^2 - \frac{1}{2k} \frac{w^2}{2} + h \quad n \ge 1$$
 (18)

From the Eq.18 one can show that for,

$$\left| k \left(\frac{n\pi}{l(t)} \right)^2 + \frac{w^2}{4k} \right| > |h| \tag{19}$$

the eigenvalues are negative, moreover, for all $n \ge 1$ the eigenvalues $\lambda_n \to -\infty$ as $n \to +\infty$ and $|\lambda_{n+1} - \lambda_n| \to +\infty$ as $n \to +\infty$, which implies that the spectrum of \mathcal{L} , i.e. $\sigma(\mathcal{L})$, is:

$$\sigma(\mathcal{L}) = \{\lambda \in \mathbb{R} | \inf_{n \ge 1} |\lambda - \lambda_n| > 0\} \cup \{\lambda_0\}$$
(20)

Therefore, $\overline{\{\lambda_n, n \in \mathbb{N}\}}$ is totally disconnected. Calculating the *Wronskian* determinant $\mathcal{W}(\phi_n, \phi_m)$ evaluated at the boundaries and application of *Abel's Theorem* gives that the eigenvalues $\{\lambda_n, n \in \mathbb{N}\}$ are simple, see [18].

The corresponding set of eigenvectors, $\{\phi_n, n \in \mathbb{N}\}$, can be determined as,

$$\phi_n(\xi) = B_n e^{\frac{w}{2k}\xi} \left[\cos\left(\frac{n\pi}{l(t)}\xi\right) - \frac{w}{2k\frac{n\pi}{l(t)}}\sin\left(\frac{n\pi}{l(t)}\xi\right) \right]$$
(21)

and form an orthonormal basis of $\mathcal{D}(\mathcal{L})$ given the coefficients calculated using the orthogonality relation $\langle \phi_n, \phi_m \rangle_{\rho} = \delta_{nm}$, which yields,

$$B_n(t) = \sqrt{\frac{2}{l(t)}} \left[1 + \left(\frac{w}{2k\frac{n\pi}{l(t)}}\right)^2 \right]^{-\frac{1}{2}}$$
(22)

The adjoint eigenvectors $\{\psi_n, n \in \mathbb{N}\}$ form an orthonormal basis of $\mathcal{D}(\mathcal{L}^*)$ defined in Proposition 1 can be determined by utilizing the weight function ρ as $\psi_n(\xi) = e^{-\frac{w}{k}\xi}\phi_n(\xi)$. Taking the inner product, one gets $\langle \phi_m, \psi_n \rangle = \delta_{mn}$ such that $\{\phi_n, \psi_n, n \in \mathbb{N}\}$ are biorthonormal and form a Riesz basis of $\mathbb{L}^2(0, l)$. Then every $f \in \mathbb{L}^2(0, l)$ can be represented uniquely by, see [3],

$$f = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \phi_n = \sum_{n=1}^{\infty} c_n \phi_n$$
(23)

Denoting the finite sum $\sum_{n=1}^{N} c_n \phi_n$, we have,

$$\left\| f - \sum_{n=1}^{N} c_n \phi_n \right\|^2 = \|f\|^2 - \sum_{n=1}^{N} c_n^2 \ge 0$$
 (24)

so that as $N \to \infty$ we have Bessel's Inequality, that implies $c_n \to 0$ as $n \to \infty$ and that $\sum_{n=1}^N c_n^2 \le ||f||^2$. Assuming c_n is square summable we look at the convergence of the sequence f_N to f in the mean square, see [3]. Denoting the partial sum of $f_N = \sum_{n=1}^N c_n \phi_n$ and assuming Parseval's equality, $\sum_{n=1}^\infty c_n^2 = ||f||^2$, is satisfied then we have that,

$$\lim_{N \to \infty} \|f - f_N\|^2 = \lim_{N \to \infty} \left[\|f\|^2 - \sum_{n=1}^N c_n^2 \right] \to 0 \quad (25)$$

That is, every sequence $\{f_n, n \in \mathbb{N}\} \in \mathbb{L}^2(0, l)$ converges to $f \in \mathbb{L}^2(0, l)$ such that $Sf_n \to f \in \mathbb{L}^2(0, l)$ as $n \to \infty$. Then the operator \mathcal{L} is closed. By these results, it is verified that the operator, \mathcal{L} , is a Riesz-spectral operator such that \mathcal{L} has the representation, see [3],

$$\mathcal{L}f = \sum_{n=1}^{\infty} \lambda_n \langle f, \psi_n \rangle \phi_n, \quad \text{for } f \in \mathcal{D}(\mathcal{L})$$
 (26)

$$\mathcal{D}(\mathcal{L}) = \{ f \in \mathbb{L}^2(0, l) \mid \sum_{n=1}^{\infty} |\lambda_n|^2 |\langle f, \psi_n \rangle|^2 < \infty \}$$
(27)

The semigroup $\mathcal{T}(t)$ is bounded since,

$$\|\mathcal{T}(t)\| \le M e^{\omega t} \quad \text{for} \quad t \ge 0 \tag{28}$$

for $\omega > \omega_0$, where the growth bound, ω_0 of $\mathcal{T}(t)$ is given by,

$$\omega_0 = \inf_{t>0} \left(\frac{1}{t} \log \|\mathcal{T}(t)\| \right) = \sup_{n \ge 1} Re(\lambda_n).$$
(29)

Since $\lambda_n < 0$, one obtains that \mathcal{L} is the infinitesimal generator of an exponentially stable C_0 -semigroup given by,

$$\mathcal{T}(t)(\,\cdot\,) = \sum_{n=0}^{\infty} e^{\lambda_n t} \langle\,\cdot\,,\psi_n\rangle\phi_n \tag{30}$$

The main result given here is that operator \mathcal{L} is the negative of a *Sturm-Liouville* operator S. Then from ([15], Lemma 1), \mathcal{L} is a Riesz-spectral operator and infinitesimal generator of the C_0 -semigroup in Eq.30 with eigenvalues $\{\lambda_n, n \in \mathbb{N}\}$ in Eqs.17-18 and the eigenvectors of \mathcal{L} and \mathcal{L}^* are $\{\phi_n, \psi_n, n \in \mathbb{N}\}$ respectively, which form a Riesz-basis of $\mathbb{L}^2(0, l)$.

IV. CONTROLLER FORMULATION

A. System description

We consider the following model describing the temperature evolution in the slab which is given by the parabolic PDE,

$$\frac{\partial x}{\partial t} = k \frac{\partial^2 x}{d\xi^2} - w(t) \frac{\partial x}{d\xi} + hx + F(\xi, t)$$
(31)

$$\frac{dx}{d\xi}(0,t) = 0 = \frac{dx}{d\xi}(l,t) \tag{32}$$

$$y(t) = \int_{0}^{l(t)} \hat{\delta}(\xi - \xi_c) x(\xi, t) \, d\xi$$
(33)

for $x(\xi,t) \in \mathcal{D}(\mathcal{L})$, where $F(\xi,t) = b(\xi)u(t)$ with $b(\xi) = 1$ is the uniform heat source input over the domain and y(t)is the output measurement where $\hat{\delta}(\xi - \xi_c)$ is the squareintegrable function in $\mathbb{L}^2(0,l)$ approximating the Dirac delta function which specifies the output measurements location. Eqs.31-32-33 are coupled with the domain evolution, l(t) = $\{l(t), t \in [t_0, t_f]\} > 0$, through the boundary evolution which is determined by the actuator pulling the slab with dynamics governed by,

$$M\frac{d^{2}l(t)}{dt^{2}} + \nu\frac{dl(t)}{dt} + \eta l(t) = F_{m}(t)$$
(34)

where M, η are the positive coefficients of the mass and elasticity of the system and $\nu < 0$ is the dampening coefficient. The input for the mechanical subsystem is the force applied by the actuator, $F_m(t)$. The corresponding state-space form of the infinite-dimensional system augmented with the finitedimensional subsystem is given by,

$$\begin{bmatrix} \dot{z}_{1}(t) \\ \dot{z}_{2}(t) \\ \dot{\mathbf{x}}(t) \end{bmatrix} = \begin{bmatrix} 0 & 1 & \mathbf{0} \\ a_{1} & a_{2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathcal{A}(t) \end{bmatrix} \begin{bmatrix} z_{1}(t) \\ z_{2}(t) \\ \mathbf{x}(t) \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ b_{1} & 0 \\ \mathbf{0} & \mathcal{B}(t) \end{bmatrix} \begin{bmatrix} F_{m} & \mathbf{u} \end{bmatrix}$$
(35)

$$y(t) = \begin{bmatrix} c_1 & 0 & \mathbf{0} \\ 0 & c_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathcal{C}(t) \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \\ \mathbf{x}(t) \end{bmatrix}$$
(36)

with states $z_1(t) = l(t)$ and $z_2(t) = \dot{l}(t)$ where $a_1 = -\frac{\eta}{M}$, $a_2 = -\frac{\nu}{M}$ and the PDE state $x(\xi, t) = \sum_{n=0}^{\infty} x_i(t)\phi_n(\xi, t)$ where $\{\phi_n(\xi), n \in \mathbb{N}\}$ are the eigenvectors in Eq.21 with coefficients in Eq.22 and the infinite dimensional state vector is denoted $\mathbf{x}(t) = [x_1(t) \ x_2(t) \cdots]^T$. The matrix $\mathcal{A}(t)$ is associated with the infinite dimensional system representation which is obtained from the exact

modal decomposition of the time-dependent spatial operator \mathcal{L} utilizing the Galerkin method, such that $\mathcal{A}(t)$ is the diagonal matrix of corresponding time varying eigenvalues in Eqs.17-18, see [16]. The input matrix $\mathcal{B}(t) = \langle b(\xi), \phi(\xi, t) \rangle$ contains the modal decomposed terms associated with the input, **u**, to the infinite dimensional system.

The ensuing sections consider the optimal control problem for cases on the finite and infinite time interval for Eq.35-36 where,

$$\dot{\mathbf{Z}}(t) = \mathbf{A}(t)\mathbf{Z}(t) + \mathbf{B}(t)\mathbf{U}(t)$$
(37)

$$\mathbf{Y}(t) = \mathbf{C}(t)\mathbf{Z}(t) \tag{38}$$

defines the linear state system $\Sigma(\mathbf{A}, \mathbf{B}, \mathbf{C})$ with the matrices:

$$\mathbf{A} = \begin{bmatrix} A_1 & 0 \\ 0 & \mathcal{A} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} C & 0 \\ 0 & \mathcal{C} \end{bmatrix} \quad (39)$$

The optimal input is determined from the solution, $\Pi(t)$, of the continuous-time differential Riccati equation,

$$\dot{\Pi} = \mathbf{A}^* \Pi + \Pi \, \mathbf{A} + \mathbf{C}^* \mathbf{C} - \Pi \, \mathbf{B} \mathbf{R}^{-1} \mathbf{B}^* \Pi \qquad (40)$$

where $\Pi(t)$ is symmetric, positive semi-definite and self adjoint and $\mathbf{R} \in \mathbb{L}^2(0, l)$ is coercive. The case that the optimal control problem solution for the finite and infinite dimensional systems is decoupled corresponds to having the off diagonal elements of $\Pi(t)$ as infinite dimensional zero matrices in addition noting the terms $B_1B_2^*$ and $B_2B_1^*$ arising from Eq.40 vanish. The solution matrix $\Pi(t)$ has the form,

$$\Pi = \begin{bmatrix} \Pi_1 & \mathbf{0} \\ \mathbf{0} & \Pi_2 \end{bmatrix}, \quad \Pi_1 = \begin{bmatrix} \pi_1 & \pi_2 \\ \pi_2 & \pi_3 \end{bmatrix}$$
(41)

for Π_1 and Π_2 respectively corresponding to the finitedimensional and infinite-dimensional systems.

B. Optimal state trajectories of mechanical subsystem

Let us consider the finite-dimensional problem associated with the mechanical subsystem. For the case of full state measurement then Π_1 is the stationary solution of the algebraic Riccati equation,

$$\Pi_1 A_1 + A^* \Pi_1 + C^* C - \Pi_1 B_1 r^{-1} B_1^* \Pi_1 = 0$$
 (42)

where r > 0 is the input penalty term. The elements π_1, π_2, π_3 of Π are the set of solutions obtained from the following algebraic equations implicitly given as:

$$\pi_1 = \frac{b_1^2}{r} \pi_2 \pi_3 - a_2 \pi_2 - a_1 \pi_3 \tag{43}$$

$$\pi_2 = \frac{r}{b_1^2} \left(a_1 \pm r \sqrt{a_1^2 r + b_1^2 c_1^2} \right) \tag{44}$$

$$\pi_3 = \frac{r}{b_1^2} \left(a_2 \pm r \sqrt{a_2^2 r + 2b_1^2 \pi_2 + b_1^2 c_2^2} \right) \quad (45)$$

For a semi-stabilizing solution to exist, Π_1 must be positive semi-definite. In terms of the principle minors of Π_1 , the requirement is to ensure that each of,

$$\pi_1 \geq 0 \tag{46}$$

$$\pi_1 \pi_3 - \pi_2^2 \ge 0 \tag{47}$$

are satisfied where strictly positive principle minors give stabilizing solutions of Π_1 .

For the case that the states are not measured, i.e. C = 0, the optimal state trajectories of the mechanical subsystem require the determination of Π_1 from the algebraic Riccati equation,

$$\Pi_1 A_1 + A_1^* \Pi_1 - \Pi_1 B_1 r^{-1} B_1^* \Pi_1 = 0$$
(48)

The elements π_1, π_2, π_3 of Π_1 are determined from the solution of the following set of equations:

$$2a_1\pi_2 - \frac{b_1^2}{r}\pi_2^2 = 0 \tag{49}$$

$$\pi_1 + a_2 \pi_2 + a_1 \pi_3 - \frac{b_1^2}{r} \pi_2 \pi_3 = 0$$
 (50)

$$2\pi_2 + 2a_2\pi_3 - \frac{b_1^2}{r}\pi_3^2 = 0 \tag{51}$$

A family of solutions for Π_1 can be determined from Eqs.49-50-51. For $\pi_2 = 2a_1 \frac{r}{b_1^2}$, two possible solutions of Eq.50 denoted π_3^{\pm} can be determined and if the following condition,

$$\frac{r}{b_1^2} \left(a_2 \pm a_1 \sqrt{a_2^2 + 4a_1} \pm \sqrt{a_2^2 + 4a_1} - a_1 a_2 \right) \ge 0 \quad (52)$$

is satisfied, then Π_1^{\pm} is positive semi-definite such that the feedback gain, $K = r^{-1}B_1^T\Pi_1$, for the finite-dimensional subsystem is semi-stabilizing. The solution $\pi_2 = 0$ again leads to two possible values of π_3 . For $\pi_3 = 0$, Π_1 is the zero matrix and semi-stabilizing. For $\pi_3 = 2a_2\frac{r}{b_1^2}$, one gets the solution matrix Π_1 as,

$$\Pi_1 = \begin{bmatrix} -2a_1a_2\frac{r}{b_1^2} & 0\\ 0 & 2a_2\frac{r}{b_1^2} \end{bmatrix}$$
(53)

Noting that $a_1 = -\frac{\eta}{M}$ and $a_2 = -\frac{\nu}{M}$ with $\nu < 0$, one obtains that Π_1 is positive-definite so the optimal feedback gain for the finite-dimensional system is stabilizing and the expression for the optimal input $F_m(t)$ is given as,

$$F_m(t) = -B_1^* \Pi_1 z(t) = \begin{bmatrix} 0 & -\frac{2a_2}{b_1} \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix}$$
(54)

The optimal state trajectories, $z_1 = l(t)$ and $z_2 = \dot{l}(t)$, for the mechanical system can be easily obtained in the analytic form. Further, under the feedback given by Eq.54 feedback the asymptotic stability of the closed loop system can be verified depending on the parameters a_1 and a_2 . That is, the closed loop system $\dot{z} = (A_1 + B_1 F_m)z$ satisfies $||K(t)|| \leq me^{-\alpha t}$ for positive constants m and α , where $K(t) = e^{(A_1 + B_1 F_m)t}$ is the *Cauchy* matrix solution of the finite-dimensional subsystem, see [19].

The optimal feedback laws for the remaining cases of partial state measurement of the mechanical subsystem can be determined in a similar procedure as the two cases given.

C. The optimal control law of infinite-dimensional system on the finite-time interval

The Riesz-spectral operator \mathcal{L} is an infinitesimal generator of the C_0 -semigroup, \mathcal{T} , which defines the evolution of the x(t) state, see Eq.28-29-30. The respective input and output operators, \mathcal{B} and \mathcal{C} , are bounded linear operators with well defined mappings from the input into the state space and from the state to the output space. The state evolution is given as,

$$x(t) = \mathcal{T}(t)x_0 + \int_0^t \mathcal{T}(t-s)\mathcal{B}u(s)ds \qquad (55)$$

$$y(t) = Cx(t) \tag{56}$$

where $x_0 \in \mathbb{L}^2(0, l)$ is the initial condition, see [3].

The associated cost functional for the finite-time interval for $t \in [0, t_f]$ is given by,

$$J(x_0; u; 0, t_f) = \langle x(t_f), Qx(t_f) \rangle + \int_0^{t_f} \langle y(s), y(s) \rangle + \langle u(s), Ru(s) \rangle ds$$
(57)

where the state penalty matrix Q self-adjoint and nonnegative and the input penalty matrix R is coercive. The decoupling of the finite and infinite dimensional systems by the structure of $\Pi(t)$ in Eq.41 requires determination of the optimal stabilizing input $\mathbf{u} = u^{\min}(x_0, t)$ for the infinite-dimensional state linear system $\Sigma(\mathcal{A}, \mathcal{B}, \mathcal{C})$ that depend on the time varying solutions $\Pi_2(t)$ of a differential Riccati equation, see [3]. Since \mathcal{A} , associated with \mathcal{L} , is not self-adjoint we utilize the biorthonormal set of eigenvectors that form a Riesz-basis of $\mathbb{L}^2(0, l)$ with $\{\phi_0, \phi_m, m \ge 1\} \in \mathcal{D}(\mathcal{L}),$ $\{\psi_0, \psi_n, n \ge 1\} \in \mathcal{D}(\mathcal{L}^*)$ and $\Pi_2(t)\phi_m \in \mathcal{D}(\mathcal{L}^*)$. The differential Riccati equation is,

$$\frac{d}{dt}\langle\psi_n,\Pi_2\phi_m\rangle = -\langle\psi_n,\Pi_2\mathcal{A}\phi_m\rangle - \langle\mathcal{A}\psi_n,\Pi_2\phi_m\rangle - \langle\mathcal{C}\psi_n,\mathcal{C}\phi_m\rangle + \langle\Pi_2\mathcal{B}R^{-1}\mathcal{B}^*\Pi_2\psi_n,\phi_m\rangle$$
(58)

$$\langle \psi_n, \Pi_2(t_f)\phi_m \rangle = \langle \psi_n, Q_{nm}\phi_m \rangle = Q_{nm}\delta_{nm}$$
(59)

The solution of Eqs.58-59 is of the form $\Pi_2(t)x = \sum_{n,m} \Pi_{2,nm}(t) \langle x, \psi_n \rangle \phi_m$ with the relation,

$$\Pi_{2,nm} = \langle \psi_n, \Pi_2 \phi_m \rangle \tag{60}$$

Noting that $\Pi_{2,nm}(t) = 0$ for $n \neq m$, one is left with the following expression for $\Pi_{2,nn}(t)$,

$$\dot{\Pi}_{2,nn} = -2\lambda_n \Pi_{2,nn} - \mathcal{C}_{nn}^2 + \mathcal{E}_{nn} \Pi_{2,nn}^2$$
(61)
$$\Pi_{2,nn}(t_f) = Q_{nn}$$
(62)

where $\mathcal{E} = \mathcal{B}R^{-1}\mathcal{B}^*$. By defining the following expressions,

$$a_n = -\mathcal{E}_{nn}^{-1} \left(\lambda_n + \sqrt{\lambda_n^2 + \mathcal{E}_{nn} \mathcal{C}_{nn}^2} \right)$$
(63)

$$b_n = -\mathcal{E}_{nn}^{-1} \left(\lambda_n - \sqrt{\lambda_n^2 + \mathcal{E}_{nn} \mathcal{C}_{nn}^2} \right)$$
(64)

$$d_n = 2\mathcal{E}_{nn}^{-1}\sqrt{\lambda_n^2 + \mathcal{E}_{nn}\mathcal{C}_{nn}^2}$$
(65)

$$g_n(t) = (\Pi_{2,nn} + a_n)^{-1}$$
(66)

one obtains the linear ODE,

$$\dot{g}_n(t) = -1 - d_n g_n(t)$$
 (67)

$$g_n(t_f) = (Q_{nn} + a_n)^{-1}$$
 (68)

The solution $g_n(t)$ is determined to be,

$$g_n(t) = \frac{-(Q_{nn} + a_n) + (Q_{nn} + b_n)e^{-d_n(t - t_f)}}{(Q_{nn} + a_n)d_n}$$
(69)

From Eq.66, one obtains the solution of $\Pi_{2,nn}(t)$,

$$\Pi_{2,nn} = \frac{(Q_{nn} + a_n)b_n - a_n(Q_{nn} + b_n)e^{-d_n(t - t_f)}}{-(Q_{nn} + a_n) + (Q_{nn} + b_n)e^{-d_n(t - t_f)}}$$
(70)

Then the finite-time interval optimal control law for the infinite-dimensional system is determined as,

$$u^{\min}(x_{0};t) = -R^{-1}\mathcal{B}^{*}\Pi_{2}(t)x_{0}$$

$$= -R^{-1}\mathcal{B}^{*}\sum_{n=0}^{\infty}\Pi_{2,nn}\langle x_{0},\psi_{n}\rangle\phi_{n}$$

$$= -R^{-1}\mathcal{B}^{*}\left\{\int_{0}^{l(t)}B_{0}(t)x_{0}(\xi)\,d\xi + \sum_{n=1}^{\infty}\frac{(Q_{nn}+a_{n})b_{n}-a_{n}(Q_{nn}+b_{n})e^{-d_{n}(t-t_{f})}}{-(Q_{nn}+a_{n})+(Q_{nn}+b_{n})e^{-d_{n}(t-t_{f})}} \cdot \int_{0}^{l(t)}x_{0}(\xi)\psi_{n}(\xi)d\xi\,\phi_{n}(\cdot)\right\}$$
(71)

For the case when state measurement is not considered, i.e. C = 0, the differential Riccati equation becomes,

$$\frac{d}{dt}\langle\psi_n,\Pi_2\phi_m\rangle = -\langle\psi_n,\Pi_2\mathcal{A}\phi_m\rangle - \langle\mathcal{A}\psi_n,\Pi_2\phi_m\rangle + \langle\Pi_2\mathcal{B}R^{-1}\mathcal{B}^*\Pi_2\psi_n,\phi_m\rangle$$
(72)

$$\langle \psi_n, \Pi_2(t_f)\phi_m \rangle = Q_{nm}\delta_{nm}$$
 (73)

Proceeding as before, one is left with the following expression for $\Pi_{2,nn}(t)$ as,

$$\dot{\Pi}_{2,nn} = -2\lambda_n \Pi_{2,nn} + \mathcal{E}_{nn} \Pi_{2,nn}^2$$
 (74)

$$\Pi_{2,nn}(t_f) = Q_{nn} \tag{75}$$

The ODE in Eq.74 is separable and has solution,

$$\Pi_{2,nn} = \frac{2\lambda_n Q_{nn} e^{-2\lambda_n (t-t_f)}}{2\lambda_n - \mathcal{E}_{nn} Q_{nn} + \mathcal{E}_{nn} Q_{nn} e^{-2\lambda_n (t-t_f)}}$$
(76)

Given that the following condition is satisfied,

$$1 - e^{-2\lambda_n(t - f_f)} > 0 \tag{77}$$

then Eq.76 is positive definite and the finite-time optimal control law for C = 0 is determined as,

$$u^{\min}(x_0;t) = -R^{-1}\mathcal{B}^* \left\{ \int_0^{l(t)} B_0(t) x_0(\xi) d\xi + \sum_{n=1}^\infty \frac{2\lambda_n Q_{nn} e^{-2\lambda_n(t-t_f)}}{2\lambda_n - \mathcal{E}_{nn} Q_{nn} + \mathcal{E}_{nn} Q_{nn} e^{-2\lambda_n(t-t_f)}} \cdot \int_0^{l(t)} x_0(\xi) \psi_n(\xi) d\xi \phi_n(\cdot) \right\}$$
(78)

D. The optimal control law of infinite-dimensional system on the infinite-time interval

The optimal control law for the infinite-time interval, $t \in [0, \infty]$, is obtained by considering the associated cost functional given by,

$$J(x_0; u) = \int_0^\infty \langle y(s), y(s) \rangle + \langle u(s), Ru(s) \rangle ds$$
(79)

The optimal control law can be obtained by determining the stationary operator $\Pi_2 \in \mathcal{D}(\mathcal{L}^*)$ as the solution to the algebraic Riccati equation (ARE), see [3]:

$$0 = \langle \mathcal{A}\phi_m, \Pi_2\psi_n \rangle + \langle \Pi_2\phi_m, \mathcal{A}\psi_n \rangle + \langle \mathcal{C}\phi_m, \mathcal{C}\psi_n \rangle - \langle \mathcal{B}^*\Pi_2\phi_m, R^{-1}\mathcal{B}^*\Pi_2\psi_n \rangle$$
(80)

where $\phi_m \in \mathcal{D}(\mathcal{L})$ and $\psi_n \in \mathcal{D}(\mathcal{L}^*)$ with $\Pi_2 \phi_n \in \mathcal{D}(\mathcal{L}^*)$. As previously defined, $\Pi_{2,nm} = \langle \psi_n, \Pi_2 \phi_m \rangle = \delta_{nm}$, and the ARE becomes,

$$0 = 2\lambda_n \Pi_{2,nn} + \mathcal{C}_{nn}^2 - \mathcal{E}_{nn} \Pi_{2,nn}^2$$
(81)

where $\mathcal{E} = \mathcal{B}R^{-1}\mathcal{B}^*$. The explicit, nonnegative solution is determined to be,

$$\Pi_{2,nn} = \mathcal{E}_{nn}^{-1} \left(\lambda_n + \sqrt{\lambda_n^2 + \mathcal{E}_{nn} \mathcal{C}_{nn}^2} \right)$$
(82)

Then, the optimal control law for the infinite-time interval is given by,

$$u^{\min}(x_0;t) = -R^{-1}\mathcal{B}^* \sum_{n=0}^{\infty} \mathcal{E}_{nn}^{-1} \cdot \left(\lambda_n + \sqrt{\lambda_n^2 + \mathcal{E}_{nn}\mathcal{C}_{nn}^2}\right) \langle x_0, \psi_n \rangle \phi_n(\cdot)$$
(83)

For the case when state measurement is not considered, i.e. C = 0, the ARE is reduced to,

$$0 = 2\lambda_n \Pi_{2,nn} - \mathcal{E}_{nn} \Pi_{2,nn}^2 \tag{84}$$

with two possible solutions,

$$\Pi_{2,nn} = \begin{cases} 0\\ 2\mathcal{E}^{-1}\lambda_n \end{cases}$$
(85)

Since $\lambda_n < 0$ in Eqs.17-18 given that Eq.19 holds, the only nonnegative solution is $\Pi_{2,nn} = 0$ and the optimal input is given by,

$$u^{\min}(x_0;t) = 0 \tag{86}$$

Note that the state linear system $\Sigma(\mathcal{A}, \mathcal{B}, 0)$ is not exponentially detectable and therefore the ARE does not admit a unique nonnegative solution $\Pi_{2,nn}$ that guarantees the stability of the closed loop system, $\Sigma(\mathcal{A} - \mathcal{B}R^{-1}\mathcal{B}^*\Pi_{2,nn}, \mathcal{B}, 0)$, see [3].



Fig. 2. Domain and boundary velocity evolution for M = 10, $\eta = 1.5$ and $\nu = -2.75$, and under control law given by Eq.54 with input penalty term r = 1.



Fig. 3. Optimal control input given by Eq.83 for infinite-dimensional system with control parameters $Q_{2,nn} = 15$ and $R_{nn} = 0.5$.

V. SIMULATION AND NUMERICAL RESULTS

The system in Eq.37-38 was simulated with optimal control laws for the finite and infinite-dimensional systems given in Eq.54 and Eq.83, respectively. The normalized eigenvectors in Eq.21 with Eq.22 were utilized for exact modal decomposition of the parabolic PDE system, Eq.31-32-33, with no internal reactionary sources, i.e. h = 0, see [2]. The two systems are coupled through the mechanical subsystem states which are injected into the infinite-dimensional system at each time instance. The domain evolution and boundary velocity for the closed-loop system are shown in Fig.2. The optimal heat input profile is shown in Fig.3 and the evolution of the temperature distribution in the time-varying crystal domain is shown in Fig.4.

VI. SUMMARY

In this paper, a parabolic PDE model describing the transport dynamics of a diffusion-reaction process with domain changing along a velocity field was derived from first principles continuum mechanics. The associated time-varying spatial operator was demonstrated to be a Riesz-spectral operator and generator of an exponentially stable C_0 -semigroup. The multiscale control problem formulation of the Czochralski crystal growth process considered the crystal temperature distribution given by the derived PDE with infinite-dimensional state-space representation, coupled



Fig. 4. Closed-loop temperature evolution in domain with crystal slab conductivity k = 1.5 and initial conditions $x(\xi, 0) = x^2$.

through the domain boundary motion determined by the mechanically actuated pulling arm, with dynamics governed by a linear second order ODE with finite-dimensional state space representation. The control objectives were optimal the stabilization of the temperature distribution by heat applied along the domain boundary and by the optimal pulling rate. The LQR optimal control synthesis of the coupled infinite and finite-dimensional linear state system $\Sigma(\mathbf{A}, \mathbf{B}, \mathbf{C})$ was considered. The optimal minimizing inputs for finite and infinite-time intervals, requiring the respective solutions to associated algebraic and time-dependent differential Riccati equations, were determined using the Riesz-spectral properties of the time-varying spatial operator. Numerical simulations provide an insight into the optimal stabilization of crystal slab temperature as the domain undergoes as timevarying change.

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