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# Computation of Empirical Eigenfunctions of Parabolic PDEs with Non-trivial Time-varying Domain

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*Abstract*— **In this article, a methodology to compute the empirical eigenfunctions for the order-reduction of parabolic partial differential equation (PDE) systems with time-varying domain is explored. In this method, a mapping functional is obtained, which relates the time-evolution of the solution of parabolic PDE with the time-varying domain to a fixed reference domain, while preserving space invariant properties of the raw solution ensemble. Subsequently, the Karhunen-Lòeve decomposition is applied to the solution ensemble with fixed spatial domain resulting in a set of optimal eigenfunctions that capture the most energy of data. Further, the low dimensional set of empirical eigenfunctions is mapped ("pushed-back") on the original time-varying domain by an appropriate mapping resulting in the basis for the construction of the reduced-order model of the parabolic PDE system with time-varying domain. Finally, this methodology is used for the order-reduction of the Czochralski crystal growth process model which is a two dimensional parabolic PDE system on a time-varying domain with non-trivial geometry. The transformations which relate the raw data on the time-varying and time-invariant domains are designed to preserve dynamic features of the scalar physical property and comparisons among reduced and high order fidelity models are provided.**

## I. INTRODUCTION

The modeling of a transport process is the most important issue in system analysis and control design. It is currently addressed by phenomenological modeling arising from theoretical first-principles, experimental studies or/and with the help of system identification theory. In many industries including chemical, petrochemical and pharmaceutical plants, model-based control has been very successful; where in majority of them, the underlying plant model is low dimensional and linear. In general, the mathematical models of many industrial relevant transport processes are obtained from conservation laws, such as mass, momentum and/or energy, and yield the forms given by partial differential equations (PDEs). In addition, many of these processes involve the change in the shape and properties of the material which can be characterized by phenomena associated with the phase change, generation and consumption of chemical species through the chemical reaction mechanism, and mass transfer.

Low dimensional model identification of distributed parameter systems governed by PDEs attracted attention of the significant number of researchers in recent years. Among many, the most notable contributions came from Gay and Ray [1], [2], Park and coworkers [3], [4], Christofides and coworkers [5], [6], and Hoo and coworkers [7], [8]. In these contributions, the common interpretation is that the dissipative distributed parameter systems could be modeled and reduced to a low finite dimensional system representation which captures the dominant dynamics while the infinite-dimensional complement associated with the fast and stable dynamics can be neglected. The similar conceptual representation appears in the hydrodynamics where "coherent structures" are associated with the most dominant modes [4], [9], [10].

In general, the model order-reduction can be achieved through the Galerkin's method which assumes the exact knowledge of the model and requires an analytic solution for the eigenvalue problem associated with the spatial operator of parabolic PDE. However, in the case of the nonlinear spatial operator there is no general analytic solution to the eigenvalue problem and the exact description of the underlying distributed parameter system is not known, so the input-output data based approach have been proposed and explored [1]. A well-known approach in the extraction of spatial characteristics (modes) of distributed parameter systems is the use of Karhunen-Loève (KL) expansion on an ensemble of solutions obtained from numerical or experimental resolution of the system (for example see [3]). These modes, known as empirical eigenfunctions, are used as the basis set of functions in Galerkin's method. This approach is widely used in the derivation of accurate reduced-order approximations of many diffusion-reaction systems and fluid flows [4], [9], [10].

Compared to the aforementioned extensive research efforts on identification and model reduction of distributed parameter systems modeled by parabolic PDEs, there are only few studies to address order-reduction of parabolic PDE systems with spatial time-varying domain [11], [12]. In [11], [12] the model identification is realized and includes the synthesis of linear optimal controllers , and design of nonlinear distributed state estimators using stochastic methods [13]. Along the same line, Armaou and Christofides used a mathematical transformation to represent the nonlinear parabolic PDE on a time-invariant spatial domain and applied KL decomposition to obtain the set of eigenfunctions on the fixed domain [14], [15]. This approach cannot be used in general, since the mathematical transformation does not always have the analytical form, e.g. for non-trivial geometry. To obtain a reduced-order approximation of systems governed by PDEs that have a traveling wave solution, Glavaski and coworkers processed the available data set using a "centring" procedure prior to performing KL [16]. This procedure involves giving an appropriate definition of the centre of a wave and moving

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it to a standard position. In the contribution by Fogleman *et al.* the proper orthogonal decomposition (POD) is applied to obtain the *phase invariant POD modes* of internal combustion engine flows [17]. In their contribution, the velocity fields are *stretched* in one dimension to obtain data on a fixed grid such that the divergence-free (continuity) property of the original velocity field is preserved.

Following these ideas, a systematic approach is proposed to obtain a set of empirical eigenfunctions of a set of data given on an spatially time-dependent domain that captures the most energy of the system's dynamics while preserving some physical invariant property. We propose the following methodology which will be discussed in detail in the consecutive sections:

1) The solution to the parabolic PDE can be found as raw data by the experiments or high fidelity numerical simulations which describe the time evolution of dissipative distributed parameter system on a time-varying domain. Having the set of solutions, the transformation that maps data to a fixed domain is defined which preserves some invariant property of the original data.
2) Then, the KL decomposition is applied on the mapped solutions to extract a low dimensional set of eigenfunctions that contains most of the energy of system on fixed domain.
3) Using the inverse of the transformation found in step 1, these eigenfunctions are mapped on the time-varying domain. As a result, a set of time-varying empirical eigenfunctions are obtained and can be used as the reduced-order representation of the initially given distributed parameter system.

Along our previous work [18], the focus of this study is to apply this methodology to a more realistic problem for which the geometry of the time-varying domain is not trivial. The example provided here is a two-dimensional axisymmetric diffusion systems and the efficiency of the proposed methodology is shown in the simulation section. Also, we point out that domain boundary evolution knowledge is essential in this approach.

## II. MATHEMATICAL FORMULATION

### A. Transformation Preserving Invariant Property

It is intended to obtain a set of time-varying empirical eigenfunctions $\{\phi_i(\xi,t)\}, i = 1,2,\cdots,K$ that capture the most energy of the ensemble of solutions $\{x(\xi,t_i)\}, i = 1,2,\cdots,N \gg K$ of the parabolic PDE:

$$\frac{\partial x(\xi,t)}{\partial t} = \mathcal{L}(x(\xi,t)) + u(\xi,t), \tag{1}$$

defined on the time-varying spatial domain $\Omega(t) \subset \mathbb{R}^n$. Here, $\xi \in \Omega(t)$ is the spatial coordinate, $t \in [0,\infty)$ is time, $x(\xi,t)$ is the state variable, $\mathcal{L}(x(\xi,t))$ is the differential operator and PDE is subjected to appropriately defined boundary and initial conditions. It is assumed that the evolution of domain $\Omega(t)$ is known as it can be easily measured in many process systems (for example phase change in the crystal growth processes).

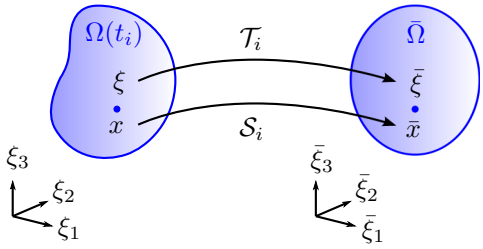


Fig. 1. At each time $t_i$, $\mathcal{T}_i$ maps time-varying domain $\Omega$ to fixed domain $\bar{\Omega}$. Also, the transformation $\mathcal{S}_i$ maps the state $x(\xi,t_i)$ from time-varying domain to $\bar{x}(\xi_i)$ on the fixed domain

Suppose that, there exists a sufficiently smooth, orientation preserving, and invertible mapping $\mathcal{T}_i$ that maps the domain $\Omega(t_i)$ to a fixed reference configuration $\bar{\Omega}$ as $\mathcal{T}_i : \xi \in \Omega(t_i) \mapsto \bar{\xi} \in \bar{\Omega}$ given by: (see Fig. 1)

$$\bar{\xi} = \bar{\xi}(\xi). \tag{2}$$

Having the state $x(\xi,t_i)$, we are interested to obtain the *same* property $\bar{x}_i(\bar{\xi})$ at each point in $\bar{\Omega}$ such that the property $f(t_i)$ (e.g. temperature) is invariant and therefore preserved for the element $d\Omega$ by the relation:

$$df = g(x(\xi,t_i))d\Omega = g(\bar{x}_i(\bar{\xi}))d\bar{\Omega}, \tag{3}$$

where $g(x)$ is the function defining $f$. Starting with the left-hand side of (3), one obtains:

$$df = g(x(\xi,t_i))d\Omega = g(x(\xi,t_i))J^{-1}d\bar{\Omega}, \tag{4}$$

where $J^{-1}$ is the determinant of the inverse of Jacobian matrix $J = \partial\xi/\partial\bar{\xi}$ which exists, since $\mathcal{T}_i$ is smooth and invertible. Then, by comparing (3) and (4):

$$g(x(\xi,t_i))J^{-1} = g(\bar{x}_i(\bar{\xi})), \tag{5}$$

or the function $\bar{x}$ is given by:

$$\bar{x}_i(\bar{\xi}) = g^{-1}(g(x(\xi,t_i))J^{-1}). \tag{6}$$

Therefore, (6) can be regarded as the transformation $\mathcal{S}_i$ that maps the state $x(\xi,t_i)$ on the time-varying domain to the state $\bar{x}_i(\bar{\xi})$ on the fixed reference domain preserving the invariant property $f$. Note that, $\mathcal{T}_i$ maps the domain (geometry) of interest, while $\mathcal{S}_i$ maps the state (see Fig. 1).

### B. Karhunen-Loève Decomposition

The Karhunen-Loève decomposition (KL) is a procedure for representation of an stochastic field with minimum number of degrees of freedom [19], [20]. In this subsection we briefly outline the KL procedure which is used to calculate the empirical eigenfunctions from the data on the fixed domain.

Consider the space of square integrable real-valued functions $\bar{x}(\bar{\xi})$ with inner product $\langle \bar{x}, \bar{y} \rangle_{\bar{\xi}}$. Given an ensemble of states $\{\bar{x}_i(\bar{\xi})\}$, $i = 1,2,\cdots,N$, whose ensemble average is denoted by:

$$\widehat{\bar{x}_i(\bar{\xi})} = \frac{1}{N}\sum_{i=1}^{N} \bar{x}_i(\bar{\xi}), \tag{7}$$

it is intended to obtain a function $\bar{\phi}(\bar{\xi})$ that maximizes $\widehat{\langle \bar{\phi}, \bar{x}_i \rangle}^2_{\bar{\xi}}$, i.e. $\bar{\phi}(\bar{\xi})$ is closest to all $\bar{x}_i(\bar{\xi})$. This problem can be expressed as finding $\max_{\bar{\phi}(\bar{\xi})} \lambda$ where:

$$\lambda = \frac{\widehat{\langle \bar{\phi}, \bar{x}_i \rangle}^2_{\bar{\xi}}}{\langle \bar{\phi}, \bar{\phi} \rangle_{\bar{\xi}}}. \tag{8}$$

Defining the two-point correlation function $K(\bar{\xi}, \bar{\eta}) = \widehat{\bar{x}_i(\bar{\xi}) \bar{x}_i(\bar{\eta})}$ for $\bar{\xi}, \bar{\eta} \in \bar{\Omega}$ and the linear operator $R$ as:

$$R\bar{\phi} = \left\langle K(\bar{\xi}, \bar{\eta}), \bar{\phi}(\bar{\eta}) \right\rangle_{\bar{\eta}},$$

it can be shown [3] that (8) reduces to the following operator eigenvalue problem:

$$R\bar{\phi} = \lambda \bar{\phi}. \tag{9}$$

Equation (9) can be solved using the Schmidt-Hilbert technique or *the method of snapshots* [21]. In this method, the eigenfunction $\bar{\phi}(\bar{\xi})$ is assumed to be a linear combination of ensemble elements as:

$$\bar{\phi}(\bar{\xi}) = \sum_{i=1}^{N} \alpha_i \bar{x}_i(\bar{\xi}). \tag{10}$$

The set of eigenfunctions $\bar{\phi}_i(\bar{\xi}), i = 1, 2, \cdots, K$ associated with the $K$ largest eigenvalues of $R$ forms an optimal basis in the sense of representation of $\bar{x}(\bar{\xi})$ in terms of $\bar{\phi}_i(\bar{\xi})$ with minimum error.

### C. Time-Varying Empirical Eigenfunctions

Once the set of $K$ eigenfunctions $\bar{\phi}(\bar{\xi})$ are found, they can be transformed to the time-varying domain $\Omega$ at each time $t_i$ using the inverse of $\mathcal{S}_i$ (see (6)). Therefore, we have the basis of $K$ time-varying eigenfunctions $\phi(\xi, t)$ which can be used to represent the state $x(\xi, t)$ on the time-varying domain $\Omega(t)$.

## III. NUMERICAL PROCEDURE AND SIMULATION

In this section, the proposed methodology is applied to a diffusive process where the geometry of the time-varying domain is non-trivial. Although this method can be used for the order-reduction of nonlinear PDEs in general, here we consider a linear parabolic PDE for simplicity. It is important to emphasize that, domain evolution is known *a priori*.

Consider the two-dimensional axisymmetric diffusive system described by the following parabolic PDE:

$$\frac{\partial x}{\partial t} = k \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial x}{\partial r} \right) + \frac{\partial^2 x}{\partial z^2} \right] - \dot{L}(t) \frac{\partial x}{\partial z} + u(t), \tag{11}$$

for $x(r, z, t)$ in time-varying domain $\Omega(t)$ shown in Fig. 2, subject to boundary conditions:

$$\begin{aligned} x(r, z = 0, t) = x(r, z = L(t), t) = 0, \\ \left. \frac{\partial x(r, z, t)}{\partial r} \right|_{r=0} = \left. \frac{\partial x(r, z, t)}{\partial r} \right|_{r=R(t)} = 0, \end{aligned} \tag{12}$$

with non-dimensional process parameter $k = 0.25$ and $\dot{L}(t)$ represent derivative of length function $L(t)$ with respect to time. This system is a model that describes the non-dimensionalized crystal temperature distribution in Czochralski crystal growth process. In this method, the crystal rod is pulled out vertically from the surface ($z = 0$) of a heated pool of melt contained in a crucible. A simplified radius control strategy results the domain evolution in terms of $L(t)$ and $R(t)$ as shown in Fig. 3.

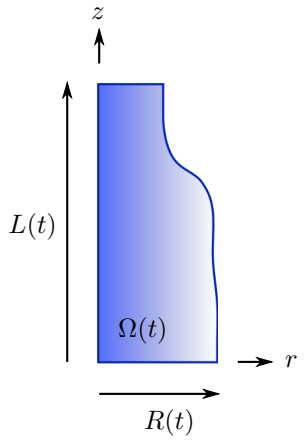


Fig. 2. Schematic representation of crystal growth in Czochralski process. $L(t)$ and $R(t)$ are the length and radius of crystal at time $t$.

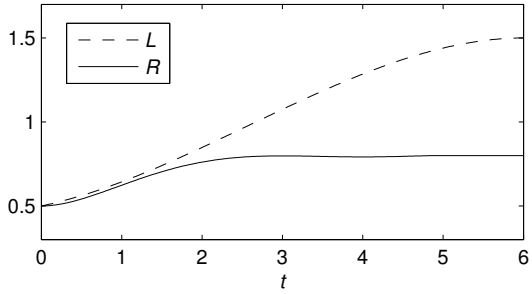


Fig. 3. Evolution of the time-varying domain with non-trivial geometry.

The ensemble of solution of (11) is obtained using finite element method. Since the geometry of domain is time-varying, a moving mesh scheme is used to spatially discretize domain of interest as shown in Fig. 4. The finite element mesh consists of $14 \times 20$ linear 4-noded elements which discretizes geometry to 285 degrees of freedom. The evolution of the time-dependent set of ordinary differential equations obtained from finite element discretization is realized by first-order implicit time integration with time step $dt = 0.025$, while implementing the input $u(t)$ as shown in Fig. 5.

To apply the proposed methodology, the reference configuration $\bar{\Omega}$ on which the solutions of (11) are mapped is considered to be a rectangular with dimensions $\bar{R} = 0.8$ and $\bar{L} = 1.5$. The mapping $\mathcal{T}_i$ can be numerically constructed by introducing sets of computational grid points ($40 \times 80$ points in $r - z$ plain in this example) on both time-varying and fixed domains, as shown in Fig. 6. Associating each grid

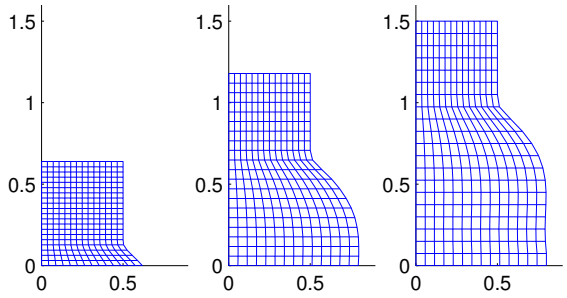

Fig. 4. Finite element moving mesh at $t = 1, 3.5$, and, 6.

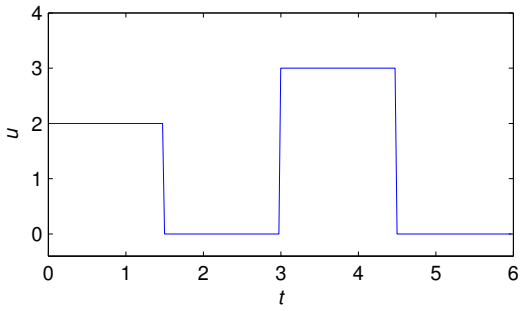


Fig. 5. Input to the PDE system.

point of time-varying domain with one and only one grid point on fixed-domain defines the one-to-one and onto (and hence invertible) mapping $\mathcal{T}_i$. It is important to emphasize that the Jacobian matrix of transformation in this case is space-dependant.

If the state $x(r, z, t)$ represents the temperature at $(r, z) \in \Omega$, the invariant property $f(t_i)$ can be considered to be thermal energy:

$$df = \alpha x d\Omega, \tag{13}$$

where $\alpha$ is a constant, and from (6), the map $\mathcal{S}_i$ found as:

$$\bar{x}_i(\bar{r}, \bar{z}) = J^{-1} x(r, z, t_i). \tag{14}$$

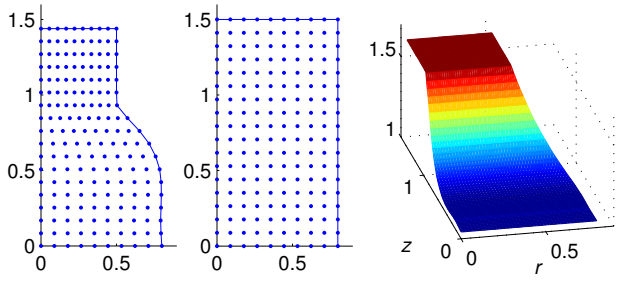

Fig. 6. Computational grid points that define the mapping $\mathcal{T}_i$ by associating each point of the time-varying domain at $t = 5$ (left panel) with one point in fixed domain (middle panel). For illustration, here a $10 \times 18$ grid is shown in this figure, but we used a $40 \times 80$ for computations. Right panel shows $J^{-1}(r, z)$.

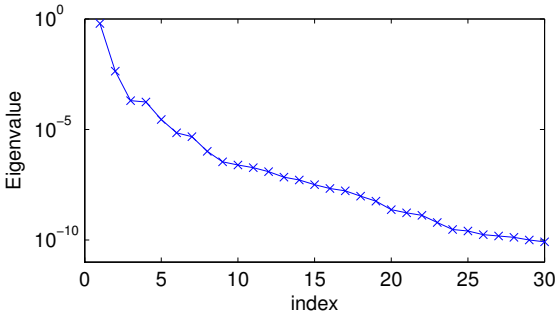


Fig. 7. The first 30 eigenvalues of KL decomposition.

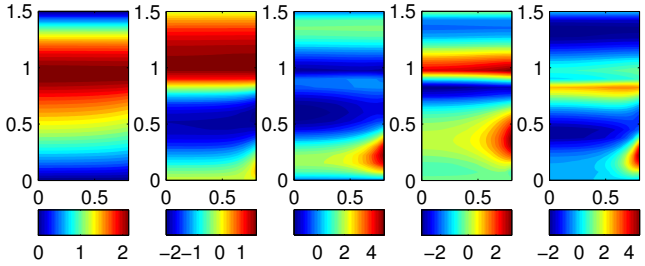

Fig. 8. The first five eigenfunctions extracted from the data mapped to the fixed domain.

Having the temperature distribution $\bar{x}_i(\bar{r}, \bar{z})$ on the fixed domain $\bar{\Omega}$, one can perform KL decomposition to extract empirical eigenmodes $\bar{\phi}_i(\bar{r}, \bar{z}), i = 1, 2, \cdots, K$ of the data with inner product defined as:

$$\langle \bar{x}, \bar{y} \rangle_{(\bar{r},\bar{z})} = \int_{\bar{\Omega}} \bar{r} \bar{x} \bar{y} d\bar{r} d\bar{z}. \tag{15}$$

Fig. 7 shows the first 30 eigenvalues of KL decomposition (see (9)), the first mode captures 99.2% of the energy solutions. Fig. 8 shows the first five eigenmodes on the fixed domain.

Having the set of time-varying eigenfunctions, Galerkin's method is used to obtain the reduced-order model by replacing $x(r, z, t) = \sum_{i=1}^{K} a_i(t)\phi(r, z, t)$ in (11) and projecting on the basis $\phi_j$ to get

$$\dot{a}(t) = A(t)a(t) + B(t)u(t), \tag{16}$$

where

$$\begin{aligned} &a = [a_1 \ a_2 \ \cdots a_K]^T, \\ &A = C^{-1}K, \quad B = C^{-1}F, \\ &C_{ij} = \langle \phi_i, \phi_j \rangle_{(r,z)}, \\ &K_{ij} = \left\langle k \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi_i}{\partial r} \right) + \frac{\partial^2 \phi_i}{\partial z^2} \right] - \dot{L} \frac{\partial \phi_i}{\partial z} - \frac{\partial \phi_i}{\partial t}, \phi_j \right\rangle, \\ &F_i = \langle 1, \phi_i \rangle. \end{aligned} \tag{17}$$

Equation (16) represents the reduced-order model of (11).

Fig. 9 compares the evolution of the norm of the states for reconstruction of the solutions of (11) with the same input

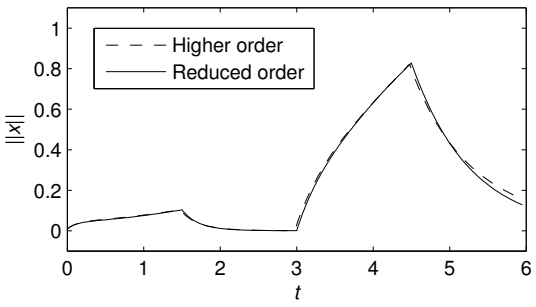


Fig. 9. Comparison of the norm of the state for higher-order finite element and reduced-order Galerkin's method resolutions of the parabolic PDE.

with two time-varying eigenfunctions used in (16). The norm is given by:

$$\|x\| = \langle x, x \rangle_{(r,z)}^{\frac{1}{2}} . \tag{18}$$

As it can be seen the reduced-order model perfectly matches the profile obtained from the high-order simulation, the finite element model with order of 285 is reduced to a second-order system. Reconstructed states resulting from the reduced-order model are shown in Fig. 10 against the finite element solutions.

## IV. Conclusions

In this paper, we proposed a method to obtain a set of time-varying empirical eigenfunctions of a set of data given on an spatially time-dependent domain. In this method the solutions of PDE system on a time-varying domain are mapped to a fixed reference configuration in such a way that invariant properties of the data are preserved. Then, KL decomposition is applied on the mapped solutions to extract a small set of eigenfunctions that contains most of the energy of system on fixed domain. These eigenfunctions are mapped back on the time-varying domain yielding a set of time-varying empirical eigenfunctions that can be used as the reduced-order representation of the main PDE system. The focus is to present the procedure for the problems that have time-varying domain with non-trivial geometry. We applied this approach to the two-dimensional axisymmetric problem of temperature distribution of Czochralski crystal growth process governed by parabolic PDE. The results show the capability of the method as a useful tool in representation of the reduced-order system with time-varying non-trivial domain.

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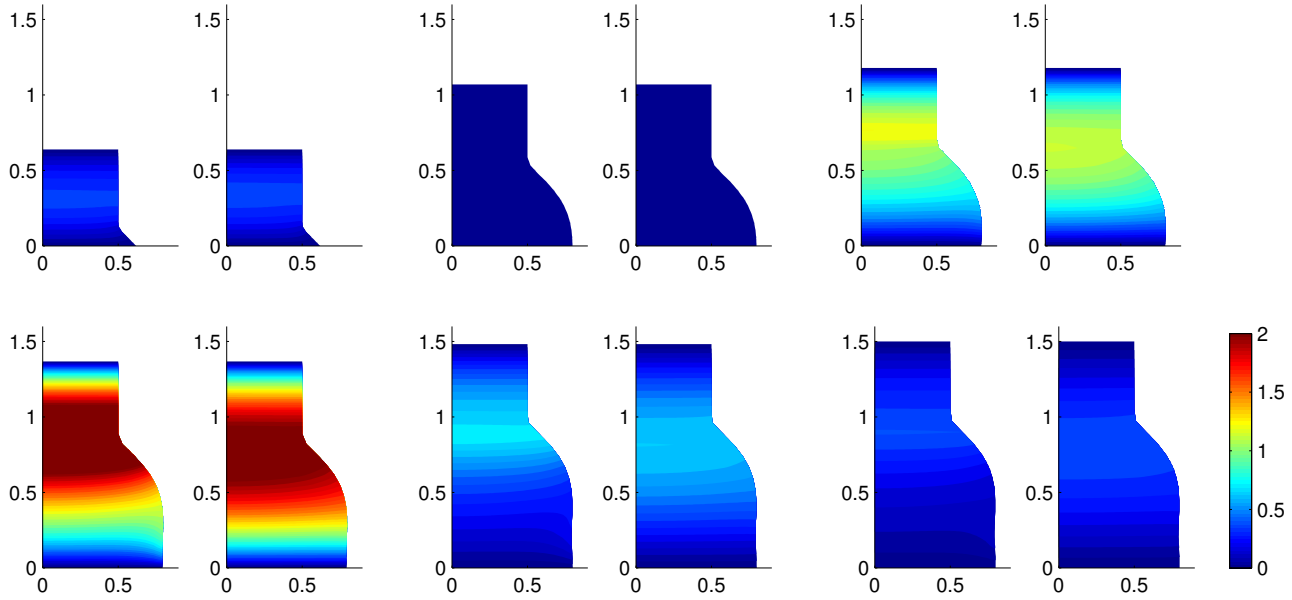


Fig. 10. Solution of the two-dimensional diffusion-reaction system with time-dependent spatial domain using reduced-order (left) and higher-order finite element (right) model at $t = 1, 3, 3.5, 4.5, 5.5,$ and $6$.