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Model Approximation of Thermo-Fluidic Diffusion Processes in Spatially Interconnected Structures

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Abstract— **This work develops a graph-theoretic framework to model thermo-fluidic diffusion processes as a network of distributed parameter systems. A three-step procedure has been proposed to reduce such a network to a finite dimensional system while preserving the boundary conditions. The viability of the developed procedure is illustrated through simulation results under physically realistic scenario.**

I. INTRODUCTION

The study of heat and mass transfer is a popular field of research with a wide range of applications in numerous disciplines. Two major aspects of this research involve the transport of thermal energy in different materials and the dynamic behavior of the fluid flows [1]. Due to the difference in their physical structure, the energy exchange between a solid body and fluid is significant when their physical interaction is allowed. Thermo-fluidic diffusion processes are a specific class of such phenomena where the influence of the thermal energy on the mutual interaction among various solids and fluids is dominantly diffusive [2]. In this way, the motion of the fluid is discarded to acquire the effective interaction between solids and fluids as diffusion processes. These thermo-fluidic diffusion processes can be observed in numerous engineering applications. For example, in the commercial printing and packaging industries, the drying of paper, cardboard, wood, etc. typically involve heat and moisture diffusion through composite materials [3]. In food processing technology, the drying of food items involves diffusion of liquid ingredients under the influence of external heat sources. In semiconductor industries, the doping of impurities in an intrinsic semiconductor involves diffusion of n or p-type species in the different layer of semiconductors [4]. There are two salient features of thermo-fluidic processes in these applications, namely, a) diffusion in multiple physical quantities that are possibly coupled and b) simultaneous interaction of various materials (solids and fluids) in a spatially distributed structure. This paper proposes a generic framework to model a network of coupled diffusion processes in an arbitrary geometrical configuration. Furthermore, we develop a methodology to derive a finite dimensional approximate solution while respecting the mutual interaction among different materials. This reduced order model can be used for simulation, prediction, shape optimization and real-time control of spatially interconnected thermo-fluidic diffusion processes.

In modeling and simulation, little research has been carried out that a) preserves the conservation laws of thermodynamics and mass flows at model boundaries and b) explicitly solves the coupling among physical quantities in materials with different properties. In [1], [5], the model for chemical processes is modeled as a diffusion equation. But the coupled effect is neglected. In [6], [7], the coupled heat and moisture diffusion is considered but this model has not been extended to the diffusion processes in spatially interconnected networks. In [8], [9] and the references therein, a detailed account is provided of various numerical approximation and reduction techniques. However, most of these techniques are focused on methods that are only applicable to decoupled single variable models and the models without spatial interconnection.

In this paper, our contributions are on two aspects:

1) We develop a generic framework to model a network of spatially interconnected diffusion processes that are defined by possibly more than one physical quantities.

2) We develop a three-step procedure to derive a reduced order solution that preserves the interaction among connected materials. Specifically, we characterize the feasibility of deriving a solution with respect to its consistency with the boundary conditions.

The remainder of this paper is organized as follows. The framework to model thermo-fluidic diffusion processes in a spatially interconnected structure is developed in Section II. The corresponding problem for model order reduction is defined in Section III. The formulated problem is solved in Section IV by a discussion of underlying methodologies. Section V analyses the feasibility of the proposed methodologies. Section VI discusses the achieved results with a simulation example. At last, Section VII provides conclusions and directions for future work.

II. FRAMEWORK FOR SYSTEM MODELING

In this section we develop a generic framework to model thermo-fluidic processes over an arbitrary spatial interconnection.

A. Geometrical Configuration

We consider the spatial interconnection of multiple thermo-fluidic processes as a network of systems under an arbitrary topology. A finite connected graph $\mathscr{G}$ describes such a network with a set of nodes $\mathscr{N}$ and edges $\mathscr{E}$

$$\mathscr{G} = (\mathscr{N},\ \mathscr{E}). \tag{1}$$

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Let $\mathbb{M} := \{1, \cdots, M\}$ be the set of indices corresponding to each node. Each element $\mathscr{N}_i$ in the set $\mathscr{N}$, $i \in \mathbb{M}$, describes a specific thermo-fluidic processes in a non-homogeneous material with specific physical properties. To denote the topology of $\mathscr{G}$ we first define an adjacency matrix $A \in \mathbb{Z}^{M\times M}$ whose elements are either zero or one depending on whether the adjacent nodes $\mathscr{N}_i$ and $\mathscr{N}_j$ are physically interconnected or not. Precisely, its entries

$$A_{i,j} = \begin{cases} 1, & \text{if } \mathscr{N}_i \text{ and } \mathscr{N}_j \text{ are interconnected} \\ 0, & \text{otherwise.} \end{cases}$$

The adjacency matrix is symmetric and hence $\mathscr{G}$ is undirected. The set of edges $\mathscr{E} = \{\mathscr{E}_{i,j} \,|\, \text{for all } (i,j) \text{ with } A_{i,j} = 1\}$ describes the interconnection among adjacent nodes. For further details on the graph theoretic properties of its topology we refer to [10]. The geometric configuration of every node $\mathscr{N}_i$ is characterized by a d-dimensional bounded set $\mathbb{S}_i \subseteq \mathbb{R}^d$. Its boundary is defined by the limit-points as

$$\mathbb{B}_i = \mathbb{S}_i \setminus \mathbb{S}_i^\circ,$$

where $\mathbb{S}_i^\circ$ denotes the interior of $\mathbb{S}_i$. The dynamics of $\mathscr{N}_i$ is confined in the spatial domain $\mathbb{S}_i^\circ$ and is constrained by the boundary conditions in $\mathbb{B}_i$. Each $\mathscr{E}_{i,j}$ describes the interconnection between two adjacent nodes ($\mathscr{N}_i$ and $\mathscr{N}_j$) on the their common boundary which is defined by $\mathbb{B}^I_{i,j} \subset \mathbb{B}_i \cap \mathbb{B}_j$. Therefore, the complete boundary $\mathbb{B}_i$ can be divided by an interface boundary $\mathbb{B}^I_{i,j}$ through which adjacent nodes are interconnected and the boundary $\mathbb{B}^{\text{ext}}_i$ through which the node is influenced by external condition. In other words, $\mathbb{B}_i = \mathbb{B}^{\text{ext}}_i + (\bigcup_j \mathbb{B}^I_{i,j})$ where the union applies to all the nodes $\mathscr{N}_j$ which are connected with the particular node $\mathscr{N}_i$. It is assumed that $\mathbb{B}^{\text{ext}}_i \cap \mathbb{B}^I_{i,j}$ is an empty set. Figure 1 illustrates an example topology of thermo-fluidic processes in spatially interconnected structure.

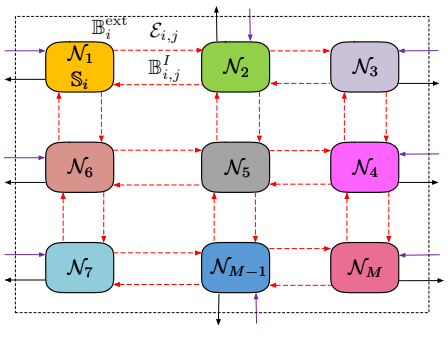

Fig. 1: Topological schematic of M thermo-fluidic processes. $\rightarrow$ indicates the inputs. $\dashrightarrow$ indicates the interconnection between adjacent nodes in $\mathbb{B}^I_{i,j}$.

B. Signal Description

Spatially interconnected distributed parameter systems consist of signals that are functions of space and time. The time axis is denoted as a set of non-negative real numbers $\mathbb{T} := [t_0,\ \infty] \subseteq \mathbb{R}_{\geq 0}$. For any given pair $(s,t) \in (\mathbb{S}_i \times \mathbb{T})$, the thermo-fluidic processes of a mutually interconnected $\mathscr{N}_i$ and $\mathscr{N}_j$ are characterized by the signals given in Figure 2.

States: The state variables z_i are defined on a state space Z_i as an n_i-dimensional vector $z_i : \mathbb{S}_i \times \mathbb{T} \to \mathbb{R}^{n_i}$. Moreover, the cumulative states over the entire graph is defined by $z = \text{col}(z_1, \cdots, z_M) \in Z := \prod_{i=1}^M Z_i$ with dimension $n_z = \sum_{i=1}^M n_i$.

Inputs: The inputs are classified into in-domain inputs and the inputs via external boundaries. The in-domain inputs $q^{\text{int}}_i(s,t)$ act on a subset of $\mathbb{S}_i^\circ \times \mathbb{T}$ and are defined on the in-domain input space Q^{int}_i as an m_i-dimensional vector $q^{\text{int}}_i : \mathbb{S}_i^\circ \times \mathbb{T} \supseteq \mathbb{B}^{\text{int}}_i \times \mathbb{T} \to \mathbb{R}^{m_i}$. On the other hand, the inputs $q^{\text{ext}}_i(s,t)$ act through the external boundary $\mathbb{B}^{\text{ext}}_i$ as a result of the ambient conditions. External inputs are defined on the boundary-input space Q^{ext}_i as a n_i-dimensional vector $q^{\text{ext}}_i : \mathbb{B}^{\text{ext}}_i \times \mathbb{T} \to \mathbb{R}^{n_i}$. For a particular $\mathbb{B}^{\text{ext}}_i$, every state has a corresponding boundary condition and therefore the dimension of the boundary-input vector is identical to the state vector. The cumulative boundary inputs over the entire graph are defined by $q^{\text{ext}} = \text{col}(q^{\text{ext}}_1, \cdots, q^{\text{ext}}_M) \in Q^{\text{ext}} := \prod_{i=1}^M Q^{\text{ext}}_i$ with dimension $n_z = \sum_{i=1}^M n_i$. Similarly, the in-domain boundary inputs over the entire graph are defined by $q^{\text{int}} = \text{col}(q^{\text{int}}_1, \cdots, q^{\text{int}}_M) \in Q^{\text{int}} := \prod_{i=1}^M Q^{\text{int}}_i$ with dimension $n_m = \sum_{i=1}^M m_i$

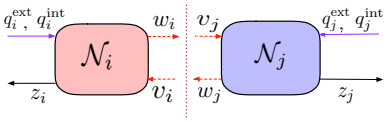

Fig. 2: Signal flow of two thermo-fluidic processes $\mathscr{N}_i$ and $\mathscr{N}_j$. For each node $\rightarrow$ indicates the boundary and in-domain inputs. $\rightarrow$ indicates the state-variables. $\dashrightarrow$ indicates the interaction signals.

Interaction Signals: The spatially distributed structure allows interaction among mutually interfaced thermo-fluidic diffusion processes. The edge $\mathscr{E}_{i,j}$ is characterized by the interaction output signals w_i, w_j and input signals v_i, v_j. In particular, $w_i, v_i : \mathbb{B}^I_{i,j} \times \mathbb{T} \to \mathbb{R}^{n_i}$ belongs to the interface state space $W_i, V_i \subseteq Z_i$ defined on the interface boundary $\mathbb{B}^I_{i,j}$. These interaction signals restrict the transport of state variables among nodes based on the net energy balance.

C. System Dynamics

At each node $\mathscr{N}_i$, we describe the thermo-fluidic diffusion processes D_i as n_i coupled linear parabolic partial differential equations. Here, we also consider the physical parameters to be spatially varying functions with sufficient smoothness. An operator based state space model defines D_i as

$$\mathcal{E}_i \frac{\partial z_i}{\partial t} = \mathcal{A}_i z_i + \mathcal{B}^{\text{int}}_i q^{\text{int}}_i \qquad (\text{D}_i)$$

Here, $\mathcal{A}_i : Z_i \to Z_i$ denotes an LTI differential operator. Precisely, $\mathcal{A}_i z_i := [\nabla \cdot K_i(s) \nabla] z_i$. The operator $\mathcal{E}_i$ is defined as $\mathcal{E}_i := E_i(s)$. Here, $K_i(s)$ and $E_i(s)$ are positive symmetric matrices that respectively represent the physical conductivity and specific capacity. Furthermore, $\mathcal{B}^{\text{int}}_i : Q^{\text{int}}_i \to Z_i$ is the in-domain input operator.

D. Boundary Conditions

The spatio-temporal evolution of the state variables z_i are constrained at the boundary $\mathbb{B}_i$ with the help of physically realistic conditions. They are a) the boundary conditions $\mathrm{B}_i^{\mathrm{ext}}$ describing the effect of external conditions across $\mathbb{B}_i^{\mathrm{ext}}$ and b) the boundary conditions $\mathrm{B}_{i,j}^{I}$ describing exchange among (w_i,v_i) and (w_j,v_j) across $\mathbb{B}_{i,j}^{I}$.

1) External Boundary Conditions: $\mathrm{B}_i^{\mathrm{ext}}$ describes the effect of q_i^{ext} as a loss of net flux across $\mathbb{B}_i^{\mathrm{ext}}$ by the following non-homogeneous boundary conditions (cf. [5]):

$$\mathcal{H}_i^{\mathrm{ext}}\ z_i\big|_{s\in\mathbb{B}_i^{\mathrm{ext}}} = q_i^{\mathrm{ext}}. \tag{$\mathrm{B}_i^{\mathrm{ext}}$}$$

Here, $\mathcal{H}_i^{\mathrm{ext}} : Z_i \to Q_i^{\mathrm{ext}}$ is a boundary operator (possibly unbounded). Precisely, this boundary condition describes the net loss of flux across the outward normal direction $\mathbf{b}_i^{\mathrm{ext}}$ according to

$$\mathcal{H}_i^{\mathrm{ext}}\ z_i := [\kappa_i(s)\frac{\partial}{\partial \mathbf{b}_i^{\mathrm{ext}}} + H_i^{\mathrm{ext}}(s)]z_i.$$

H_i^{ext} is a symmetric matrix that represents the state transfer coefficient with the external environment. The above relation describes a Dirichlet condition if $\kappa_i(s) = 0$, $H_i^{\mathrm{ext}}(s) \succ 0$ and a Newman condition if $\kappa_i(s) = K_i(s)$, $H_i^{\mathrm{ext}}(s) = 0$. Otherwise, it defines a mixed boundary condition (cf. [5]).

2) Interface Boundary Conditions: For the interconnected nodes $\mathscr{N}_i$ and $\mathscr{N}_j$, we consider that $\mathrm{col}(w_i,\ w_j)$ and $\mathrm{col}(v_i,\ v_j)$ are algebraically related by an operator $\mathcal{L}_{i,j}$ according to

$$\begin{bmatrix} w_i \\ w_j \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}}_{\mathcal{L}_{i,j}} \begin{bmatrix} v_i \\ v_j \end{bmatrix}. \tag{2}$$

The edge $\mathscr{E}_{i,j}$ defines an interface boundary condition $\mathrm{B}_{i,j}^{I}$ over $\mathbb{B}_{i,j}^{I}$ in terms of the these interaction inputs and outputs. We define an interaction input operator $\mathcal{P}_{i,j}^{v} : Z_i \times Z_j \to V_i \times V_j$ that maps from the mutual state space to the interface state space. Similarly, the interaction output operator is $\mathcal{P}_{i,j}^{w} : Z_i \times Z_j \to W_i \times W_j$. As a result, we can rewrite (2) in terms of $\mathrm{col}(z_i,\ z_j)$ and obtain the following equality:

$$\underbrace{\begin{bmatrix} \mathcal{P}_{i,j}^{w} - \mathcal{L}_{i,j}\mathcal{P}_{i,j}^{v} \end{bmatrix}}_{\mathcal{P}_{i,j}^{I}} \begin{bmatrix} z_i \\ z_j \end{bmatrix} = 0. \tag{$\mathrm{B}_{i,j}^{I}$}$$

Now the definitions of $\mathcal{P}_{i,j}^{w}$ and $\mathcal{P}_{i,j}^{v}$ vary based on the net loss of energy across the interface boundary. They are

Lossy Interface: Here, losses are allowed across the outward normal direction $\mathbf{b}_{i,j}^{I}$ with

$$\mathcal{P}_{i,j}^{w} := \begin{bmatrix} K_i(s)\frac{\partial}{\partial \mathbf{b}_{i,j}^{I}} + H_{i,j}^{I}(s) & 0 \\ 0 & K_j(s)\frac{\partial}{\partial \mathbf{b}_{i,j}^{I}} \end{bmatrix}, \mathcal{P}_{i,j}^{v} := \begin{bmatrix} K_i(s)\frac{\partial}{\partial \mathbf{b}_{i,j}^{I}} & 0 \\ 0 & H_{i,j}^{I}(s) \end{bmatrix}.$$

$H_{i,j}^{I}$ is a positive symmetric matrix that represents the state transfer coefficient across $\mathbb{B}_{i,j}^{I}$.

Loss-less Interface: Here, no loss is allowed across the outward normal direction $\mathbf{b}_{i,j}^{I}$ with

$$\mathcal{P}_{i,j}^{w} := \begin{bmatrix} I & 0 \\ 0 & K_j(s)\frac{\partial}{\partial \mathbf{b}_{i,j}^{I}} \end{bmatrix}, \mathcal{P}_{i,j}^{v} := \begin{bmatrix} K_i(s)\frac{\partial}{\partial \mathbf{b}_{i,j}^{I}} & 0 \\ 0 & I \end{bmatrix}.$$

III. PROBLEM DEFINITION

Suppose that the following definitions are given

G.1 A finite and connected graph $\mathscr{G} = (\mathscr{N}, \mathscr{E})$.

G.2 A symmetric adjacency matrix A.

G.3 Every node $\mathscr{N}_i$ as

$$\mathscr{N}_i = (\mathbb{S}_i, \mathbb{B}_i^{\mathrm{ext}}, \mathbb{B}_i^{\mathrm{int}}, \mathrm{D}_i, \mathrm{B}_i^{\mathrm{ext}}).$$

G.4 Every edge $\mathscr{E}_{i,j}$ as

$$\mathscr{E}_{i,j} = (\mathbb{B}_{i,j}^{I}, \mathrm{B}_{i,j}^{I}).$$

G.5 Initial condition $z(t_0) := \mathrm{col}(z_1(t_0), \cdots, z_M(t_0))$ which must be compatible with the boundary conditions.

The aim of this paper is to derive a unique solution $z := \mathrm{col}(z_1, \cdots, z_M)$ of the complete graph $\mathscr{G}$ that satisfies (G.1)-(G.5). Standard numerical techniques often lead to a very large scale system which are computationally expensive [8]. In order to circumvent such difficulties, model reduction techniques are typically employed where the infinite dimensional solution is replaced by an approximated finite dimensional solution. To this end, in this paper, the problem amounts to developing a generic model reduction technique that will yield a computationally cheaper finite dimensional model which will satisfy such spatially interconnected model structure keeping all the boundary conditions preserved.

IV. METHODOLOGIES

In this section, we propose a three-step procedure to determine the solution $z := \mathrm{col}(z_1, \cdots, z_M)$ for the entire graph satisfying all the external and interface boundary conditions. First, we derive an abstract state space model that describes the dynamical behaviour of the graph. At the second stage, the solution of this model is decomposed as the spectral expansion of spatially and temporally varying functions which are parametrized to ensure a unique definition of z. At the third stage, this solution is projected onto a finite dimensional space to obtain a reduced order model.

A. State Space Model via Separation of Solution

To incorporate the non-homogeneous action of q_i^{ext} in the boundary condition ($\mathrm{B}_i^{\mathrm{ext}}$), we use the linearity of the system operator to postulate that

$$z(s,t) := x(s,t) + \mathcal{G}\ q^{\mathrm{ext}}(s,t), \tag{3}$$

with $x = \mathrm{col}(x_1, \cdots, x_M)$. The equation (3) must satisfy (G.1)–(G.5) when every q_i^{int} is set to zero. Here, $\mathcal{G} : Q^{\mathrm{ext}} \to Z$ is a uniquely defined bounded operator that describes the effect of each possible q_i^{ext} on z. The boundary conditions impose the following constraints on the definition of $\mathcal{G}$

$$\mathcal{H}^{\mathrm{ext}}\mathcal{G}\ q^{\mathrm{ext}} = q^{\mathrm{ext}}, \quad \mathcal{P}^{I}\mathcal{G}\ q^{\mathrm{ext}} = 0. \tag{4}$$

Here, $\mathcal{H}^{\text{ext}}$ and $\mathcal{P}^I$ are block-diagonal operators whose entries are $\mathcal{H}_i^{\text{ext}}$ and $\mathcal{P}_{i,j}^I$ with $i,j \in \mathbb{M}$. Thus a suitable operator $\mathcal{G}$, under the constraints (4), describes the effect of boundary inputs. Subsequently, the solution of $x(s,t) : \bigcup_{i=1}^{M} \mathbb{S}_i \times \mathbb{T} \to \mathbb{R}^{n_z}$ amounts to substituting (3) in (D_i), (B_i^{ext}) and ($\text{B}_{i,j}^I$). Given that $q_i^{\text{ext}} \in C^2(\mathbb{T}, Q_i^{\text{ext}})$ and $q_i^{\text{int}} \in C^1(\mathbb{T}, Q_i^{\text{int}})$ (cf. [11], [12]), an extended state space model is derived in the following abstract form

$$\underbrace{\begin{bmatrix} \mathcal{E} & 0 \\ 0 & I \end{bmatrix}}_{\mathbf{E}} \frac{\partial x^e}{\partial t} = \underbrace{\begin{bmatrix} \mathscr{A} & \mathcal{A}\mathcal{G} \\ 0 & 0 \end{bmatrix}}_{\mathbf{A}} x^e + \underbrace{\begin{bmatrix} \mathcal{B}^{\text{int}} & -\mathcal{E}\mathcal{G} \\ 0 & I \end{bmatrix}}_{\mathbf{B}} u. \tag{5}$$

Here the extended state vector $x^e := \text{col}(x, q^{\text{ext}})$ is defined on $Z^e := Z \times Q^{\text{ext}}$ as an extension of the original state space over the boundary input spaces for all the connected nodes. Similarly, the input vector $u := \text{col}(q^{\text{int}}, \frac{\partial q^{\text{ext}}}{\partial t})$ is defined on $Q^e := Q^{\text{int}} \times Q^{\text{ext}}$. Moreover, $\mathcal{A}$, $\mathcal{E}$ and $\mathcal{B}^{\text{int}}$ are block diagonal operators whose entries are the corresponding operators that belong to the respective node. The operator $\mathscr{A} : \text{dom}(\mathscr{A}) \to Z$ is related to the system operator $\mathcal{A}$ by constraining it to the boundary conditions (B_i^{ext}) and ($\text{B}_{i,j}^I$). Precisely,

$$\mathscr{A} := \Big(\mathscr{A}x = \mathcal{A}x | \forall x \in Z, \mathcal{H}^{\text{ext}} x = 0, \mathcal{P}^I x = 0 \Big). \tag{6}$$

To summarize, with the initial condition $x^e(t_0) := \text{col}(z(t_0) - \mathcal{G}\ q^{\text{ext}}(t_0),\ q^{\text{ext}}(t_0))$, the equation (5) defines the extended state space model of the entire graph satisfying all the boundary conditions. The above methodology is an extension of classical homogenization approach used in multi-varibale calculus (cf. [12]).

B. Decomposition and Parametrization of Solution

In the current subsection, the solution of (5) is associated with a set of known functions which are generated by the corresponding operators. These functions are subsequently parameterized by a set of coefficients which act as degrees of freedom to the chosen functions. As a result, obtaining a unique set of these coefficients will ensure a unique solution for x^e. Due to the infinite dimensional nature of Z^e in the state space model (5), the spectral factorization (cf. [13]) of x^e is expressed as an infinite sum where each component of the sum is a product of spatial basis functions and temporal coefficient functions as

$$x^e(s,t) = \begin{bmatrix} x(s,t) \\ q^{\text{ext}}(s,t) \end{bmatrix} = \sum_{m=1}^{\infty} \underbrace{\begin{bmatrix} \Theta_m^x(t) & 0 \\ 0 & \Theta_m^q(t) \end{bmatrix}}_{\Theta_m(t)} \underbrace{\begin{bmatrix} \Phi_m^x(s) \\ \Phi_m^q(s) \end{bmatrix}}_{\Phi_m(s)}. \tag{7}$$

Here, Z^e is spanned by a countable set of basis functions $\{\Phi_m(s) := \text{col}(\Phi_m^x, \Phi_m^q) | m \in \mathbb{Z}^+\}$. $\Phi_m^x(s)$ and $\Phi_m^q(s)$ are n_z dimensional vectors whose elements are $\phi_{i,m}^{x,j}(s)$ and $\phi_{i,m}^{q,j}(s)$ corresponding to x_i^j and $q_i^{\text{ext},j}$ respectively. The coefficient matrices $\Theta_m^x(t)$ and $\Theta_m^q(t)$ are diagonal whose entries $\theta_{i,m}^{x,j}(t)$ and $\theta_{i,m}^{q,j}(t)$ are the coefficients to the respective basis. Additionally, we consider $\phi_{i,m}^{k,j}(s)$ is defined according to

$$\phi_{i,m}^{k,j}(s) = \alpha_{i,m}^{k,j} f_{i,m}^{k,j}(\omega_m, s) + \beta_{i,m}^{k,j} g_{i,m}^{k,j}(\omega_m, s),\ k \in \{x,q\}. \tag{8}$$

Here, $f_{i,m}^{k,j}$ and $g_{i,m}^{k,j}$ are sufficiently smooth functions which are either chosen in advance or derived analytically. ω_m acts an identifier associated with each basis function to guarantee their uniqueness for every $m \in \mathbb{Z}^+$. $\alpha_{i,m}^{k,j}$ and $\beta_{i,m}^{k,j}$ are two coefficients which act as two degrees of freedom. Substituting the expansion (7) in (4) and (6) we obtain the following equations for every $m \in \mathbb{Z}^+$

$$\begin{aligned} &\mathcal{H}^{\text{ext}}\ \mathcal{G}\ \Theta_m^q(t)\ \Phi_m^q(s) = \Theta_m^q(t)\ \Phi_m^q(s), \\ &\mathcal{H}^{\text{ext}}\ \Theta_m^x(t)\ \Phi_m^x(s) = 0, \\ &\mathcal{P}^I\ \mathcal{G}\ \Theta_m^q(t)\ \Phi_m^q(s) = 0, \quad \mathcal{P}^I\ \Theta_m^x(t)\ \Phi_m^x(s) = 0. \end{aligned} \tag{9}$$

To determine the degrees of freedom for each basis function, we substitute (8) in (9). We obtain the following characteristic equation

$$\Gamma_m(\omega_m) \Xi_m(t) = 0. \tag{10}$$

Here $\Gamma_m(\omega_m)$ is a square matrix and $\Xi_m(t) := \text{col}\Big(\alpha_{i,m}^{k,j} \theta_{i,m}^{k,j},\quad \beta_{i,m}^{k,j} \theta_{i,m}^{k,j} \Big)_{i \in \mathbb{M}, j \in \mathbb{N}}^{k \in \{x,q\}}$ is a time dependent vector. If we can obtain a unique value for individual $\alpha_{i,m}^{k,j}, \theta_{i,m}^{k,j}$ and $\beta_{i,m}^{k,j}$ for every $m \in \mathbb{Z}^+$, we can uniquely parametrize x^e using (7). In Section V, we discuss various possibilities to parametrize the basis functions and their temporal coefficients.

C. Approximation of Solution

In the preceding subsections, we have described the decomposition of x^e and its corresponding parametrization. In this section, we derive a finite dimensional model to approximate the infinite dimensional solution of the entire graph.

Based on the state space model in (5), we define a residual operator $\mathbf{R} : Z^e \to Z^e$ in the following manner

$$\mathbf{R}(x^e) := \mathbf{E} \frac{\partial x^e}{\partial t} - \mathbf{A} x^e - \mathbf{B} u = 0. \tag{11}$$

A finite dimensional model is obtained by projecting both x^e and the residual (11) on a finite dimensional subspace Z_H^e of Z^e. To this end, we assume that Z^e is a separable Hilbert space with inner product defined as $\langle \cdot, \cdot \rangle : Z^e \times Z^e \to \mathbb{R}$. Let, Z_H^e be a H dimensional subspace spanned by the first H basis functions of Z^e as $\{\Phi_m(s) \mid m = 1, \cdots, H\}$. Since $Z^e := Z \times Q^{\text{ext}}$ with $\Phi_m = \text{col}(\Phi_m^x,\ \Phi_m^q)$, the finite dimensional approximation of (11) is given by solution $\hat{x}^e(s,t)$

$$\hat{x}^e(s,t) = \sum_{m=1}^{H} \Theta_m(t) \Phi_m(s), \tag{12}$$

that satisfies

$$\big\langle \Phi_m, \mathbf{R}(\hat{x}^e) \big\rangle = 0; \quad \forall m \in \{1, \cdots, H\}. \tag{13}$$

Here, the equation (13) represents a H-dimensional state space model of (11). In particular, this represents a set of ordinary differential equations in terms of $\mathbf{a}(t) := \text{col}\Big(\theta_{i,m}^{k,j} \Big)_{i \in \mathbb{M}, j \in \mathbb{N}}^{k \in \{x,q\}}$ driven by the projected input $\mathbf{b}(t) := \langle \Phi_m, u \rangle$. In order to solve them, the time derivative can be approximated as $\dot{\mathbf{a}}(t)|_l \approx \frac{\mathbf{a}(t_{l+1}) - \mathbf{a}(t_l)}{T_d}$ with $l = \{0, \ldots, N\}$ and the sampling period T_d. Using stable time marching methods

[14] $\mathbf{a}(t_l)$ can be solved in an iterative fashion. The evaluation of the first iteration $\mathbf{a}(t_0)$ can be derived by projecting the initial condition $x^e(t_0)$ onto Z_H^e in a similar fashion.

V. FEASIBILITY ANALYSIS

The three-step procedure largely depends on the unique parametrization of individual $\alpha_{i,m}^{k,j}$,$\beta_{i,m}^{k,j}$ and $\theta_{i,m}^{k,j}$. The feasibility of finding its unique values amounts to verifying whether we can obtain a non-trivial set of all parameters in the kernel-space of $\Gamma_m(\omega_m)$. However, the construction of (10) strongly depends on the choice of structuring $\Phi_m(t)$ and $\Theta_m(t)$ in (8). Here, we define two feasibility criteria and apply them to verify different choices of building (8).

Definition 5.1: If the choice of parametrizing $\Phi_m(s)$ and $\Theta_m(t)$ is such that (10) leads to a constant (t independent) vector Ξ_m which uniquely spans the kernel-space of $\Gamma_m(\omega_m)$ for every $m \in \mathbb{Z}^+$, then the selected parametrization has '*continual feasibility*' to satisfy (9).

Definition 5.2: Consider that the time axis is discretized with equidistant samples such that $t_{l+1} = t_l + T_d$ with T_d the sampling period and $l = \{1, \cdots, N\}$. If the parametrization of $\Phi_m(s)$ and $\Theta_m(t)$ is such that (10) leads to a unique $\Xi_m(t_l)$ for every t_l and $m \in \mathbb{Z}^+$, then the selected parametrization has '*recurrent feasibility*' to satisfy (9) at the time sample t_l.

1) Case 1: A possible structure of (7) would be to consider identical basis functions for every element in $\Phi_m(s)$. In other words, $\phi_{i,m}^{k,j}(s) = \phi_m(s)$ for all i, j, k and Z^e is spanned by $\{\phi_m(s) \mid m \in \mathbb{Z}^+\}$. Hence, $x^e(s,t)$ is defined according to

$$x^e(s,t) = \sum_{m=1}^{\infty} \Theta_m(t)\phi_m(s). \tag{14}$$

Theorem 5.1: The solution decomposition in (14) satisfying (9) is not feasible.

Proof: We use the definition (8) to re-write it in terms of two parameters as $\phi_m(s) = \alpha_m f(\omega_m, s) + \beta_m g(\omega_m, s)$. As a result, (10) takes the form $\Xi_m(t) := \text{col}\Big(\alpha_m \theta_{i,m}^{k,j}(t),\ \beta_m \theta_{i,m}^{k,j}(t)\Big)_{i\in\mathbb{M}, j\in\mathbb{N}}^{k\in\{x,q\}}$. If we consider the time axis to be sampled, with $\theta_{i,m}^{k,j}(t_l)$ being recursively calculated, finding a unique α_m and β_m from $\Xi_m(t_l)$ is still not feasible. ■

2) Case 2: Another choice of parametrization is to keep the same structure as (7), i.e. different basis functions and different temporal coefficients for all the elements in x^e. Precisely,

$$x^e(s,t) = \sum_{m=1}^{\infty} \Theta_m(t)\Phi_m(s). \tag{15}$$

Theorem 5.2: The parametrization of the solution decomposition in (15) satisfying (9) has recurrent feasibility.

Proof: For sampled time set we obtain unique $\Xi_m(t_l)$ from $\Gamma_m(\omega_m)\Xi_m(t_l) = 0$. Precisely, $\Xi_m(t_l) := \text{col}\Big(\alpha_{i,m}^{k,j}\theta_{i,m}^{k,j}(t_l),\ \beta_{i,m}^{k,j}\theta_{i,m}^{k,j}(t_l)\Big)_{i\in\mathbb{M}, j\in\mathbb{N}}^{k\in\{x,q\}}$. If we recursively calculate $\theta_{i,m}^{k,j}(t_l)$ from initial condition $\theta_{i,m}^{k,j}(t_0)$, $\Xi_m(t_l)$ can be uniquely parametrized leading to recurrent feasibility. ■

3) Case 3: The third choice of parametrizing $x^e(s,t)$ would be to consider identical temporal functions $\theta_m(t)$ for each element in $\Theta_m(t)$ and keep different basis functions in $\Phi_m(s)$. In other words, $\theta_{i,m}^{k,j}(t) = \theta_m(t)$. As a result $x^e(s,t)$ takes the following form

$$x^e(s,t) = \sum_{m=1}^{\infty} \theta_m(t)\Phi_m(s). \tag{16}$$

Theorem 5.3: The parametrization of the solution decomposition in (16) satisfying (9) has continual feasibility.

Proof: Using (10), the definition of $\Xi_m(t)$ yields $\Xi_m(t) := \text{col}\Big(\alpha_{i,m}^{k,j}\theta_m(t),\ \beta_{i,m}^{k,j}\theta_m(t)\Big)_{i\in\mathbb{M}, j\in\mathbb{N}}^{k\in\{x,q\}}$. This definition of Ξ_m should hold for all possible non-trivial value of $\theta_m(t)$. As a result, Ξ_m becomes a time independent vector. Hence, such expansion choice leads to continual feasibility. ■

Compared to other cases, (16) leads to a unique parametrization of $\Phi_m(s)$ independent of time. As a result, the expansion in (16) can be a better choice than (15).

VI. SIMULATION RESULTS

To demonstrate the discussed methodologies, we simulate one dimensional heat diffusion in a composite material. A composite material is a non-homogeneous substance which are constructed by interconnecting layers of different materials [3]. The simulation of heat diffusion in such structure allows to analyze the thermal effects of different material when they are mutually interconnected.

A. Graph Definition

Figure 3 illustrates a three-layered composite material in a spatially interconnected structure.

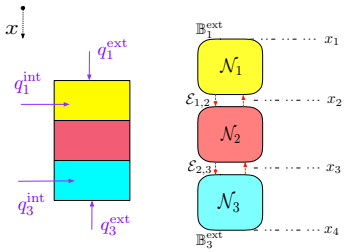

Fig. 3: Diffusion problem in composite materials.

The definitions related to the entire graph $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ are specified in the following items:

1) The graph $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ is equipped with 3 nodes and 2 edges. The nodes are $\{\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3\}$. The edges are $\{\mathcal{E}_{1,2}, \mathcal{E}_{2,3}\}$. The state variable $z_i = T_i$ is temperature($^\circ$C).
2) The adjacency matrix A is a 3×3 symmetric matrix as
$$A = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$
3) For every node $\mathcal{N}_i$, $\mathbb{S}_i = [x_i, x_{i+1}]$ for $i = \{1, 2, 3\}$. $\mathbb{B}_1^{\text{ext}} = x_1$, $\mathbb{B}_3^{\text{ext}} = x_4$ and $\mathbb{B}_2^{\text{ext}}$ is an empty set. In the equation (D_i), $K_i(x)$ is a piece-wise constant with $\mathcal{A}_i z_i := k_i \frac{\partial^2 z_i}{\partial x}$. Similarly, $E_i(x) = \rho_i C_{p,i}$. In the equation (B_i^{ext}), $H_i^{\text{ext}}(x)$

is similarly defined as $H_i^{\text{ext}}(x) = h_i$. Moreover, $\mathbb{B}_1^{\text{int}} = [x_1, x_2]$, $\mathbb{B}_3^{\text{int}} = [x_3, x_4]$ and $\mathbb{B}_2^{\text{int}}$ is an empty set, indicating that there is no input in the second node. $\mathcal{B}_i^{\text{int}}$ is chosen such that q_i^{int} is applied on the whole domain uniformly.

4) For every edge $\mathscr{E}_{i,j}$, $\mathbb{B}_{1,2}^I = x_2$ and $\mathbb{B}_{2,3}^I = x_3$. We assume that, the interface among nodes are loss-less.
5) The initial condition is chosen as $z(t_0) = \mathcal{G}\ q^{ext}$. We consider $q_1^{\text{ext}} = 30°\text{C}$ and $q_3^{\text{ext}} = 15°\text{C}$ as constant values.

B. Heat Transfer in Composite Material

We compare the solution of the proposed method with respect to the solution produced by PDE toolbox in MATLAB that utilizes finite difference method (cf. [14]) on a discretized domain. The comparison between these two simulation results is given in Figure 4. Additionally, Figure 5 shows the temperature difference between the proposed method and the finite difference method. For the considered

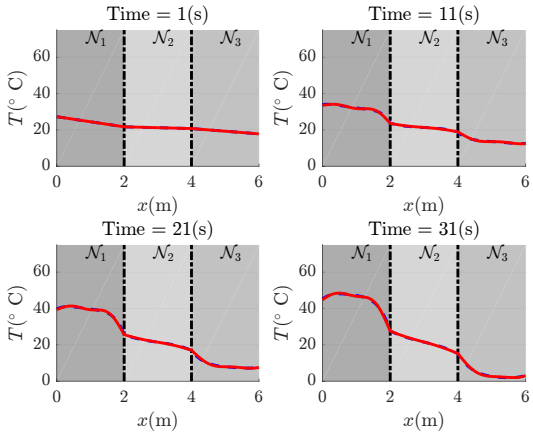

Fig. 4: Temperature distribution of the proposed method with dimension 20 (red line) with respect to the finite difference approach of dimension 50 (blue dotted line) at four time instances. $\mathcal{N}_1$ is heated up with +50 watt/m^2 and $\mathcal{N}_3$ is cooled down with -50 watt/m^2.

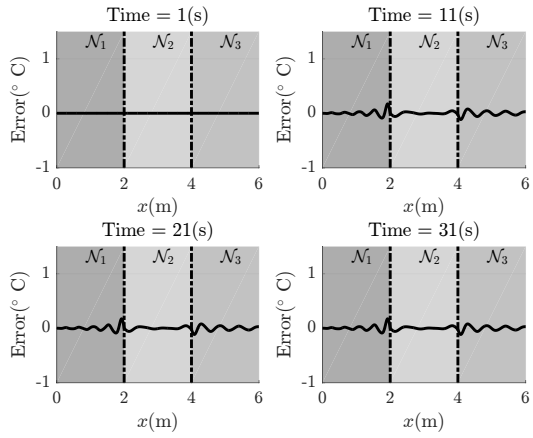

Fig. 5: The temperature difference between the proposed method with finite difference method.

heat diffusion problem, we use linear functions of x to parametrize $\mathcal{G}$ which takes the form $Ax + B$ and can be solved using (4). The basis functions in (7) are chosen as orthonormal Fourier basis [13]. As the state consists of only one variable, the parametrization of Fourier basis in (8) is continually feasible. Based on the Figure 4 and 5, the difference in temperature between two methods is below $\pm 0.2°$C. At the same time, with the proposed method, we are able to achieve significant reduction in the dimension (20 compared to 50). The proposed method also captures the mutual effect of simultaneously heating and cooling the different layers.

VII. CONCLUSIONS

A graph-theoretic framework has been developed where a set of nodes models the network of thermo-fluidic processes, and the edges describes their mutual interconnections. The proposed model is generic for an arbitrary network of spatially interconnected thermo-fluidic processes. The exchange of energy across the interconnection is also taken into account by introducing interface boundary conditions. The three step approximation procedure guarantees feasibility of obtaining a finite dimensional model which preserves the boundary conditions.

However, extending the modeling framework to include other physical behaviour (e.g., fluid dynamics, structural mechanics) is not addressed in this paper. Additionally, the possibility of applying different model reduction techniques for fast computation has also to be further explored. The proposed framework also expedites excellent opportunity to solve model based problems which require further research.

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