Parametric low-order models in transient heat diffusion by MIM. Estimation of thermal conductivity in a 2D slab

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Abstract. Classical modeling methods based on spatial discretization of local governing equations lead to fine meshes, resulting in large size models which require huge computing times. In applications such as on-line inverse or real-time feedback control problems, this issue becomes crucial. Several techniques have been developed for building low-order models, involving a smaller set of equations and able to reproduce the thermal behavior of a reference large-size model or an actual system, whatever the time-varying boundary conditions and/or heat source terms, or for a range of values of a thermophysical parameter. But low-order models able to mimic heat transfer dynamics for both a time-varying thermal load and a physical parameter range are not frequently encountered. Such a problem is addressed here, through an extension of the Modal Identification Method. The approach is illustrated on a simple linear 2D transient heat diffusion problem, with a time-varying heat flux density applied on one side and a thermal conductivity in the 15 to 45 W.m⁻¹.K⁻¹ range. The low-order model is used for the estimation of the thermal conductivity from the knowledge of both the applied heat flux and a simulated transient temperature measurement on the opposite side. The approach remains valid for 3D cases in complex geometries involving more independent thermal loads.

1. Introduction
In the frame of heat transfer modeling, classical methods based on spatial discretization of local governing equations, such as the Finite Element, Finite Volume or Finite Difference Methods for instance, lead to very fine meshes involving a huge amount of cells, especially for 3D problems in complex geometries. The so-built large size heat transfer models require large computing times. Although progress in computer technology and development of massive parallel computations are continuously pushing back the limits of allowed modeling, thermal problems nowadays involve coupled heat transfer modes, nonlinearities, transient boundary conditions and/or source terms, that always require more computing resources. This becomes penalizing in applications for which the model has to be run a large amount of times, such as optimization problems (estimation of physical parameters, shape optimization, etc.). In the frame of feedback control in real-time, classical models

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can not even be used. In order to cope with this crucial issue, several model reduction methods have been developed in the last decades for building Low Order Models (LOM) involving a small set of equations compared to the large number of degrees of freedom of the classical models. LOMs aim at reproducing the behavior of a reference large-size model or an actual thermal system, whatever the time-varying boundary conditions and/or heat source terms, or for a range of values of a thermophysical parameter. Among reduction methods, let us cite those based on Proper Orthogonal Decomposition (POD) followed by a Galerkin projection. For instance, an inverse problem of nonlinear heat diffusion with a time-varying heat source has been handled in [1]. Suppression of vortex shedding past a circular cylinder has been performed with an adaptive POD reduced model taking into account an actuator defined by two parameters [2]. The Branch Eigenmodes Reduction Method [3] allows building reduced models for systems with multiple time-varying thermal loads. The Reduced Basis approximation based on Galerkin projection onto a Lagrange space [4] is more adapted to parametric reduced models construction. Both the goal oriented model-constrained approach developed in [5] and the Proper Generalized Decomposition [6] offer the capability to generate LOM able to mimic the heat transfer dynamics of a thermal system for both a time-varying thermal load and a physical parameter range. However, the former requires to perform a POD and then to solve an optimization problem, whereas the latter appears to provide a discrete solution in time and parametric space rather than a continuous LOM, hence its use for optimization purposes does not seem an obvious option. The construction of a heat transfer LOM valid for both a time-varying thermal load and a physical parameter in a specific range is addressed in the present work, through an extension of the Modal Identification Method (MIM). LOM built by MIM have proved to be efficient for solving inverse problems [7] [8] and recently thermal feedback control problems [9]. Details about MIM may be found in [8], especially the handling of multiple independent thermal loads (boundary conditions, heat sources) and the extensions to nonlinear problems. Although the approach remains valid for 3D cases in complex geometries, we will here focus for illustration purpose on a simple linear 2D heat sources) and the extensions to nonlinear problems. Although the approach remains valid for 3D transient heat diffusion problem, with a time-varying heat flux density applied on one side and a thermal conductivity in the 15 to 45 W.m$^{-1}$.K$^{-1}$ range. Once built and validated against test cases, the LOM is used in an inverse problem for the estimation of the thermal conductivity from the knowledge of both the applied heat flux and a simulated transient temperature measurement on the opposite side.

2. General linear heat diffusion problem

Let us consider a linear thermal system on a domain $\Omega$. Such system is governed by the heat equation:

$$\rho c_p \frac{\partial T}{\partial t}(\vec{x}, t) = k_{th} \nabla \vec{T}(\vec{x}, t) \quad \forall \vec{x} \in \Omega , \forall t \in [0; t_f]$$

(1)

$T(\vec{x}, t)$ is the temperature at location $\vec{x}$ ($\vec{x}$ is here a generic point of the spatial domain $\Omega$) and time $t$. $\rho$ (kg.m$^{-3}$) is the density, $c_p$ (J.kg$^{-1}$.K$^{-1}$) the specific heat and $k_{th}$ (W.m$^{-1}$.K$^{-1}$) the thermal conductivity throughout the domain. These properties are assumed to be temperature-independent. The boundary $\Gamma$ of $\Omega$ is partitioned as follows:

i. a sub-boundary $\Gamma_n$ on which a Neumann-type boundary condition is applied:

$$k_{th} \nabla T \cdot \vec{n} = \varphi(t)$$

(2)

ii. a sub-boundary $\Gamma_f$ with a Fourier-type boundary condition:

$$k_{th} \nabla T \cdot \vec{n} = h(\vec{x}) (T_a(t) - T(\vec{x}, t))$$

(3)

$\vec{n}$ is defined as the outward unit vector normal to each considered sub-boundary. $\varphi(t)$ (W.m$^{-2}$) is the prescribed heat flux density on $\Gamma_n$, $h(\vec{x})$ (W.m$^{-2}$.K$^{-1}$) is the heat exchange coefficient distribution between sub-boundary $\Gamma_f$ and the ambient environment at temperature $T_a(t)$.

Although (1) is linear in $T$ and the relation between thermal loads $\varphi(t)$ and $T_a(t)$ and resulting temperature field is also linear, temperature is nonlinear with respect to thermal conductivity $k_{th}$. Our goal is here to build a low order model parameterized by $k_{th}$ and able to take into account the time-varying boundary condition $\varphi(t)$ ($T_a$ will be set constant, equal to 0°C).
3. A simple example: 2D slab submitted to a prescribed wall heat flux density

Let us consider a 2D slab as shown in Figure 1 whose dimensions are 0.24 m x 0.16 m, made of some steel whose thermal conductivity is assumed to be constant, however lying in the range [15 W.m\(^{-1}\).K\(^{-1}\), 45 W.m\(^{-1}\).K\(^{-1}\)], and whose volumetric heat capacity is supposed to be constant and equal to 4x10\(^6\) J.m\(^{-3}\).K\(^{-1}\). The slab is submitted to a prescribed time-varying heat flux density \(q(t)\) on the left side. The upper side is insulated and on both other sides there is a convective heat exchange with an ambient environment at constant temperature \(T_a = 0 \ ^\circ\text{C}\). The heat exchange coefficient \(h\) is supposed to be uniform on both boundaries and equal to 100 W.m\(^{-2}\).K\(^{-1}\). The reference model has been built using the Finite Volume Method, with a 49x33 mesh for a total number of \(N = 1617\) discretization nodes.

4. Modal Identification Method: overview

The Modal Identification Method (MIM) consists in three main steps:

1) Define the structure of the Low Order Model (LOM) equations able to adequately describe the involved physics (see section 5),

2) Generate some input-output data representative of the system dynamics. Those data come from in-situ measurements or from numerical simulations (see section 6),

3) Identify the parameters of the LOM equations through the minimization of a functional based on the quadratic residuals between the previously generated output data of the system on the one hand and the outputs of the LOM on the other hand, for the same input data (see section 7).

The MIM therefore aims to adjust the LOM constitutive parameters using optimization techniques, in order for the LOM to mimic the data characterizing the input-output dynamics of the system. It is hence important to note that the MIM is a not a method for building a model from the knowledge of system geometry, involved materials, governing PDE and boundary conditions, like the Finite Volume Method for instance. The MIM does not rely on a spatial discretization scheme: there is no mesh on which balance equations are written, the knowledge of the geometry is therefore not required.

5. Low order model formulation

5.1. General approximation of temperature field

It is assumed that the temperature field may be written as a sum of functions, each one being the product of a function of space by a function of time:

\[
T(\vec{x}, t) \approx \sum_{i=1}^{n} \phi_i(\vec{x})X_i(t) \tag{4}
\]

where the spatial functions \(\phi_i(\vec{x}), i = 1, \ldots, n\), are a truncation of a basis of the Hilbert space \(L_2(\Omega)\). Of course, our goal will be to find a low order model, hence corresponding to a small number \(n\) of functions used in the temperature field decomposition.

5.2. Galerkin projection

Let us now define \(\mathcal{R}(\vec{x}, t)\) as the residual of heat equation (1):

\[
\mathcal{R}(\vec{x}, t) = \rho C_p \frac{\partial T}{\partial t}(\vec{x}, t) - k_{th} \vec{\nabla} \cdot \vec{\nabla} T(\vec{x}, t) \tag{5}
\]

The Galerkin projection consists in forcing the residual \(\mathcal{R}(\vec{x}, t)\) (written with the decomposition (4)), to be orthogonal to each \(\phi_i(\vec{x}), i = 1, \ldots, n\), so that the projection of the residual onto the subspace of \(L_2(\Omega)\) generated by the \(\phi_i(\vec{x}), i = 1, \ldots, n\), would be null. Defining the inner product \(\langle \cdot, \cdot \rangle\) as \(\langle u, v \rangle = \int_\Omega uv d\Omega\), one hence writes:

\[
\langle \mathcal{R}(\vec{x}, t), \phi_k(\vec{x}) \rangle = \int_\Omega \mathcal{R}(\vec{x}, t) \phi_k(\vec{x}) d\Omega = 0 \quad \forall k \in [1; n] \tag{6}
\]
For introducing explicitly the boundary conditions (2) and (3), the diffusion term $k_{th}\nabla \overline{\nabla} T(\bar{x}, t)$ is integrated by parts, using the first Green formula:

$$
\int_{\Omega} f \nabla \cdot \overline{\nabla} u d\Omega = \int_{\Gamma} f \overline{\nabla} u \cdot d\Gamma - \int_{\Omega} \overline{\nabla} f \cdot d\Omega
$$

(7)

After integration by parts, (6) is written as:

$$
\sum_{i=1}^{n} I_{ki} \frac{dX_i(t)}{dt} - k_{th} \sum_{i=1}^{n} (L_D)_{ki} X_i(t) - \sum_{i=1}^{n} (L_C)_{ki} X_i(t) - P_k \phi(t) - V_k T_a(t) = 0
$$

(8)

where $\forall k \in [1; n], \forall i \in [1; n]$:

$$
l_{ki} = \rho C_p \int_{\Omega} \phi_i(\bar{x}) \phi_k(\bar{x}) d\Omega, \quad (L_D)_{ki} = \int_{\Omega} \overline{\nabla} \phi_i(\bar{x}) \cdot \overline{\nabla} \phi_k(\bar{x}) d\Omega, \quad (L_C)_{ki} = -\int_{\Gamma} h(\bar{x}) \phi_i(\bar{x}) \phi_k(\bar{x}) d\Gamma, \quad P_k = \int_{\Gamma} h(\bar{x}) \phi_k(\bar{x}) d\Gamma, \quad V_k = \int_{\Gamma} h(\bar{x}) \phi_k(\bar{x}) d\Gamma.
$$

Equation (8) corresponds to the LOM parameterized by thermal conductivity, obtained by Galerkin projection.

Notes:
1. Matrices $L_D \in \mathbb{R}^{n \times n}$ and $L_C \in \mathbb{R}^{n \times n}$ are both associated to linear terms in $X_i(t)$. $L_D$ is associated to diffusive terms whereas $L_C$ is associated to convective ones arising from the Fourier boundary condition. In the present work, these two matrices are used instead of a single one $L = k_{th} L_D + L_C$ in order to make the parameter $k_{th}$ appear explicitly in the low order model.
2. When dealing with several independent boundary conditions of the same type but with different time-varying values, similar terms are introduced, each one associated to a specific boundary condition.
3. The spatial functions $\phi_i$ used in the decomposition (4) of the temperature field could be obtained by Proper Orthogonal Decomposition (POD). In this case, the system (8) constitutes a so-called « POD-Galerkin » low order model. However, in the frame of MIM used in this paper, those functions will be in fact embedded in matrices whose parameters are identified in an optimization procedure, as briefly described in section 7.

5.3. Final form of the low order model to be identified

Let us call $W = [P \quad V]$ and define $U(t)$ as the input vector gathering both thermal loads:

$$
U(t) = \left[ \begin{array}{c} \phi(t) \\ T_a(t) \end{array} \right]
$$

(9)

Matrix $I \in \mathbb{R}^{n \times n}$ is supposed to be invertible. Let us call $X(t) = [X_1(t) \quad \ldots \quad X_n(t)]^T$ and define:

$$
A_D = I^{-1} L_D \in \mathbb{R}^{n \times n}, \quad A_C = I^{-1} L_C \in \mathbb{R}^{n \times n}, \quad A_B = I^{-1} W \in \mathbb{R}^{n \times 2}.
$$

Equation (8) now writes under matrix form:

$$
\frac{dX(t)}{dt} = (k_{th} A_D + A_C) X(t) + B U(t)
$$

(10)

In most cases, the thermal analyst is interested in a restricted set of outputs, that is a set of $q$ observable temperatures at specific locations $\bar{x}_j, j = 1, \ldots, q$ throughout the spatial domain $\Omega$. Using the decomposition (4), those $q$ temperatures are written as:

$$
Y_j(t) = T(\bar{x}_j, t) = \sum_{i=1}^{n} \phi_i(\bar{x}_j) X_i(t) \quad j = 1, \ldots, q
$$

(11)

We now define the output matrix $C \in \mathbb{R}^{q \times n}$ such as:

$$
C_{ji} = \phi_i(\bar{x}_j) \quad \forall j \in [1; q], \quad \forall i \in [1; n]
$$

Equation (11) for the output vector $Y(t) \in \mathbb{R}^q$ hence writes, under matrix form:

$$
Y(t) = CX(t)
$$

(12)

It is now assumed that matrix $A_D$ can be diagonalized. Let’s call $D$ the diagonal matrix of eigenvalues of $A_D$ and $M$ a matrix whose columns are eigenvectors of $A_D$. One hence has $D = \ldots$
\(M^{-1}A_p M\). Introducing the change of basis \(X(t) = MX'(t)\) in (10) and (12), and defining \(E = M^{-1}A_c M, G = M^{-1}B\) and \(H = CM\) one gets:

\[
\frac{dX(t)}{dt} = (k_{th}D + E)X'(t) + GU(t)
\]

and

\[
Y(t) = HX'(t)
\]

Equations (13) and (14) constitute the low order model form, whose state vector is \(X'(t) \in \mathbb{R}^n\).

6. Input-output data for model construction

The database for the LOM identification is composed of \(N_{set} = 11\) sets of \(q = 4\) temperatures \(T_1\) to \(T_4\) located in the middle of each boundary (see Figure 1), computed at \(N_{t} = 15001\) instants (time step between snapshots was \(\Delta t = 10s\)) with the reference Finite Volume model. Each set corresponds to a fixed constant value of the thermal conductivity \(k_{th}\): \(k_{th}(set 1) = 15 \text{ W.m}^{-1}.\text{K}^{-1}\), \(k_{th}(set 2) = 18 \text{ W.m}^{-1}.\text{K}^{-1}\), ..., \(k_{th}(set 11) = 45 \text{ W.m}^{-1}.\text{K}^{-1}\). The input signal \(\varphi(t)\) used to compute these data sets is shown in Figure 2. As examples, resulting temperatures \(T_2\) and \(T_3\) for two values of \(k_{th}\) (15 and 45 \(\text{W.m}^{-1}.\text{K}^{-1}\)) are shown in Figure 3, with the label “DM” standing for “Detailed Model”.

7. Low order model identification

The Modal Identification Method consists in building a model similar in form to equations (13) and (14), but without prior computation of functions \(\varphi_i\). In fact, for a given model order \(n\), the goal of the MIM is to determine the values of the components of matrices \(D = \text{diag}(D_i) \in \mathbb{R}^{n \times n}\), \(E \in \mathbb{R}^{n \times n}\), \(G \in \mathbb{R}^{n \times 2}\) and \(H \in \mathbb{R}^{q \times n}\). In MIM, the problem of the determination of all these components is recast in a parameter estimation problem. Unknown components of \(D, E, G, H\) are hence identified through the minimization of a quadratic criterion \(J_{id}^{(n)}\) built on an output error, defined as:

\[
J_{id}^{(n)}(D, E, G, H) = \sum_{k=1}^{N_{set}} \sum_{i=1}^{q} \sum_{j=1}^{N_{t}^i} (Y_{kl}(D, E, G, H ; t_j) - Y_{kl}^{data}(t_j))^2
\]

where:

- \(Y_{kl}(D, E, G, H ; t_j)\) is the temperature at point \(i\) and time \(j\) for the set \(k\), computed by the LOM and which depends on \(D, E, G, H\),
- \(Y_{kl}^{data}(t_j)\) is the corresponding output data value, which is either computed with a numerical simulation (solution of a reference model as in the present work) or composed of measured values recorded on the real system. Here the reference model is assumed to be “perfect”, however the computed data could have been corrupted with some artificial noise.

\(Y(D, E, G, H ; t)\) and \(Y^{data}(t)\) correspond to the same input vector \(U(t)\) applied to the LOM and to the reference model (or actual plant) respectively.

\(J_{id}^{(n)}\) is minimized for successive values of \(n\) until a stopping criterion is satisfied:

1. \(n \leftarrow 1\)
2. Minimization of \(J_{id}^{(1)} \Rightarrow \text{identification of } (\text{diag}(D))_1, (E)_1 \times 1, (G)_1, (H)_{q \times 1}\)
3. \(n \leftarrow n + 1\)
4. Minimization of \(J_{id}^{(n)} \Rightarrow \text{identification of } (\text{diag}(D))_n, (E)_n \times n, (G)_n, (H)_{q \times n}\)
5. Test of stopping criterion, classically based on the value of the mean quadratic discrepancy (i.e. root mean square of the residuals) \(\sigma_y^{id,(n)} = \sqrt{J_{id}^{(n)}(D, E, G, H) / (N_{set} \times q \times N_{t}^i)}\) between data \(Y^{data}(t)\) to be fitted and LOM outputs \(Y(D, E, G, H ; t)\). If \(\sigma_y^{id,(n+1)} \approx \sigma_y^{id,(n)}\) or \(\sigma_y^{id,(n+1)} \leq \sigma_y^2\), where \(\sigma_y^2\) is the standard deviation corresponding to the accuracy wished by the user, then STOP else go to 3.
Notes:
1. MIM allows building LOMs only on the outputs of interest for the user. Here we choose temperature at 4 locations but LOMs could have been built for temperature at all the mesh nodes of the reference model. In this case, we would have had \( q = N \).
2. The LOM size \( n \) is not related to the number \( q \) of outputs. In fact \( n \) is the number of state components \( X'_i(t) \) needed to reproduce the main dynamics of the thermal system behaviour.
3. Parameters of the order \( n \) LOM are used as initial guesses for the corresponding parameters to be identified in the order \( n + 1 \) LOM.
4. Eigenvalues of matrix \( k_{th} \mathbf{D} + \mathbf{E} \) are constrained to be real and negative in the minimization procedure, to ensure the dynamical stability of the LOM.
5. The optimization algorithms used in the identification procedure are the Particle Swarm Optimization method [10] and the Ordinary Least Squares method.
6. Details about handling multiple inputs and identification of nonlinear LOMs may be found in [7] [8] [9], among others.

Using the 11 data sets generated in section 6, a series of LOMs of order \( n = 1 \) to 7 has been built. The root mean square of the residuals \( \sigma_Y^{id,(n)} \) is given in Figure 4 as a function of the order \( n \) of the identified reduced model. For the order 7 model, this value comes down to 5.4 \( \times 10^{-3} \) °C. As examples, temperatures \( T_2 \) and \( T_3 \) for two values of \( k_{th} \) (15 and 45 W.m\(^{-1}\).K\(^{-1}\)) are shown in Figure 3, for both the Finite Volume model (labelled “DM” for “Detailed Model”) and the LOM of order 7. Temperatures are quasi-superimposed and the residuals almost never exceed 0.1°C.
8. Test case for low order model validation
The order 7 LOM previously identified is now tested with another input signal \( U(t) = \varphi(t) \) shown in Figure 5, different from the one used for the building phase, and a thermal conductivity \( k_{th} = 20 \text{ W.m}^{-1}\cdot\text{K}^{-1} \), a value that was not used in the data set for construction. As shown in Figure 6, temperatures \( T_1 \) to \( T_4 \) computed with both the Finite Volume model and the LOM are quasi-superimposed. The residuals almost never exceed 0.1°C.

Figure 5. Heat flux \( \varphi(t) \) for LOM validation.

Figure 6. LOM validation: temperatures computed by DM and by LOM of order 7.

9. Inverse problem for estimation of thermal conductivity
In this section, the parametric LOM of order 7 is used to solve an inverse problem. The goal is to estimate the value of the thermal conductivity \( k_{th} \). The exact value of \( k_{th} \) to be retrieved in the inverse problem test case is 20 W.m\(^{-1}\).K\(^{-1}\). As in section 8, this value is in the building range \([15;45]\) but is not part of the database used for the LOM identification. The slab is heated with a known heat flux density \( \varphi(t) \), here a step signal of magnitude 5000 W.m\(^{-2}\). In order to simulate temperature measurements, resulting temperature \( T_3 \) computed with the reference model has been corrupted with an additive Gaussian noise of standard deviation \( \sigma = 0.2^\circ\text{C} \). Temperature \( T_3 \), which is located on the opposite side to the heated side, is shown in Figure 7. From the knowledge of both the thermal load \( \varphi(t) \) and the simulated measurement \( T_3^n \) at \( N_t = 2001 \) time instants with a time step \( \Delta t = 10\text{s} \), the thermal conductivity \( k_{th} \) is estimated through an inverse problem recast in an optimization problem:

\[
\tilde{k}_{th} = \text{Argmin}\{\mathcal{F}(k_{th})\} = \text{Argmin} \sum_{j=1}^{N_t} \left( T_3(k_{th} ; t_j) - T_3^n(t_j) \right)^2 \tag{16}
\]

The minimization of the objective function \( \mathcal{F}(k_{th}) \) has been performed by the Fletcher-Reeves variant of the conjugate gradient method. The required sensitivities \( \partial T_3(k_{th} ; t_j) / \partial k_{th} \) are easily and quickly computed thanks to the LOM. From (14), one has indeed:

\[
\frac{\partial T_3(t)}{\partial k_{th}} = [H_{31} \ldots H_{37}] \frac{\partial X'(t)}{\partial k_{th}} \tag{17}
\]

where \([H_{31} \ldots H_{37}]\) is the 3\(^{rd}\) row of matrix \( H \in \mathbb{R}^{4\times 7} \), associated to \( T_3 \), and, according to equation (13), \( \partial X'(t) / \partial k_{th} \) is solution of:

\[
d \frac{\partial X'(t)}{\partial k_{th}} \bigg/ dt = (k_{th} D + E) \frac{\partial X'(t)}{\partial k_{th}} + DX'(t) \tag{18}
\]

Inversion results are summarized in Figure 8, where, starting from \( k_{th} = 40 \text{ W.m}^{-1}\cdot\text{K}^{-1} \) as initial guess, the convergence to the exact value \( k_{th} = 20 \text{ W.m}^{-1}\cdot\text{K}^{-1} \) is obtained after 4 iterations. It can also be observed that the value of \( a_{T_3}^{inv} = \sqrt{\mathcal{F}(k_{th}) / N_t} \) converges to the standard deviation \( \sigma = 0.2^\circ\text{C} \) of the measurement error, thus in accordance with the discrepancy principle.
10. Conclusions and prospects

An extension of the Modal Identification Method has been proposed, for building low order models able to mimic the heat transfer dynamics of a thermal system for both a time-varying thermal load and a physical parameter in a specific range. The approach is illustrated on a simple linear 2D transient heat diffusion toy problem, with a time-varying heat flux density applied on one side and a thermal conductivity in the 15 to 45 W.m\(^{-1}\).K\(^{-1}\) range. The general form of the low order model to identify is obtained thanks to a Galerkin projection, assuming a decomposition of the temperature field on a small set of space functions and time functions. After a brief presentation of the model identification procedure, a series of low order models parameterized by the thermal conductivity has been built. A low order model is then used for solving efficiently an inverse problem for the estimation of the thermal conductivity. An extension to the case of another parameter or several other parameters, such as convective exchange coefficients, may be similarly developed. The approach remains valid for 3D cases in complex geometries and will be tested in such more interesting problems in future works.

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