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Fast and accurate two-field reduced basis approximation for parametrized thermoelasticity problems

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ABSTRACT

This paper concerns a two-field reduced basis algorithm for the metamodelling of parametrized one-way coupled thermoelasticity problems based on the constitutive relation error (CRE) estimation. The coupled system consists of parametrized thermal diffusion and elastostatic equations which are explicitly coupled in a one-way manner. The former can be solved in advance independently and the latter can be solved afterwards using the solution of the former. For the fast and accurate analysis of the coupled system, we developed an algorithm that can choose adaptively the number of reduced basis functions of the temperature field to approximate the CRE equality of the mechanical field. We compute *approximately* the upper bound for the true errors of displacement and stress fields in energy norms. To enable this, a two-field greedy sampling strategy is adopted to construct the displacement and stress fields in an efficient manner. The computational efficiency of the proposed approach is demonstrated with computing the effective coefficient of thermal expansion of heterogeneous materials.

1. Introduction

Coupled systems exist in many engineering applications such as fluid-structure interaction, thermo-mechanical, electro-mechanical, electro-magnetic, and so on. The coupling is caused by the interaction between different subsystems describing different physical quantities such as temperature, displacement, velocity, pressure, etc. After discretizing coupled systems with certain traditional numerical methods such as finite-element and finite-volume methods, their resulting algebraic systems are often complex and very large. Such a complex and large algebraic system entails difficulties for the real-time computation which is vital for tailoring responses of the complex system via computational system design approach. To circumvent such difficulties, the purpose of this work is to develop a two-field model order reduction (MOR) technique that can enable metamodelling of the coupled system for the fast and accurate computation.

In the following, we provide a brief literature review on the use of MOR techniques for coupled problems, as a more exhaustive overview on this topic can be found in Refs. [1,2]. The first MOR technique to deal with coupled systems is the component mode synthesis method proposed for structural dynamics problems [3–5]. After that, different MOR techniques have been proposed and can be categorized into several types. For examples, MOR techniques based on systems and control theory such as balanced truncation [6,7], MOR techniques based on approximation theory such as moment-matching [8,9], MOR techniques such as the reduced basis (RB) method [10,11], proper orthogonal decomposition (POD) method [12,13] and proper generalized decomposition method [14] have been successfully applied to coupled systems, and have shown significant efficiency for various multi-physics problems.

In this work, we focus on the application of a reduced order model (ROM) for the class of one-way coupled thermoelasticity problems. In particular, a one-way coupled thermoelasticity problem shall include one thermal elliptic partial differential equation (PDE) and one elastic elliptic PDE, where the former can be solved *in advance* independently and the latter is solved *afterwards* using the solution of the former [15,16]. Due to this special property, the application of the ROM for the thermal PDE is straightforward and simple: any available ROM with associated error estimation technique (e.g., a snapshot-proper orthogonal decomposition method [17–20], a hyper-reduction technique [21,22], a proper generalized decomposition method [23], reduced basis with a successive constraint method [24,25], or a recent two-field reduced basis method (TF-RBM) [26]) will work well for such thermal problem. However, *a posteriori* error estimation for the

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ROM of the elastic PDE is complicated because of the passing of the approximated ROM temperature field from the thermal PDE to the elastic one. To the best of our knowledge, there is no work in literature to evaluate such an error of the elastic PDE in this context. As references, the application of ROM techniques for the class of coupled thermoelasticity problems can be found in, for example, [7,27]. These works belong to the class of either balance truncation or moment-matching methods which were described briefly in the previous paragraph.

In this paper, we pursue the RB methodology with a CRE estimation to handle such parametrized coupled thermoelasticity problems. In particular, we use the TF-RBM with the CRE estimation technique [26] to approximate *certifiably* both thermal and elastic PDEs. As mentioned in the previous paragraph, while such an approach to handle the thermal PDE is straightforward, that to handle the elastic PDE is not trivial and requires some special modifications. This is due to the appearance of expansion terms which depend on the true error of the RB temperature field, besides the usual true errors of the RB displacement and stress fields in the CRE equality.

Therefore, the first purpose of this paper is to propose an algorithm to choose *adaptively* the number of RB basis functions of the temperature field in such a way that these expansion terms are eliminated — thus recovers *approximately* the CRE equality. In other words, we recover the upper boundedness of the CRE estimator for true errors of RB displacement and stress fields [26]. In turn, this CRE estimator is used in a two-field greedy sampling algorithm to build the corresponding reduced spaces of these displacement and stress fields. The second purpose of this paper is to extend the CRE upper error bound to goal-oriented error bounds for several quantities of interest (QoIs), where these QoIs are linear functionals of the displacement field. (Note that the QoIs of the thermal PDE are addressed in the RB approximation of the thermal PDE *in advance*.) Based on these goal-oriented error bounds, the final objective is to compute the *certified* ROM approximations of the effective coefficient of thermal expansion (CTE) for parametrized coupled thermoelasticity problems.

The remainder of the paper is organized as follows. In section 2, we state the exact parametrized coupled thermoelasticity problem and its finite-element discretization. In section 3, we describe our ROM approximations for the thermal equation in section 3.1 and the elastic equation in section 3.2. While section 3.1 repeats briefly the work in Ref. [26], section 3.2 and section 4 present all the novel proposed theory of this paper. In particular, section 3.2 is devoted to the CRE estimator, the proposed algorithm to select appropriately the number of RB basis vectors for the temperature field, and the two-field greedy sampling algorithm. Goal-oriented error bounds and the extension to compute the effective CTE are presented in section 4. In section 5, the performance of all the proposed algorithms is investigated for a 2D material homogenization problem. Finally, we provide some concluding remarks in section 6.

2. Parametrized explicitly coupled thermoelasticity equations

2.1. Exact formulation

2.1.1. Strong form

We consider the problem of determining the displacement field $u(x)$ and the (excess) temperature field $\theta(x)$[1] within a static thermoelastic body occupying the physically spatial domain $\Omega \in \mathbb{R}^d$ $(d = 2, 3)$. The displacement field $u \in \mathcal{U}(\Omega) = \left(H^1(\Omega)\right)^d$ and the temperature field $\theta \in \Theta(\Omega) = H^1(\Omega)$ satisfy the nonhomogeneous Dirichlet boundary conditions $u = w$ and $\theta = \vartheta$ on the parts Γ^u and Γ^θ of the boundary Γ, respectively. Here, $H^1(\Omega) = \left\{v \in L^2(\Omega) \mid \nabla v \in (L^2(\Omega))^d\right\}$ is a Hilbert space and $L^2(\Omega)$ is the space of square integrable functions over Ω. The body may also be subjected to prescribed tractions t, body forces b, prescribed flux h and heat source f on the boundary parts Γ^t, Ω, Γ^h and Ω, respectively.

We define a set of input parameters $\mathcal{D} \subset \mathbb{R}^P$, a typical point of which is denoted by $\mu \equiv (\mu_1, \ldots, \mu_P)$. In particular, the force densities b, t; the heat densities h, f; the Dirichlet boundary conditions w, ϑ and the material properties of the structure may be functions of parameter μ. We assume that Ω, Γ^u and Γ^θ do not undergo any parametric changes.

For a given parameter μ, the strong formulation is stated as: obtain $(\theta(\mu), u(\mu))$ by solving the following one-way coupled system

$$\text{Heat equation} \begin{cases} -k(\mu)\nabla^2\theta(\mu) = f(\mu) & \text{on} \quad \Omega, \\ \theta = \vartheta & \text{on} \quad \Gamma^\theta, \\ q(\mu) = k(\mu)\cdot\nabla\theta(\mu) & \text{on} \quad \Omega, \end{cases} \tag{1}$$

$$\text{Elastic equation} \begin{cases} -div\,(\sigma(u(\mu))) = b(\mu) & \text{on} \quad \Omega, \\ u = w & \text{on} \quad \Gamma^u, \\ \sigma(u(\mu)) = D(\mu) : \epsilon(u(\mu)) - D(\mu) : \epsilon_0(\theta(\mu)) & \text{on} \quad \Omega. \end{cases} \tag{2}$$

Here, $q(\mu)$ is the flux field and $k(\mu)$ is the heat conductivity tensor for the heat equation. For the elastic equation, $\epsilon(v) = \frac{1}{2}\left(\nabla v + \nabla v^T\right)$ is the strain field, $\sigma(\mu)$ is the Cauchy stress field, $D(\mu)$ is the fourth-order Hooke's elasticity tensor which depends on the two Lamé constants $\lambda(\mu)$ and $G(\mu)$, $\epsilon_0(\theta(\mu))$ is the thermal strain which depends on the temperature field $\theta(\mu)$ that was solved from Eq. (1) (see for instance Eq. (1.9) in Ref. [28] or Eq. (8.23) in Ref. [29]). System (1) and (2) is thus one-way coupled in this sense. (Interested readers can refer to the full coupled thermomechanical system, for instance, arising in shear band modelling application [30,31].)

2.1.2. Weak form

For a given parameter μ, the corresponding weak form is described by

$$-\int_\Omega q(\mu)\cdot\nabla v_1\,d\Omega + \int_\Omega f(\mu)\cdot v_1\,d\Omega + \int_{\Gamma^h} h(\mu)\cdot v_1\,d\Gamma = 0, \quad \forall v_1 \in \Theta^{\mathrm{Ad},0}(\Omega), \tag{3a}$$

$$-\int_\Omega \sigma(\mu) : \epsilon(v_2)\,d\Omega + \int_\Omega b(\mu)\cdot v_2\,d\Omega + \int_{\Gamma^t} t(\mu)\cdot v_2\,d\Gamma = 0, \quad \forall v_2 \in \mathcal{U}^{\mathrm{Ad},0}(\Omega). \tag{3b}$$

Here, $\Theta^{\mathrm{Ad}}(\Omega;\mu) = \{v \in \Theta(\Omega) \mid v_{|\Gamma^\theta} = \vartheta(\mu)\}$ and $\Theta^{\mathrm{Ad},0}(\Omega) = \{v \in \Theta(\Omega) \mid v_{|\Gamma^\theta} = 0\}$ are the spaces which contain the full and homogeneous temperature fields; $\mathcal{U}^{\mathrm{Ad}}(\Omega;\mu) = \left\{v \in \mathcal{U}(\Omega) \mid v_{|\Gamma^u} = w(\mu)\right\}$ and $\mathcal{U}^{\mathrm{Ad},0}(\Omega) = \left\{v \in \mathcal{U}(\Omega) \mid v_{|\Gamma^u} = 0\right\}$ are the spaces which contain the full and homogeneous displacement fields. The solution to the parametrized heat conduction problem (3a) is an admissible pair $(\theta(\mu), q(\mu)) \in \Theta^{\mathrm{Ad}}(\Omega;\mu) \times \mathcal{Q}^{\mathrm{Ad}}(\Omega;\mu)$ that verifies the isotropic linear constitutive law

$$q(\mu) = k(\mu)\cdot\nabla\theta(\mu). \tag{4}$$

Similarly, the solution to the parametrized problem of elasticity is an admissible pair $(u(\mu), \sigma(\mu)) \in \mathcal{U}^{\mathrm{Ad}}(\Omega;\mu) \times \mathcal{S}^{\mathrm{Ad}}(\Omega;\mu)$ that verifies the isotropic linear constitutive law

$$\sigma(\mu) = D(\mu) : \epsilon(u(\mu)) - D(\mu) : \epsilon_0(\theta(\mu)). \tag{5}$$

By substituting (4) into (3a) and (5) into (3b), the parametric problem of thermoelasticity can be written in the following primal variational form: for any $\mu \in \mathcal{D}$, find $\theta(\mu) \in \Theta^{\mathrm{Ad}}(\Omega;\mu)$ and $u(\mu) \in \mathcal{U}^{\mathrm{Ad}}(\Omega;\mu)$ such that

[1] $\theta^{\mathrm{tot}}(x) = \theta^{\mathrm{ref}} + \theta(x)$ where $\theta^{\mathrm{tot}}(x)$ is the total (absolute) temperature and θ^{ref} is the reference temperature corresponding to the zero thermal strains state, which motivates the notion *excess* temperature for θ.