Comput. Methods Appl. Mech. Engrg. 209–212 (2012) 144–155

Contents lists available at SciVerse ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

Certified reduced basis methods for parametrized parabolic partial differential equations with non-affine source terms

Dirk Klindworth [a], Martin A. Grepl [b,*], Georg Vossen [a]

[a] RWTH Aachen University, Nonlinear Dynamics of Laser Processing, Steinbachstraße 15, 52074 Aachen, Germany
[b] RWTH Aachen University, Numerical Mathematics, Templergraben 55, 52056 Aachen, Germany

ARTICLE INFO

Article history:
Received 12 April 2011
Received in revised form 31 August 2011
Accepted 11 October 2011
Available online 15 October 2011

Keywords:
Reduced basis methods
Parabolic PDEs
Non-affine parameter dependence
A posteriori error estimation
Empirical interpolation method
Welding process

ABSTRACT

We present rigorous *a posteriori* output error bounds for reduced basis approximations of parametrized parabolic partial differential equations with non-affine source terms. The method employs the empirical interpolation method in order to construct affine coefficient-function approximations of the non-affine parametrized functions. Our *a posteriori* error bounds take both error contributions explicitly into account—the error introduced by the reduced basis approximation *and* the error induced by the coefficient function interpolation. To this end, we employ recently developed rigorous error bounds for the empirical interpolation method and develop error estimation and primal–dual formulations to provide rigorous bounds for the error in specific outputs of interest. We present an efficient offline–online computational procedure for the calculation of the reduced basis approximation and associated error bound. The method is thus ideally suited for many-query or real-time contexts. As a specific motivational example we consider a three-dimensional mathematical model of a welding process. Our numerical results show that we obtain efficient and reliable mathematical models which may be gainfully employed in manufacturing and product development.

1. Introduction

The role of numerical simulation in engineering and science has become increasingly important. System or component behavior is often modeled using a set of parametrized partial differential equations (PDEs) and associated boundary and initial conditions, where the parameters, or inputs, μ—such as material properties and geometry—serve to identify a particular configuration. Since the analytical solution to these problems is generally unavailable, a discretization procedure such as the finite element method (FEM) is used in practice. In a design, optimization, and control context one often requires repeated, reliable, and real-time prediction of the system or component outputs, s^e, such as heat fluxes or flow rates.[1] These outputs are typically functionals of field variables, y^e—such as temperatures or velocities—associated with the parametrized PDE. The relevant system behavior is thus described by an implicit input–output relationship, $s^e(\mu)$, evaluation of which demands solution of the underlying parametrized PDE.

More specifically, the motivation of this work is to develop an efficient mathematical model for the heat flow in a welding process [1–5]. An accurate knowledge of the temperature distribution within the workpiece is crucial in determining the quality of the weld: two such quality measures are the weld pool depth—indicating the strength of the joint—and the shape distortion of the workpiece.

A complete model of the welding process which couples and accounts for all of the physical processes involved does not yet exist. In actual practice, the heat flux input is therefore modeled as a parametrized volume heat source [2,6,7]. The non-dimensionalized temperature distribution, $y^e(x,t;\mu)$, within the workpiece is governed by the (appropriately) non-dimensionalized unsteady convection–diffusion equation

$$\frac{\partial}{\partial t} y^e(x,t;\mu) + \mathrm{v}\cdot\nabla y^e(x,t;\mu) - \kappa\nabla^2 y^e(x,t;\mu) = q(x;\mu)\,u(t), \quad x\in\Omega, \quad t\in I, \tag{1}$$

with initial condition (say) $y^e(x,t=0;\mu)=0$. Here, $\Omega\subset\mathbb{R}^3$ is the three-dimensional spatial domain, a point in which shall be denoted by $x=(x_1,x_2,x_3)$, the time interval of interest is $I=]0,t_f]$ with final time $t_f>0$, v corresponds to the velocity of the torch,[2] κ is the thermal diffusivity, and $u(t)$ is the source strength. In this paper, we consider the so called *hemispherical volume heat source* given by

$$q(x;\mu) := e^{-x_1^2/\sigma_1^2}\, e^{-x_2^2/\sigma_2^2}\, e^{-x_3^2/\sigma_3^2}, \quad x\in\Omega. \tag{2}$$

* Corresponding author. Tel.: +49 241 8096470; fax: +49 241 80696470.
E-mail address: grepl@igpm.rwth-aachen.de (M.A. Grepl).

[1] Here, superscript "e" shall refer to "exact." We shall later introduce a "truth approximation" which will bear no superscript.

[2] We consider a coordinate system moving with the same velocity as the torch. In this coordinate system, the torch is stationary and the velocity enters as a convective term in the governing equation; see Section 3.1.3.

0045-7825/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.cma.2011.10.010

The standard deviations σ_i, $i = 1, 2, 3$, and the thermal diffusivity κ shall serve as our parameter, i.e., our parameter of interest is $\mu = (\sigma_1, \sigma_2, \sigma_3, \kappa)$. The source type (2) is a special case of the *double ellipsoid source* which was first introduced by Goldak et al. [6] to model the heating effect of a welding torch. We note, however, that the methods developed in this paper are not restricted to the particular welding process considered here, i.e., Gaussian source terms play an important role in many applications in science and engineering-another prominent example is the simulation of airborne contaminants [8–10]. Furthermore, our approach of course also directly applies to other types of non-affine functions besides Gaussians.

The main task in the analysis and modeling of the welding process is to find parameters $(\sigma_1, \sigma_2, \sigma_3)$ such that the simulated temperature at one or several measurement points on the surface of the workpiece predicted by (1) and (2) matches the experimental measurements [11]. Given the parameter estimates, we may subsequently aim to control the welding process to achieve a desired weld pool depth [12,13,3]. The parameter estimation problem needs to be solved in real-time, requiring a rapid and reliable evaluation of the PDE (1). Our goal here is thus to develop numerical methods to efficiently and reliably evaluate the forward problem, i.e., the PDE-induced input output relationship (1), in the limit of many queries or in real-time.

To achieve this goal we pursue the reduced basis method. The reduced basis method is a model-order reduction technique which provides efficient yet reliable approximations to solutions of parametrized partial differential equations in the many-query or real-time context; see [14] for a recent review of contributions to the methodology. In this paper we focus on parabolic problems with a non-affine parameter dependence in the source term—a typical example is given by the Gaussian function (2). To this end we employ the empirical interpolation method (EIM) [15] which serves to construct affine approximations of non-affine parametrized functions. The method is frequently applied in reduced basis approximations of parametrized PDEs with non-affine parameter dependence [15–19]; the affine approximation of the coefficient function is crucial for computational efficiency.

A posteriori error estimators for non-affine elliptic and parabolic problems have been proposed in [17,19,20], respectively. However, these estimators do not provide a provable rigorous upper bound for the true error due to the contribution of the interpolation error. Only recently, Eftang et al. [21] introduced a rigorous error analysis for the EIM. Furthermore, reduced basis output approximations and associated output bounds may suffer from a slow convergence, thus requiring a large dimension of the reduced order model to achieve a desired accuracy. Primal–dual formulations were proposed in [22] to circumvent this problem and improve the accuracy of the output prediction. These ideas have been successfully applied also in the FEM context, e.g. in [23,24], and in the reduced basis context, e.g. in [25–27]. However, these previous reduced basis works only considered *affine* problems. The contributions here are thus (i) rigorous *a posteriori* error bounds for reduced basis approximations of non-affine parabolic problems, and (ii) the development of primal–dual formulations for non-affine problems to ensure rapid convergence of the reduced basis output approximation and output error bound.

This paper is organized as follows: in Section 2 we present a short review of the EIM and corresponding rigorous error analysis. The abstract problem formulation and reduced basis approximation for linear coercive parabolic problems with non-affine source terms are introduced in Section 3. In Section 4 we develop our *a posteriori* error estimation procedures and in Section 5 we briefly discuss the sampling technique to generate the reduced basis space. Numerical results for the welding process are presented in Section 6. Finally, we offer concluding remarks in Section 7.

2. Empirical interpolation method

In this section we briefly review the EIM and associated *a posteriori* error estimation procedures [15,16,21].

2.1. Coefficient function approximation

We assume we are given a function $g : \Omega \times \mathcal{D} \to \mathbb{R}$ with $g(\cdot;\mu) \in L^\infty(\Omega)$ for all $\mu \in \mathcal{D}$, where $\mathcal{D} \subset \mathbb{R}^p$ is the set of admissible parameters, $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, is a bounded domain, and $L^\infty(\Omega) := \{v | \operatorname{ess\,sup}_{v\in\Omega} |v(x)| < \infty\}$. We introduce a finite but suitably large parameter train sample $\Xi^{\text{EIM}}_{\text{train}} \subset \mathcal{D}$ which shall serve as our surrogate for $\mathcal{D}$, and a triangulation $\mathcal{T}_{\mathcal{N}}(\Omega)$ of Ω with $\mathcal{N}$ vertices over which we shall in practice realize $g(\cdot;\mu)$ as a piecewise linear function.

The construction of the EIM approximation space W^g_M and set of interpolation points $T^g_M = \{\hat{x}^1, \ldots, \hat{x}^M\}$ is based on a greedy algorithm [28]: we first choose $\mu^1 := \arg\max_{\mu\in\Xi^{\text{EIM}}_{\text{train}}} \|g(\cdot;\mu)\|_{L^\infty(\Omega)}$, set $\hat{x}^1 := \arg\operatorname{esssup}_{x\in\Omega} |g(x;\mu^1)|$, and obtain the first (normalized) EIM basis function $\hat{g}^1(x) := g(x;\mu^1)/g(\hat{x}^1;\mu^1)$. We define $W^g_1 := \operatorname{span}\{\hat{g}^1(\cdot)\}$ and introduce the nodal value matrix $G^1 \in \mathbb{R}^{1\times 1}$ with the single element $G^1_{1,1} := \hat{g}^1(\hat{x}^1) = 1$.

Then, for $1 \leqslant M \leqslant M_{\max} - 1$, we compute the approximation $g_M(\cdot;\mu)$ to $g(\cdot;\mu)$ from

$$g_M(x;\mu) := \sum_{m=1}^{M} \omega_m(\mu)\hat{g}^m(x), \tag{3}$$

where the coefficient vector $\underline{\omega}(\mu) = [\omega_1(\mu), \ldots, \omega_M(\mu)]^{\mathrm{T}} \in \mathbb{R}^M$ is given by the solution of the linear system

$$G^M \underline{\omega}(\mu) = [g(\hat{x}^1;\mu), \ldots, g(\hat{x}^M;\mu)]^{\mathrm{T}}. \tag{4}$$

We choose the next parameter

$$\mu_{M+1} := \arg\max_{\mu\in\Xi^{\text{EIM}}_{\text{train}}} \|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)} \tag{5}$$

and define the residual $r^g_M(x) := g(x;\mu_{M+1}) - g_M(x;\mu_{M+1})$. The next interpolation point is then set to $\hat{x}^{M+1} := \arg\max_{x\in\Omega} |r^g_M(x)|$, and the next EIM basis function is given by $\hat{g}^{M+1}(x) := r^g_M(x)/r^g_M(\hat{x}^{M+1})$. We define $W^g_{M+1} := \operatorname{span}\{\hat{g}^m(\cdot) | 1 \leqslant m \leqslant M+1\}$, and update our nodal value matrix $G^{M+1} \in \mathbb{R}^{(M+1)\times(M+1)}$ with components $G^{M+1}_{m,n} := \hat{g}^n(\hat{x}^m), 1 \leqslant m, n \leqslant M+1$. This procedure is either terminated if the maximum dimension of the EIM space $M_{\max}$ is reached or if the maximum of $\|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)}$ over all $\mu \in \Xi^{\text{EIM}}_{\text{train}}$ is smaller than some desired tolerance $\varepsilon_{\text{tol}} > 0$. We note that the determination of the coefficients $\underline{\omega}(\mu)$ requires only $\mathcal{O}(M^2)$ computational cost since G^M is lower triangular with unity diagonal and that $\{\hat{g}^m\}^M_{m=1}$ is a basis for W^g_M [15,16].

Finally, we define a "Lebesgue constant" [29] $\Lambda_M := \sup_{x\in\Omega} \sum_{m=1}^M |V^M_m(x)|$, where $V^M_m(x) \in W^g_M$ are the characteristic functions of W^g_M satisfying $V^M_m(x_n) \equiv \delta_{mn}, 1 \leqslant m, n \leqslant M$; here, δ_{mn} is the Kronecker delta symbol. We recall that (i) the set of all characteristic functions $\{V^M_m\}^M_{m=1}$ is a basis for W^g_M, and (ii) the Lebesgue constant Λ_M satisfies $\Lambda_M \leqslant 2^M - 1$, see [15,16]. In applications, the actual asymptotic behavior of Λ_M is much better, as we shall observe subsequently.

2.2. A Posteriori error estimation

Given an approximation $g_M(x;\mu)$ to $g(x;\mu)$, we first define the interpolation error as

$$\varepsilon^g_M(\mu) := \|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)}. \tag{6}$$

We recall that, if $g(\cdot;\mu) \in W^g_{M+1}$, the interpolation error satisfies $\varepsilon^g_M(\mu) = \hat{\delta}^g_M(\mu)$, where the error estimator, $\hat{\delta}^g_M(\mu)$, is defined as $\hat{\delta}^g_M(\mu) := |g(x_{M+1};\mu) - g_M(x_{M+1};\mu)|$, see [15,16]. Since $\hat{\delta}^g_M(\mu)$ is very inexpensive to evaluate, it is used as an estimator for the function