C. R. Acad. Sci. Paris, Ser. I 349 (2011) 1229–1232

Contents lists available at SciVerse ScienceDirect

C. R. Acad. Sci. Paris, Ser. I

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Partial Differential Equations

A level set reduced basis approach to parameter estimation

Une méthode à bases réduites du type « level set » pour estimer des paramètres

Martin A. Grepl [a], Karen Veroy [b]

[a] *Institut für Geometrie und Praktische Mathematik (IGPM), RWTH Aachen University, 52056 Aachen, Germany*
[b] *Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, 52056 Aachen, Germany*

A R T I C L E I N F O

Article history:
Received 22 June 2011
Accepted 20 October 2011
Available online 9 November 2011

Presented by Philippe G. Ciarlet

A B S T R A C T

We introduce an efficient level set framework to parameter estimation problems governed by parametrized partial differential equations. The main ingredients are: (i) an "admissible region" approach to parameter estimation; (ii) the certified reduced basis method for efficient and reliable solution of parametrized partial differential equations; and (iii) a parameter-space level set method for construction of the admissible region. The method can handle nonconvex and multiply connected regions. Numerical results for two examples in design and inverse problems illustrate the versatility of the approach.

R É S U M É

Nous présentons ici une recette « level set » efficace pour résoudre des problèmes d'estimation de paramètres régis par des équations aux dérivées partielles. Ses ingrédients principaux sont: (i) une « région admissible » sur laquelle procéder à l'estimation du paramètre; (ii) la méthode éprouvée des bases réduites pour obtenir une solution efficace et fiable des équations paramétrées aux dérivées partielles; et (iii) une méthode « level set » sur l'espace des paramètres permettant de construire la « région admissible ». Cette méthode peut aussi s'appliquer à des régions multi-connectées ou non-convexes. La flexibilité de notre approche est démontrée à travers les résultats numériques obtenus lors de l'étude d'un problème de design et de celle d'un problème inversé.

1. Introduction

In this Note we address the following problem: Given a system characterized by parameters μ, determine the "admissible region," i.e., the set of all parameter values which satisfy prescribed constraints on the system. The constraints may be derived from experimental measurements in inverse problems, uncertainty or sensitivity tolerances in design, or feasibility conditions in optimization and control problems. Furthermore, in engineering analysis these constraints often involve outputs $s(\mu)$ of a parametrized partial differential equation (PDE) modeling the system behavior, whereas the parameters typically describe geometry, physical properties, boundary conditions, or loads.

Our aim is to construct an efficient and rigorous approximation to the admissible region. The admissible region approach was initially introduced in [2] for the solution of inverse problems using the reduced basis (RB) method. However, the approach presented in [2] has several limitations: first, it can only deal with simply connected and convex – or, more

E-mail addresses: grepl@igpm.rwth-aachen.de (M.A. Grepl), veroy@aices.rwth-aachen.de (K. Veroy).

1631-073X/$ – see front matter
doi:10.1016/j.crma.2011.10.020

generally, star-shaped – regions; and second, it can result in unwanted truncation of the region since the boundary is determined by only a small number of points. Here, we present a novel approach based on the level set method [5] lifting these limitations.

We first recall the RB recipe for second-order coercive elliptic PDEs (see [6] for a recent review): Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, we evaluate the (scalar) output $s^{\mathrm{e}}(\mu) = \ell(y^{\mathrm{e}}(\mu))$, where $y^{\mathrm{e}}(\mu) \in Y^{\mathrm{e}}$ satisfies $a(y^{\mathrm{e}}(\mu), v; \mu) = f(v; \mu)$, $\forall v \in Y^{\mathrm{e}}$. Here, $\mu \equiv (\mu_1, \dots, \mu_P)$ and $\mathcal{D}$ are the parameter and parameter domain, respectively; Y^{e} is a suitable Hilbert space with associated inner product $(w, v)_{Y^{\mathrm{e}}}$ and induced norm $\|\cdot\|_{Y^{\mathrm{e}}}$; $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, is our spatial domain, a point in which is denoted $(x_1, \dots, x_d)$; ℓ and f are bounded linear functionals; and, for any $\mu \in \mathcal{D}$, $a(\cdot, \cdot; \mu): Y^{\mathrm{e}} \times Y^{\mathrm{e}} \to \mathbb{R}$ is a coercive, continuous, bilinear form.

We now introduce a truth finite element (FE) space $Y \subset Y^{\mathrm{e}}$ of (typically large) dimension $\mathcal{N}$; Y inherits the inner product and norm from Y^{e}. Our truth approximation is: given $\mu \in \mathcal{D}$, evaluate $s(\mu) = \ell(y(\mu))$, where $y(\mu) \in Y$ satisfies $a(y(\mu), v; \mu) = f(v; \mu)$, $\forall v \in Y$. We define the parameter sample $S_N \equiv \{\mu_1, \dots, \mu_N\}$ and associated RB space, $Y_N = \mathrm{span}\{y(\mu_1), \dots, y(\mu_N)\}$. Given $\mu \in \mathcal{D}$, we evaluate the RB estimate $s_N(\mu) = \ell(y_N(\mu))$, where $y_N(\mu) \in Y_N$ satisfies $a(y_N(\mu), v; \mu) = f(v; \mu)$, $\forall v \in Y_N$. We can derive *a posteriori* bounds for the error in the RB output: $|s(\mu) - s_N(\mu)| \leqslant \Delta_N^s(\mu) \equiv \|\ell(\cdot)\|_{Y'} \|r(\cdot; \mu)\|_{Y'} / \alpha_{\mathrm{LB}}(\mu)$, $\forall \mu \in \mathcal{D}$. Here, the dual norm of the output and residual are defined as $\|\ell(\cdot)\|_{Y'} \equiv \sup_{v \in Y} \ell(v)/\|v\|_Y$ and $\|r(\cdot; \mu)\|_{Y'} \equiv \sup_{v \in Y} r(v; \mu)/\|v\|_Y$, respectively; the residual is given by $r(v; \mu) = f(v; \mu) - a(y_N(\mu), v; \mu)$, $\forall v \in Y$; and $\alpha_{\mathrm{LB}}(\mu): \mathcal{D} \to \mathbb{R}_+$ is a lower bound for the coercivity constant $\alpha(\mu) \equiv \inf_{v \in Y} a(v, v; \mu)/\|v\|_Y^2$. If a and f depend affinely on the parameter, e.g., $a(w, v; \mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) a^q(w, v)$, an efficient offline–online computational procedure can be developed to evaluate $s_N(\mu)$ and $\Delta_N^s(\mu)$.

We recall that certified RB approximations have also been developed for parabolic problems where – directly considering a time-discrete framework with K timesteps – the truth (resp. RB) field variable $y(t^k; \mu)$ (resp. $y_N(t^k; \mu)$), output $s(t^k; \mu)$ (resp. $s_N(t^k; \mu)$), and associated output bound $\Delta_N^s(t^k; \mu)$ are now also functions of the discrete time $t^k \equiv k\Delta t$, $1 \leqslant k \leqslant K$, with timestep Δt; see [2] for details.

2. The “admissible region” approach

We now formulate our parameter estimation problem: given prescribed constraints on the output $s(\mu)$ in the form of an interval $[a, b]$, we define the admissible region as

$$\mathcal{A} = \big\{\mu \in \mathcal{D} \,\big|\, s(\mu) \in [a, b]\big\}. \tag{1}$$

If the outputs of interest $s(\mu)$ depend on the parameters μ through the underlying parametrized PDE, then numerical methods for the construction or approximation of $\mathcal{A}$ would require repeated solution of the PDE. Unfortunately, evaluation of the truth approximation output for a single parameter value is generally quite expensive, and direct construction of the admissible region $\mathcal{A}$ thus requires great computational cost.

We thus use the RB method (see Section 1) which provides efficient certified approximations of the form

$$s(\mu) \in \big[s_N^-(\mu), s_N^+(\mu)\big] \equiv \big[s_N(\mu) - \Delta_N^s(\mu), s_N(\mu) + \Delta_N^s(\mu)\big] \tag{2}$$

where s_N^- and s_N^+ are *rigorous* upper and lower bounds to the true output $s(\mu)$. We may then replace all instances of the truth output $s(\mu)$ with the RB bound appropriate to the particular context. We illustrate this idea using two examples: a design problem and an inverse problem. We also note that these and the subsequent definitions directly extend to parabolic problems: the constraints on the output (and output bounds) then have to hold for all discrete observation times.

In *design problems*, one often needs to find the values of the parameters μ satisfying uncertainty constraints or sensitivity tolerances. These constraints are often given as intervals $[a, b] = [\tau - c, \tau + d]$, where τ is a target or desired value, and c, d represent the uncertainty or sensitivity tolerances. In this context we must guarantee that $s(\mu)$ is *definitely* in $[a, b]$, and we thus define the approximate admissible region as

$$\mathcal{A}_N^{\mathrm{des}} = \big\{\mu \in \mathcal{D} \,\big|\, \big[s_N^-(\mu), s_N^+(\mu)\big] \subseteq [a, b]\big\}. \tag{3}$$

From (1) and (2) it follows that $\mathcal{A}_N^{\mathrm{des}} \subseteq \mathcal{A}$, i.e., any $\mu \in \mathcal{A}_N^{\mathrm{des}}$ is certifiably also in $\mathcal{A}$. Thus, no errant values of μ are introduced due to the RB approximation, and the approximate tolerance is more stringent.

In *inverse problems*, the goal is to estimate the value of parameters μ consistent with experimental measurements given as intervals, $[a, b]$, reflecting measurement uncertainty. We seek the “possibility” region, the set of all parameter values which *may* be consistent with the measurements. In this context we must ensure that $s(\mu)$ is *possibly* in $[a, b]$, and we thus define the approximate admissible region as

$$\mathcal{A}_N^{\mathrm{inv}} = \big\{\mu \in \mathcal{D} \,\big|\, \big[s_N^-(\mu), s_N^+(\mu)\big] \cap [a, b] \neq \emptyset\big\}. \tag{4}$$

From (1) and (2) it follows that $\mathcal{A} \subseteq \mathcal{A}_N^{\mathrm{inv}}$, that is, all solutions μ contained in $\mathcal{A}$ are also in $\mathcal{A}_N^{\mathrm{inv}}$. Therefore, no possible solutions to the inverse problem are errantly eliminated due to the RB approximation. Our formulation thus accommodates experimental error and uncertainty (within our model assumptions).

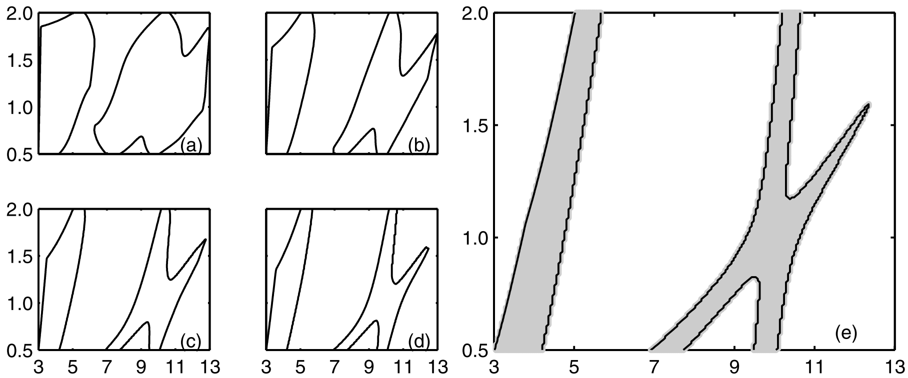

Fig. 1. Snapshots (a)–(d) of the level curve at different values of the artificial evolution time t, and (e) the level curve at steady state (with $\mathcal{A}_N^{\mathrm{des}}$ in gray), plotted with respect to the frequency ω (x-axis) and anisotropic property ρ (y-axis).

3. Level set method in parameter space

The level set method, introduced in [5], is a popular method for tracking interfaces in arbitrary dimensions. The method hinges upon the representation of (say) a curve $\Gamma \in \mathbb{R}^2$ as the zero contour of the level set function $\varphi(x,t) \in \mathbb{R}^3$, i.e., $\Gamma(t) = \{x \mid \varphi(x,t) = 0\}$, where $\varphi(x,t)$ satisfies a Hamilton–Jacobi equation of the form $\varphi_t(x,t) = v(x,t)|\nabla\varphi(x,t)|$. Here, t is an artificial evolution time and $v(x,t)$ is the speed function of the zero level set in the normal direction. It is known that the method can readily handle nonconvex and multiply connected regions, topological changes, and extends to arbitrary dimensions.

Our proposed method is based on the following key observation: we consider the boundary of the admissible region as an (initially) unknown interface in parameter space. We thus introduce a level set function $\phi(\mu,t)$ in parameter space $\mu \in \mathcal{D} \subset \mathbb{R}^P$ and initialize $\phi(\mu, t=0)$ as the signed distance function from the boundary of $\mathcal{D}$. We then evolve the zero level set $\Gamma(t) = \{\mu \mid \phi(\mu,t) = 0\}$, where $\phi(\mu,t)$ satisfies $\phi_t(\mu,t) = v(\mu)|\nabla\phi(\mu,t)|$, and choose an appropriate speed function $v(\mu)$ such that the zero contour of the steady-state solution of $\phi(\mu,t)$ is equivalent to the boundary of the admissible regions $\mathcal{A}_N^{\mathrm{des,inv}}$.

We thus need to set up a parameter dependent speed function $v(\mu)$ such that $v(\mu) = 0$ if μ lies on the boundary $\partial\mathcal{A}_N^{\mathrm{des,inv}}$, $v(\mu) > 0$ if $\mu \in \mathcal{A}_N^{\mathrm{des,inv}}$, and $v(\mu) < 0$ if $\mu \notin \mathcal{A}_N^{\mathrm{des,inv}}$. Returning to the design and inverse problems discussed in the last section, we define the associated speed functions

$$v^{\mathrm{des}}(\mu) = \min\big[b - s_N^+(\mu), s_N^-(\mu) - a\big] \quad \text{and} \quad v^{\mathrm{inv}}(\mu) = \min\big[s_N^+(\mu) - a, b - s_N^-(\mu)\big], \tag{5}$$

respectively. It is easily confirmed that the conditions on the sign of $v(\mu)$ are satisfied.

By initializing the zero level set on the boundary of $\mathcal{D}$ we ensure that we can detect multiply connected regions; we would not, however, detect the hole in a "donut" shaped region. More elaborate initializations, such as multiple circular "seeds" in $\mathcal{D}$, are of course also possible. Finally, we note that our approach can also directly be applied to detect the possibility region in a frequentistic uncertainty framework [3].

4. Numerical results

For our *design problem*, we consider a vibrating membrane where the displacement y is governed by the damped Helmholtz equation; the output of interest is the average deflection. In the framework of Section 1, we have $a(v,w;\mu) = \int_\Omega \frac{\partial w}{\partial x_1}\frac{\partial \bar{v}}{\partial x_1} + \rho\frac{\partial w}{\partial x_2}\frac{\partial \bar{v}}{\partial x_2} + (i\varepsilon\omega - \omega^2)\int_\Omega w\bar{v}$, $f(v) = \int_\Omega v(\sin(\pi x_1)\sin(\pi x_2) + \sin(\pi x_1)\sin(3\pi x_2) + \sin(3\pi x_1)\sin(\pi x_2))$, and $\ell(v) = \int_\Omega v$. Here, $\Omega =]0,1[^2$ is the domain, $Y_{\mathrm{e}} \equiv \{v = v_{\mathrm{R}} + iv_{\mathrm{I}} \mid v_{\mathrm{R}} \in H_0^1(\Omega), v_{\mathrm{I}} \in H_0^1(\Omega)\}$ is a complex Hilbert space, and $\bar{v}$ denotes the complex conjugate of v. Furthermore, $\varepsilon = 0.5$ is the damping constant, and the parameter is given by $\mu = (\omega,\rho) \in \mathcal{D} = [0.5, 2.0] \times [3.0, 13.0]$, where ω is the frequency and ρ is a material property. The FE space Y, obtained from piecewise linear triangular elements, has dimension $\mathcal{N} = 3970$. We generate an RB approximation of dimension $N = 20$ where the maximum relative output bound is less than 3%.

We seek $\mathcal{A}_N^{\mathrm{des}}$ given by (3) with $a = 0.09$, and $b = 1.00$. Given the RB approximation, we introduce a 200×200 parameter grid in $\mathcal{D}$, initialize the zero level set on the boundary of $\mathcal{D}$ and define $v^{\mathrm{des}}(\mu)$ as in (5). Figs. 1(a)–(d) show snapshots of $\Gamma(t)$ at four values of the artificial time. Fig. 1(e) shows Γ at steady state; the region in gray indicates $\mathcal{A}_N^{\mathrm{des}}$. The toolbox [4] was used for the level set calculation.

For our *inverse problem*, we consider the transient thermal nondestructive analysis of a fiber-reinforced polymer (FRP) bonded to a concrete slab (Fig. 2). The aim is to detect and characterize delaminations occurring at the FRP–concrete interface. Given measurements at various points in time on the surface, we thus need to characterize the delamination

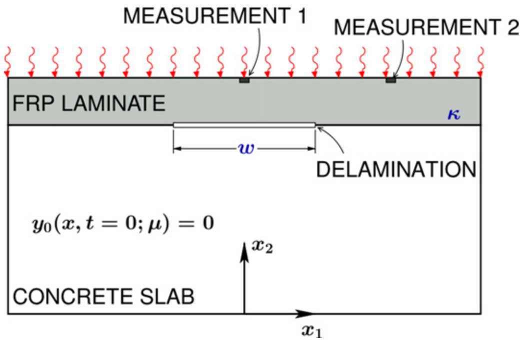

Fig. 2. Delamination sketch.

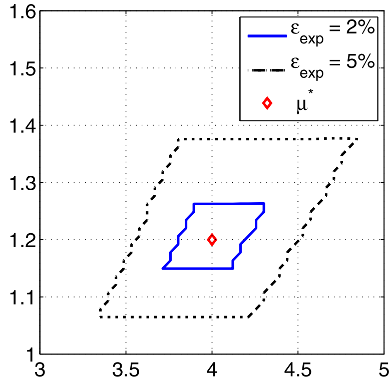

Fig. 3. Admissible regions $\mathcal{A}_N^{\text{inv}}$.

width w given an uncertainty in the conductivity ratio, κ, of the FRP and concrete. For a detailed problem description and numerical results of the RB approximation see [1].

Our parameter is $\mu = (w/2, \kappa) \in \mathcal{D} \equiv [1, 10] \times [0.4, 1.8]$. We generate noisy measurements for the (unknown) parameter $\mu^* = (4, 1.2)$: we solve the truth approximation $s(\mu^*, t^k)$ and then define $a(t^k) = s(\mu^*, t^k) - \epsilon_{\text{exp}} s_{\text{max}}$ and $b(t^k) = s(\mu^*, t^k) + \epsilon_{\text{exp}} s_{\text{max}}$, where ϵ_{exp} is the experimental error and $s_{\text{max}} = \max_{1 \leqslant k \leqslant K} s(\mu^*, t^k)$. We solve the level set equation on a grid of size 200×100 in $\mathcal{D}$. Fig. 3 shows the boundary of $\mathcal{A}_N^{\text{inv}}$ for $\epsilon_{\text{exp}} = 2\%, 5\%$. As expected $\mathcal{A}_N^{\text{inv}}$ increases with ϵ_{exp} and we observe that the corners are well defined.

This work shows that the admissible regions for design and inverse problems can be successfully constructed by combining the certified RB method with the level set framework. For our proof of concept, we used a regular grid in parameter space for the level set evolution. However, more efficient implementations using the narrow band approach and adaptive mesh refinement techniques would certainly decrease the number of required input–output evaluations, and thus increase the efficiency of the method.

Acknowledgements

We acknowledge A.T. Patera, D. Knezevic, and M. Bachmayr for fruitful discussions. This work was supported by the German Research Foundation through Grant GSC 111 and the Excellence Initiative of the German federal and state governments.

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