Physica D 240 (2011) 1228–1244

Contents lists available at ScienceDirect

Physica D

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

On optimal reconstruction of constitutive relations

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ARTICLE INFO

Article history:
Received 7 May 2010
Received in revised form
16 November 2010
Accepted 14 April 2011
Available online 10 May 2011
Communicated by T. Sauer

Keywords:
Parameter estimation
Constitutive relations
Optimization
Nonequilibrium thermodynamics
Continuum mechanics
Adjoint analysis

ABSTRACT

In this investigation we develop and validate a computational method for reconstructing constitutive relations based on measurement data, applicable to problems arising in nonequilibrium thermodynamics and continuum mechanics. This parameter estimation problem is solved as PDE-constrained optimization using a gradient-based technique in the optimize-then-discretize framework. The principal challenge is that the control variable (i.e., the relation characterizing the constitutive property) is not a function of the independent variables in the problem, but of the state (dependent) variable. The proposed method allows one to reconstruct a smooth constitutive relation defined over a broad range of the dependent variable. It relies on three main ingredients: a computationally friendly expression for the cost functional gradient, Sobolev gradients used in lieu of discontinuous L_2 gradients, and a systematic technique for shifting the identifiability region. The performance of this approach is illustrated by the reconstruction of the temperature dependence of the thermal conductivity in a one-dimensional model problem.

1. Introduction

Reliable mathematical and computational modeling of physical processes depends on our knowledge of the relevant properties of the materials involved. Obtaining such properties is particularly challenging when the materials are of a less common type. For example, when investigating thermo-fluid phenomena occurring in liquid metals, one needs to know the coefficients of viscosity, thermal diffusivity, surface tension, etc., for the specific alloys. This task is often made more difficult by the fact that these coefficients tend to depend on the temperature in a complicated way. As a result, precise information about such material properties is rarely available, except for some common materials. The goal of this investigation is to propose and validate a computational method that will allow one to reconstruct such material properties based on some measurements available for a particular process (e.g., heat conduction) and a particular material. The specific motivation for this investigation comes from our research on the optimization of multiphysics phenomena involved in advanced welding processes [1], where accurate data concerning material properties is quite important. While our intended applications concern more complicated systems, for the sake of clarity in this paper our approach is developed and validated based on a fairly simple model problem.

In principle, as regards the inverse problem of parameter estimation, one can consider two distinct formulations:

- material properties depending on the *space* variable $\mathbf{x}$ (i.e., the *independent* variable in the problem), and
- material properties depending on the *state* variable T (i.e., the *dependent* variable in the problem).

Problems of the first type have in fact received quite a lot of attention in the literature, and we refer the reader to the monographs [2] and [3,4] for surveys of the mathematical and more applied aspects of these problems, respectively. For example, as the reconstructed parameters are functions of the space variables, these problems represent the foundation of numerous imaging techniques in medical diagnostics, such as, e.g., X-ray tomography [4], as well as in geosciences [5]. Problems of this type are at least in principle relatively well understood, and there exist several established methods for their solution.

In this paper our focus will be exclusively on parameter estimation problems of the second type in which we want to determine the material properties as a function of the state (i.e., *dependent*) variable, e.g., the temperature T, rather than the position in space (the *independent* variable). In other words, we seek a relationship between the material property and the state variable that holds uniformly at *every* point $\mathbf{x}$ of the domain Ω in which the problem is formulated. This problem seems to have received less attention in the literature than the problem of estimating the space-dependent material properties. Foundations of an optimization-based approach to the solution of this problem

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0167-2789/$ – see front matter
doi:10.1016/j.physd.2011.04.006

were laid in the work of Chavent and Lemonnier [6] (which to the best of our knowledge never appeared in the English language), where the authors established the existence of solutions to the problem and derived expressions for the gradient of the least-squares error functional. They also showed the results of computations in which the cost functional gradients were obtained based on a suitably-defined adjoint system. Similar problems were also considered by Alifanov et al. [7,8], except that in their formulation the dependence of the material property on the state variable was assumed in the form of a spline interpolant, effectively resulting in a finite-dimensional optimization problem. A computational approach also based on a least-squares error functional and a linearization of the problem via a suitable change of variables was considered by Tai and Kärkkäinen [9]. An alternative technique utilizing the adjoint equations, but without making use of the error functional, was proposed by DuChateau et al. [10], whereas Janicki and Kindermann studied a method combining Green's functions and Landweber's iteration applied to the parameter-to-measurements map [11]. A different approach, based on the "equation error method", was pursued by Hanke and Scherzer [12] who also considered a discrete formulation. Some mathematical aspects of the inverse problem of determining the state-dependent diffusion coefficients were addressed by Kügler [13,14] who investigated the Tikhonov regularization, by Neubauer [15] who studied regularization using adaptive grids and also by DuChateau et al. [16,17]. Some analytical results concerning this problem posed in an infinite domain were also reported in [18]. In the present investigation we consider an optimization-based approach to the estimation of a state-dependent material property and the main contributions of our work are as follows

- we provide a novel expression for the gradient of the cost functional which is more computationally tractable than the formula originally derived in [6],
- recognizing that in the standard formulation (based on the L_2 inner products) the cost functional gradients may be discontinuous, we develop an approach ensuring a required degree of smoothness of the reconstructed material properties, and
- noting that in a given problem reconstruction is normally limited to the corresponding "identifiability region" (defined below), we propose a systematic experimental design procedure that allows one to tune inputs to the system, so that the constitutive relation can be reconstructed over a broader range of the state variable.

While adjoint analysis is now routinely used to solve partial differential equation (PDE)-constrained optimization problems [19], we emphasize that the structure of the gradients in the present problem is in fact quite different from what is encountered in typical problems [20]. The reason is that the optimization variable is a function of the dependent, rather than independent, variables in the problem. We also add that, in contrast to the results reported in some of the references quoted above, our approach is formulated in the "optimize-then-discretize" framework, i.e., while we ultimately discretize the problem for the purpose of a numerical solution, our optimality conditions and the cost functional gradients are derived in the continuous (PDE) setting. As a consequence, the main constituents of our approach are independent of the specific discretization used.

In order to ensure the applicability of our proposed approach to a broad array of problems in continuum mechanics and nonequilibrium thermodynamics, we formulate it in terms of reconstruction of constitutive relations. Thus, we will consider the optimal reconstruction of isotropic constitutive relationships between thermodynamic variables based on measurements obtained in a spatially-extended system. In other words, assuming the constitutive relation in the following general form

$$\begin{bmatrix}\text{thermodynamic}\\ \text{flux}\end{bmatrix} = k\,(\text{state variables}) \begin{bmatrix}\text{thermodynamic}\\ \text{“force”}\end{bmatrix}, \quad (1)$$

our approach allows us to reconstruct the dependence of the transport coefficient k on the state variables consistent with the assumed governing equations. Constitutive relations in the form (1) arise in many areas of nonequilibrium thermodynamics and continuum mechanics. To fix attention, but without loss of generality, in the present investigation we focus on a heat conduction problem in which the heat flux $\mathbf{q}$ represents the thermodynamic flux, whereas the temperature gradient $\boldsymbol{\nabla} T$ is the thermodynamic "force", so that relation (1) takes the specific form

$$\mathbf{q}(\mathbf{x}) = -k(T)\,\boldsymbol{\nabla} T(\mathbf{x}), \quad \mathbf{x} \in \Omega, \tag{2}$$

where $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$, is an open domain in which the problem is formulated. We note that by assuming the function $k : \mathbb{R} \to \mathbb{R}$ to be given by a constant, we recover the well-known linear Fourier law of heat conduction. While expressions for the transport coefficients such as $k(T)$ are typically obtained using methods of statistical thermodynamics, in the present investigation we will show how to reconstruct the function $k(T)$ based on some available measurements of the spatial distribution of the state variable T combined with the relevant conservation law. Such a technique could be useful, for example, to systematically adjust the form of a constitutive relationship derived theoretically to better match actual experimental data. Combining constitutive relation (2) with an expression for the conservation of energy, we obtain a partial differential equation describing the distribution of the temperature T in the domain Ω corresponding to the distribution of heat sources $g : \Omega \to \mathbb{R}$ and suitable boundary conditions (for example, of the Dirichlet type), i.e.,

$$-\boldsymbol{\nabla} \cdot [k(T)\,\boldsymbol{\nabla} T] = g \quad \text{in } \Omega, \tag{3a}$$

$$T = T_0 \quad \text{on } \partial\Omega, \tag{3b}$$

where T_0 denotes the boundary temperature. Instead of (3b), we could also consider Neumann boundary conditions involving $k(T)\frac{\partial T}{\partial n}$, where $\mathbf{n}$ is the unit vector normal to the boundary $\partial\Omega$ and pointing out of the domain, and our subsequent analysis would essentially be unchanged. In regard to reconstruction of constitutive relations, it is important that such relations be consistent with the second principle of thermodynamics [21]. There exist two mathematical formalisms, one due to Coleman and Noll [22] and another one due to Liu [23], developed to ensure in a very general setting that a given form of the constitutive relation does not violate the second principle of thermodynamics. In continuous thermodynamical and mechanical systems this principle is expressed in terms of the Clausius–Duhem inequality [24] which in the case of the present simple model problem (2)–(3) reduces to the statement that $k(T) > 0$ for all values of T. At the same time, the condition $k(T) > 0$ is also required for the mathematical well-posedness of elliptic boundary value problem (3). In addition, to ensure the existence of classical (strong) solutions of (3), we will assume that the heat source $g(\mathbf{x}) > 0$ is at least a continuous function of $\mathbf{x}$. This appears reasonable taking into account possible physical phenomena represented by this term. The positivity of g allows us to establish a lower bound on classical solutions of problem (3), cf. Appendix A.

We now define two intervals:

- $[T_\alpha, T_\beta] \triangleq [\min_{\mathbf{x}\in\overline{\Omega}} T(\mathbf{x}), \max_{\mathbf{x}\in\overline{\Omega}} T(\mathbf{x})]$ which represents the range spanned by the solution of problem (3); we note that, as demonstrated in Appendix A, the minimum T_α is attained at the boundary $\partial\Omega$; following [14], we will refer to the interval $\mathcal{I} \triangleq [T_\alpha, T_\beta]$ as the *identifiability interval*,