



Proper Orthogonal Decomposition and Radial Basis Functions in material characterization based on instrumented indentation

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ARTICLE INFO

Article history:

Received 20 November 2009

Received in revised form

26 October 2010

Accepted 2 November 2010

Available online 30 November 2010

Keywords:

Instrumented indentation

Inverse analysis

Proper Orthogonal Decomposition

Radial Basis Functions

Material characterization

Structural diagnosis

ABSTRACT

For the mechanical characterization of structural materials non-destructive tests combined with computer simulations and inverse analyses are more and more frequently and advantageously employed in various engineering fields. The contribution to such development presented in this paper can be outlined as follows. With reference to isotropic elastic–plastic material models, indentation test simulations are done preliminarily, once-for-all, by a conventional finite element forward operator. Results of these simulations are employed in a procedure which is centered on Proper Orthogonal Decomposition and Radial Basis Functions approximation and is used for fast interpolations which replace further finite element analyses in the parameter identification process. Comparative computational exercises are presented in order to point out the consequent significant reduction of computing times in test simulations and, hence, in the minimization of the discrepancy function by the Trust Region Algorithm, namely by a traditional first-order mathematical programming method. Such a parameter identification procedure may be carried out routinely and economically on small computers for in situ structural diagnoses. Both the force–penetration relationship (provided by an instrumented indenter) and the average imprint profile (achievable by laser profilometer) are considered as sources of measurable response quantities or experimental data.

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1. Introduction

The assessments of inelastic properties of materials are usually called “destructive” if laboratory tests are required on specimens extracted from structures. Indentation tests, which are becoming more and more frequent in engineering for structural diagnosis (and hardness tests which represent their historical origin) can be considered “non-destructive” (or at least “almost-nondestructive”). In fact, they usually imply neither service interruption nor a reduction of safety margins of the structure or plant involved. At micro- and nano-scales such an advantage is not exhibited by indentation but it is usually not practically important (e.g. for MEME and NEMS not considered here). Truly “nondestructive” experiments, like ultra-sonic tests, cannot provide data on material inelastic properties, a meaningful limitation from a structural mechanics standpoint.

Inverse analyses based on experimental data collected from instrumented indentation tests and on their simulations have been widely used in recent years for material parameter identification in structural engineering. Several developments of such methodology

oriented to different industrial applications can be found at present in the literature. For example, mechanical properties of functionally graded materials and of thin films have been assessed by such an approach in Refs. [1,2], respectively.

In [3] the exploitation of two kinds of experimental data was proposed and shown to be useful, namely of both the load-versus-penetration digitalized curves provided by the instrumented indenter and the residual imprint geometry measured by a laser profilometer as an additional instrument. Possible perturbations on the imprint geometry due to the inhomogeneity of material microstructures are made irrelevant by averaging imprint profiles in various directions and by adopting a penetration much larger than the typical size of that microstructure. By means of such an amplification of available experimental data, nondestructive indentation tests, originally proposed to assess hardness (see e.g. [4,5]), at present can be successfully employed if associated to test simulation and inverse analysis, in order to assess also anisotropic material properties [6], tensorial residual stresses [7] and quasi-brittle fracture properties [8]. Clearly, the above mentioned properties cannot be assessed on the basis of conventional data provided by the instrumented indenter alone. However, even if direction-independent quantities are to be assessed in the indentation specimen (like parameters in isotropic elasto–plastic constitutive models to be considered herein), two, instead of one, sources of experimental data contribute to the “regularization” in the Tikhonov

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sense of the inverse problem (namely, to the convexity of the discrepancy function to be minimized), see e.g. [9].

However, even in the presence of well-posedness, the numerical solution of inverse problems, both by traditional and modern procedures, turns out to be computationally heavy. In fact, it generally implies a sequence of direct analyses, namely of computer simulations of the test with diverse inputs of sought parameters. Such circumstances frequently represent a severe burden and handicap in engineering, when parameter identification becomes the main tool for the diagnostic search of possible structural material damages and should be done repeatedly and routinely (hopefully, if possible, in situ rather than in a computing center).

The above practical difficulty may be drastically mitigated or avoided by the procedure presented and numerically validated in this paper. A simple popular constitutive model is attributed to the (metallic, ductile) material considered for mechanical characterization (e.g. required by damage diagnosis on pipelines and power-plant components, which specifically have motivated the present study). The identification of possible deteriorated material parameters is pursued by a conventional deterministic approach, namely by minimization of a norm (called “discrepancy function”) of the differences between measurable quantities and their counterparts computed as functions of the unknown parameters.

Test simulations, namely “direct analyses”, are performed by the commercial Finite Element (FE) code ABAQUS [10]. Both the loading–unloading force-versus-penetration relationship (denominated here “indentation curves”) and the average profile of the residual imprint measured by a laser profilometer (“imprint profile”) are considered as sources of experimental data (or “pseudo-experimental”, computer-generated data), as proposed in [3].

The constrained minimization of the discrepancy function is carried out by the traditional mathematical programming algorithm called “Trust Region” (TRA), see e.g. [11], which involves first derivatives only (computed by finite differences, of course) and is available in MATLAB [12]. In order to drastically reduce the computing effort for the sequence of simulations required by TRA, the following operative procedure is adopted and investigated herein (basically similar to the one recently developed and applied to thermal problems in [13,14]): (i) construction of a Proper Orthogonal Decomposition (POD) basis of system responses (“snapshots”) in terms of both indentation curves and imprint profiles; these “snapshots” (namely vectors of measurable quantities) are computed “a-priori”, once-for-all, on the basis of “nodes” of a suitable grid selected in the space of the material parameters looked for; (ii) “truncation” as low-order approximation of the POD basis and relevant snapshot “amplitudes” (see e.g. [15]); (iii) replacement of FE direct analyses within each TRA iteration through computationally fast interpolation by means of Radial Basis Functions (RBF) (see e.g. [16,17]).

Section 2 is devoted to a brief survey of POD and RBF in view of their specific employment as mathematical tools within the present structural diagnostic analysis. The various comparative computational exercises in Section 3 on direct problems, and Section 4 on inverse problems are intended to evidence potentialities and limitations of the proposed procedure in structural engineering. Section 5 is devoted to conclusions and future prospects. The usual notation of matrix algebra is adopted (e.g. bold-face letters for matrices and vectors).

2. On Proper Orthogonal Decomposition (POD) and Radial Basis Functions (RBF) in the present context

2.1. Preliminary remarks

In the present indentation methodology for materials characterization the following two circumstances can be expected in

most real-life practical problems: (a) in the space of the parameters to identify, a domain where to confine the search can “a priori” be identified by physical considerations and/or by an “expert”; (b) if M tests are simulated by assuming different parameter vectors $\mathbf{p}_i$ ($i = 1, \dots, M$) included in the domain mentioned in (a), the N quantities which are measurable within responses to the tests can be gathered in a N -vector $\mathbf{u}$ (called a “snapshot” in the POD jargon); this vector $\mathbf{u}$ is “correlated” to all other snapshots included in the set of M vectors generated through the above simulations, since all the snapshots represent consequences due to the same external action in the same system, with only differences in material parameters.

The correlation mentioned in (b) means mechanically that changes of parameters in the domain (a) give rise to moderate changes of snapshot and, hence, geometrically that the snapshots are “almost parallel” and equally oriented in their N -dimensional space. This geometrical interpretation naturally suggests to find a new reference system whose axes will be sorted in the descending order of norm of all M snapshot projections: namely, the first new axis will have in N -dimensional space the direction that maximizes a norm of projections of the snapshots, the second one will give the second largest norm etc. In this new basis a low-order approximation of high accuracy can be achieved by preserving first $K < N$ prevailing components, i.e. by “truncating” the negligible ones.

In the present context the above “modus operandi”, which is central to POD conceptual kernel, implies the size reduction (or “compression”) of the information contained in the snapshots and concerning the essential role played by the parameters in the material specimen response to the indentation test.

2.2. Proper Orthogonal Decomposition: an outline

The mathematical procedure of POD adopted herein and briefly summarized below is consistent with the approach called Principal Component Analysis (PCA), described with details and proofs e.g. in [15]. Recurrent symbols in the sequel have the following meaning: the $S \times M$ matrix $\mathbf{P}$ gathers as columns M sets of S identifiable parameters ($\mathbf{p}_i$, $i = 1, 2, \dots, M$); the corresponding snapshots $\mathbf{u}_i$ ($i = 1, 2, \dots, M$) are collected in the $N \times M$ matrix $\mathbf{U}$; $\Phi = [\varphi^1, \dots, \varphi^N]$ denotes the $N \times N$ (or $N \times M$ matrix in the case when $M < N$) basis matrix which defines in the N -space of the measurable quantities the “optimal” reference system to be found according to the criterion suggested by the expected snapshot correlation as mentioned in Section 2.1; the $N \times M$ matrix $\mathbf{A}$ quantifies the “amplitudes” of the snapshots $\mathbf{u}_i$ in the basis Φ , namely the snapshot matrix $\mathbf{U}$ can be re-constructed when $\mathbf{A}$ is known by the relationship:

$$\mathbf{U} = \Phi \cdot \mathbf{A}. \quad (1)$$

Clearly, if the basis Φ is known, in view of its orthonormality, the amplitude matrix $\mathbf{A}$ is computed easily, namely ($\mathbf{I}$ being the identity matrix):

$$\Phi^T \cdot \Phi = \mathbf{I}, \quad \mathbf{A} = \Phi^T \cdot \mathbf{U}. \quad (2)$$

The central mathematical kernel, originally demonstrated in probability and information theories and dealt with in various publications (see e.g. [15,18]), consists of the sequential maximization of Euclidean norms of snapshot components, as mentioned in Section 2.1, whose result can be condensed into the formula which follows:

$$\tilde{\varphi}^i = \mathbf{U} \cdot \mathbf{v}^i \cdot \lambda_i^{-1/2}, \quad (i = 1, \dots, M) \quad (3)$$

where λ_i is the i th positive eigenvalue and $\mathbf{v}^i$ represents the corresponding normalized eigenvector of the following matrix

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