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Data-Driven Computational Plasticity

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Abstract

The use of constitutive equations calibrated from data collected from adequate testing has been implemented successfully into standard solvers for successfully addressing a variety of problems encountered in SBES (simulation based engineering sciences). However, the complexity remains constantly increasing due to the more and more fine models being considered as well as the use of engineered materials. Data-Driven simulation constitutes a potential change of paradigm in SBES. Standard simulation in classical mechanics is based on the use of two very different types of equations. The first one, of axiomatic character, is related to balance laws (momentum, mass, energy...), whereas the second one consists of models that scientists have extracted from collected, natural or synthetic data. Data-driven simulation consists of directly linking data to computers in order to perform numerical simulations. These simulations will use universal laws while minimizing the need of explicit, often phenomenological, models. This work revisits our former work on data-driven computational linear and nonlinear elasticity and the rationale is extended for addressing computational inelasticity (viscoelastoplasticity).

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Keywords: Computational plasticity, Computational inelasticity, Data-Driven, LATIN, Manifold learning

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1. Introduction

Big-data is becoming a key protagonist in our lives in many aspects, ranging from e-commerce to social sciences, mobile communications, healthcare, etc. However, very little has been done in the field of scientific computing, despite some very promising first attempts.

Advanced clustering techniques, for instance, not only help engineers and analysts, they become crucial in many areas where models, approximation bases, parameters, etc. are adapted depending on the local state (in space and time senses) of the system [1,2]. Machine learning needs frequently to extract the manifold structure in which the solution of complex and coupled engineering problems is living. Thus, uncorrelated parameters can be efficiently extracted from the collected data, the last coming from numerical simulations or experiments. As soon as uncorrelated parameters are identified (constituting the information level), the solution of the problem can be predicted at new locations of the parametric space, by employing adequate interpolation schemes [3,4]. On a different setting, parametric solutions can be obtained within an adequate framework able to circumvent the curse of dimensionality for any value of the uncorrelated model parameters [5].

This unprecedented possibility of directly determine knowledge from data or, in other words, to extract models from experiments in a automated way, is being followed with great interest in many fields of science and engineering. For instance, the possibility of fitting the data to a particular set of models has been explored recently in [6]. Closely related, Ortiz has developed a method that works without constitutive models, by finding iteratively the experimental data that best satisfies conservation laws [7]. In [8] authors followed a similar rationale extending the data-driven framework to nonlinear elasticity and inelasticity, where model-based simulations where replaced by data-driven simulations operating on a new kind of constitutive models defined directly from data. Thus, experiments become crucial because they are not only used for calibrating pre-assumed models (as it is the case in standard simulation approaches) but for driving directly simulations. Its main drawback is the huge amount of data required for running simulations. In the present work we will assume that all the needed data is available. We will not address the way of collecting data from adequate experiments and the use of eventual inverse techniques to enrich the behavior description, issues that will be reported in incoming works.

Usual model-based simulations proceeds by solving the equilibrium weak form defined in the domain Ω with boundary Γ

$$\int_{\Omega} \varepsilon\left(\mathbf{u}^*\right) : \sigma \; \mathrm{d}\mathbf{x} = \int_{\Gamma_t} \mathbf{u}^* \cdot \mathbf{t}_g \; \mathrm{d}\mathbf{x} \tag{1}$$

where $\Gamma = \Gamma_u \bigcup \Gamma_t$ ($\Gamma_u \bigcap \Gamma_t = \varnothing$) representing portions of the domain boundary where, respectively, displacements $\mathbf{u}_g$ (essential boundary conditions) and tractions $\mathbf{t}_g$ (natural boundary conditions) are enforced. In Eq. (1) $\mathbf{u}^*$ represents an arbitrary displacement field kinematically admissible (regular enough and satisfying the essential boundary conditions). In order to solve (1) a relationship linking kinematic and dynamic variables is required, the so-called constitutive equation. The simplest one, giving rise to linear elasticity, is known as Hooke's law (even if, more than a law, it is simply a model), and writes

$$\sigma = \lambda \mathrm{Tr}(\varepsilon)\mathbf{I} + \mu\varepsilon \tag{2}$$

where $\mathrm{Tr}(\bullet)$ denotes the trace operator, and λ and μ the two elastic coefficients. By introducing the constitutive model, Eq. (2), into Eq. (1), a problem is obtained that can be formulated entirely in terms of the displacement field $\mathbf{u}(\mathbf{x})$. By discretizing it, using for instance the standard finite element method, after performing numerically the integrals involved in Eq. (1), we finally obtain a linear algebraic system of equations, from which the nodal displacements can be obtained.

The biggest challenge could then be formulated as follows: *can simulation proceed directly from data by circumventing the necessity of establishing a mathematical expression of the constitutive model?*

In [8] authors explored different possibilities in the context of nonlinear elasticity, the less intrusive from the point of view of its implementation in standard simulation software, being the local calculation of a secant or tangent elasticity matrix. Another approach based on the direct use of data proceeds from a mixed formulation involving the two main fields, the strain $\boldsymbol{\varepsilon}$ and the stress $\boldsymbol{\sigma}$ fields respectively, as was successfully proposed in the LaTIn method [9]. The solution strategy consists of iterating between two manifolds, the first one related to couples $(\boldsymbol{\varepsilon},\boldsymbol{\sigma})$ verifying equilibrium, while the second one is related to couples $(\hat{\boldsymbol{\varepsilon}},\hat{\boldsymbol{\sigma}})$ verifying the material behavior.

If we assume that, at iteration *n*, the couple $(\boldsymbol{\varepsilon}^n,\boldsymbol{\sigma}^n)$ verifies the equilibrium, and that it does not belong to the constitutive manifold, a new couple $(\hat{\boldsymbol{\varepsilon}},\hat{\boldsymbol{\sigma}})$ is sought by considering an appropriate search direction. In fact the searched couple is no more that the intersection of the search direction with the constitutive manifold. The just updated stress-strain couple belongs to the constitutive manifold, but it does not verify equilibrium. Thus, a new equilibrated solution $(\boldsymbol{\varepsilon}^{n+1},\boldsymbol{\sigma}^{n+1})$ is searched from the former one, being the intersection of a new search direction and the equilibrium manifold. The iteration process continues until reaching the problem solution at the intersection of both manifolds. Both steps are summarized below:

- *Local step*. At each integration point $\mathbf{x}_g$, $g=1,\ldots,G$, we consider $\left(\boldsymbol{\varepsilon}^n(\mathbf{x}_g),\boldsymbol{\sigma}^n(\mathbf{x}_g)\right)$ and look for $\left(\hat{\boldsymbol{\varepsilon}}(\mathbf{x}_g),\hat{\boldsymbol{\sigma}}(\mathbf{x}_g)\right)$. Even if there are infinite possible search directions, in [8] we considered the simple projection of it onto the constitutive manifold.

- *Global step*. From the strain-stress couples satisfying the constitutive law at every integration point, we come back to the weak form, Eq. (1), in order to obtain updated strain-stress couples satisfying equilibrium $\left(\boldsymbol{\varepsilon}^{n+1}(\mathbf{x}),\boldsymbol{\sigma}^{n+1}(\mathbf{x})\right)$, $\mathbf{x}\in\Omega$. The generic search direction can be written as

$$\boldsymbol{\sigma}^{n+1}(\mathbf{x})-\hat{\boldsymbol{\sigma}}(\mathbf{x})=\mathbf{D}\left(\boldsymbol{\varepsilon}^{n+1}(\mathbf{x})-\hat{\boldsymbol{\varepsilon}}(\mathbf{x})\right) \tag{3}$$

with $\mathbf{D}$ a symmetric positive-definite matrix to ensure the problem ellipticity. Enforcing now the equilibrium, it results:

$$\int_{\Omega}\boldsymbol{\varepsilon}^*(\mathbf{x}):\left[\mathbf{D}\left(\boldsymbol{\varepsilon}^{n+1}(\mathbf{x})-\hat{\boldsymbol{\varepsilon}}(\mathbf{x})\right)+\hat{\boldsymbol{\sigma}}(\mathbf{x})\right]\,\mathrm{d}\mathbf{x}=\int_{\Gamma_t}\mathbf{u}^*\cdot\mathbf{t}_g\,\,\mathrm{d}\mathbf{x} \tag{4}$$

2. Data-Driven Inelasticity

2.1. Non-isothermal elasto-visco-plastic behavior

In the context of continuum-thermodynamics it is assumed that the state of the system can be defined at each time by a set of variables know as state-variables, some of them observable, like the total strain $\boldsymbol{\varepsilon}$, and other internal like the elastic $\boldsymbol{\varepsilon}^e$ and inelastic $\boldsymbol{\varepsilon}^p$ strain components (in what follows we assumed an additive decomposition, i.e. $\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}^e+\boldsymbol{\varepsilon}^p$), as well as the variables describing the isotropic and kinematic hardening, the scalar p and the tensor $\boldsymbol{\alpha}$ respectively. It is assumed the existence of a free energy depending on the state variables $\rho\Psi(\boldsymbol{\varepsilon}^e,p,\boldsymbol{\alpha};T)$, whose derivative allows defining the state-laws and the associated variables, the stress $\boldsymbol{\sigma}$ and both, the isotropic R and kinematic X hardening:

$$\begin{cases} \sigma = \rho \dfrac{\partial \Psi}{\partial \varepsilon^e} \\ R = \rho \dfrac{\partial \Psi}{\partial p} \\ X = \rho \dfrac{\partial \Psi}{\partial \alpha} \end{cases} \tag{5}$$

In order to obtain the evolution laws we consider the derivatives of the dissipation potential, the last depending on the associated variables $\varphi^*(\sigma, R, X; T)$:

$$\begin{cases} \dot{\varepsilon}^p = \dfrac{\partial \varphi^*}{\partial \sigma} \\ \dot{p} = -\dfrac{\partial \varphi^*}{\partial R} \\ \dot{\alpha} = -\dfrac{\partial \varphi^*}{\partial X} \end{cases} \tag{6}$$

A simple elastoviscoplastic model consists of choosing as free energy and dissipation potentials:

$$\begin{cases} \rho\Psi = \dfrac{1}{2}\mathbf{K}(T)\varepsilon^e : \varepsilon^e - \alpha^{th}(T - T_0)\mathbf{K}(T)\mathbf{I} : \varepsilon^e + h(T)g(p) + \dfrac{1}{2}C(T)\alpha : \alpha \\ \varphi^* = \dfrac{\kappa(T)}{n(T)-1}\left\langle \dfrac{f}{\kappa(T)} \right\rangle_+^{n(T)-1} \end{cases} \tag{7}$$

with the simplest yield function

$$f = \|\sigma - X\| - R - R_0(T) \tag{8}$$

that leads to the evolution laws

$$\begin{cases} \dot{\varepsilon}^p = \dot{\varepsilon}^p(\sigma, R, X) \\ \dot{p} = \dot{p}(\sigma, R, X) \\ \dot{\alpha} = \dot{\alpha}(\sigma, R, X) \end{cases} \tag{9}$$

Model-based simulations consist of considering adequate free energy and dissipation potentials to derive the state and evolution laws. As soon as they are available different solvers can be employed. An appealing strategy, the LaTIn, decouples the local and nonlinear equations related to the constitutive behavior from the global and linear ones, related to the equilibrium. When applying this strategy state equations are linearized by using an adequate change of variables, in order to transfer all the nonlinearities to the local step, that is to the evolution equations.

In the global step the normalized state-laws for (p,R) and (α,X) are enforced in a weak sense, as well as the kinematic admissibility of the total strain, whose elastic component has its own state-law. In order to use the rate of the plastic strain (coming from the behavior) the stress-formulation of the principle of virtual power is considered

$$\int_{\Omega} \dot{\varepsilon} : \sigma^{*} \mathrm{d}\mathbf{x} = \int_{\Gamma_u} \dot{\mathbf{u}}_g \cdot \left(\sigma^{*} \cdot \mathbf{n} \right) \mathrm{d}\mathbf{x} \tag{10}$$

The weak form (10) and the ones related to the verification of the state laws for (p,R) and (α,X) do not suffice for calculating the mechanical state (state and associated variables). For this reason a search direction is used. The local step uses the evolution laws complemented by an adequate search direction.

2.2. Data-Driven Inelastic Simulation

From the previous analysis, it seems clear that simulation can proceed as soon as the evolution equations (9) are known. Data-driven simulations can proceed in different manner but the simplest and minimally-invasive one consists of defining the behavior manifold from data, that is by a set of sextuplets $\hat{\mathbb{S}}_m = (\hat{\varepsilon}^p_m, \hat{p}, \hat{\alpha}, \hat{\sigma}, \hat{R}, \hat{X})$ properly collected (the question related to its collection will be addressed later).

Now different possibilities exist: (i) from the sextuplet $\mathbb{S}^n$ verifying the equilibrium and the state-laws at iteration *n*, defined at each position any time, and using an adequate search direction determine the sextuplet verifying the behavior and then computing from the global step $\mathbb{S}^{n+1}$ (usual LaTIn); (ii) from the behavior manifold determine locally around each position $\hat{\mathbb{S}}_m$ a linear relation between the rates of kinematic variables and the associate variables; and (iii) looking for polynomial approximations of the evolution laws.

It is important to note that alternatives (ii) and (iii) can be easily use in any usual nonlinear solver because here physically inspired mathematical expressions have been replaced by local or global polynomial expressions without direct physical content.

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2.3. Example involving elastoplastic behavior

In this example we consider an elasto-plastic behavior with isotropic hardening. We generated the synthetic data by using associate plasticity, a yield function expressed from the Von-Mises yield criterion and a linear hardening. Now, we considered the usual incremental weak form

$$\int_{\Omega} \varepsilon^{*} : \mathbf{K} \Delta\varepsilon \, dx = \int_{\Gamma_N} \mathbf{u}^{*} \cdot \Delta\mathbf{t} + \int_{\Omega} \varepsilon^{*} : \mathbf{K} \Delta\varepsilon^{p} \, dx \tag{11}$$

If the displacement is measurable everywhere in Ω the first integral in (11) becomes fully determined allowing the calculation of the plastic strains (involved in the last integral in (11)). This procedure allows calculating the elastic and plastic strain, and more particularly the plastic strain rate, as well as the stress. Now, we define the internal variable related to the isotropic hardening p from the accumulated plastic strain. Thus we have

$$\begin{cases} \dot{\varepsilon}^{p} = \lambda \dfrac{\partial f}{\partial \sigma} \\ f(\sigma, R) \\ \dot{p} = \lambda \end{cases} \tag{12}$$

where the yield function can be easily determined experimentally from the limit of the elastic domain. Figure 1 (left) depicts the yield surface based on data (expected representing the Von-Mises criterion). The normal to the yield surface represents the term $\partial f / \partial \sigma$ in (12), that allows calculating λ (that follows also from the total strain rate

and the elastic tensor, by making use of the persistency condition) and consequently $\dot{p}$. For calculating the associated variable, the hardening R it suffices considering the relation

$$\dot{R} = \frac{\partial f}{\partial \lambda} = \frac{\partial f}{\partial \sigma} \frac{\partial \sigma}{\partial \lambda} \tag{12}$$

that allows determining the hardening law illustrated in Fig. 1 (right), that coincides with the one used to generate the synthetic data.

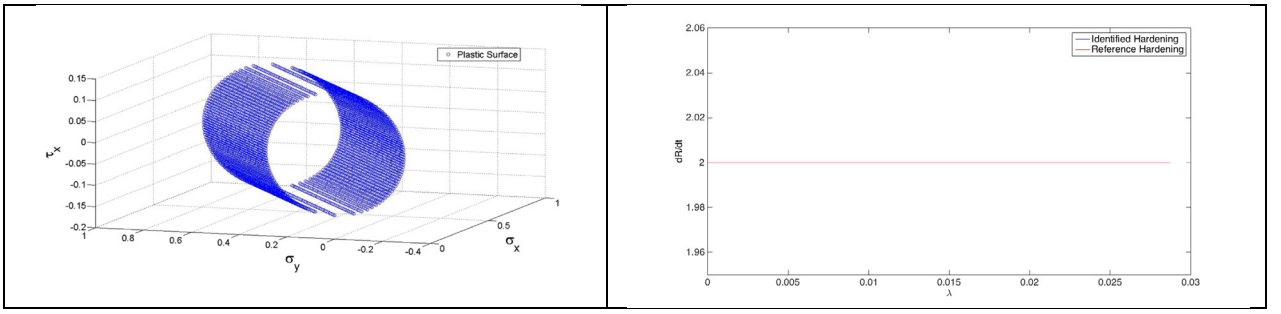

Figure 1. Measured yield stress (left) and identified hardening (right).

3. Conclusions

This work succeeded to extend the data-driven strategy proposed in our former works for addressing nonlinear elasticity to more complex scenarios involving internal variables. The proposed approach combines a rich enough behavior manifold, inspired from thermo-mechanics of continuous media, that for the simplest inelastic behaviors (e.g. elastoplastic, viscoelastoplastic, …) include the plastic strain rate, the rate of accumulated plastic deformation, and the kinematic variable associated to the kinematic hardening rate as well as their associated thermodynamic forces. In order to perform the problem discretization many techniques are available, the LaTIn being an appealing candidate because its facility to consider alternatively the enforcement of the global equilibrium and the local behavior, the last expressed from the only knowledge of the data.

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