Data-Driven Mechanics

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Abstract :

This work revisits data-driven approches and addresses a new paradigm in engineering sciences, the one of hybrid approches, in which the data could enrich existing models, without neither the necessity nor the opportunity of replacing them, while models allows enriching models in order to transform the big-data paradigm into the smart data one, able to proceed very efficiently in the low-data limit.

Key words : Data-driven, Physic-based models, Big-data, Smart-data, Hybrid paradigm

1 Introduction : Data-Driven Mechanics.

In an environment in which large scientific infrastructures produce petabytes of data every day, it was unavoidable that computational mechanics succumbed under the tsunami of big data. Science was first experimental (the so-called first paradigm of science), then was able, by means of models, to establish a theoretical paradigm. In the last decades it has become heavily computational, so as to make predictions by simulating the already established physical laws. However, very recently, the fourth paradigm of science is that of data exploration, the one that unifies data, theory and simulation.

The word *genome*, when applied out of the context of biological systems, refers to a *fundamental building block toward a larger purpose*. The materials genome is an initiative set forth by the White House in USA. to face the challenge of incorporating new, designed materials to the market twice as fast at a fraction of the nowadays cost. This initiative emphasizes the need for the design of more advanced computational techniques able to supplement physical experiments. This will be possible if data are shared and integrated across the "materials continuum" process of design. The materials genome initiative highlights the need for an integrated workflow of experiments, simulation and theory and the *development of advanced simulation tools* that are validated through experimental data. It also emphasizes the need to make digital data accessible, including combining data from experiment and computation into a searchable materials data infrastructure. This need has revealed, however, being totally insufficient. For instance, data produced in one week by the Spallation Neutron Source in the USA used to take one year of graduate student's time to analyze. Now, this research installation is producing data one hundred times faster.

Therefore, it is absolutely necessary to go substantially beyond : to develop simulation methods able to integrate and perform data acquisition, reduction, assimilation and analysis so as to be able to seamlessly integrate them in the design and fabrication processes of products involving radically new materials.

Existing computational tools still posses some other fundamental limitations. One of the biggest is the difficulty of integrating disparate time and length scales. For instance, we can model and predict the vibration of atoms in a lattice at time scales on the order of picoseconds. But this information is not suitable for the prediction of materials behavior across the course of the years. If a computational tools is needed to cope with this challenge, it will need to acquire and reduce all this huge amount of data and convert it in knowledge. Therefore, the need for model order reduction techniques is seen as a must.

Materials Informatics is a new scientific discipline that applies the principles of informatics to the design of new materials. It shares much of the spirit of the materials genome initiative. Indeed, it envisages the design of "specialized informatics tools for data capture, management, analysis, and dissemination" and the need for "advances in computing power, coupled with computational modeling and simulation and materials properties databases". Again, the possibility of sifting vast amounts of data reveals to be the bottleneck of a suitable strategy.

In an attempt to incorporate the huge possibilities of Big Data to the field of scientific computing, some proposals have been proposed very recently. The first one represents an attempt of working without constitutive laws [10]. In fact, they propose a method that works directly with balance equations and seeks for the experimental point that gives the state closest to equilibrium. To that end, it employs an optimization procedure.

This method re-opens the *epistemic controversy* between the scientific approach followed by Kepler—who, with the help of "big" data, was able to accurately describe planet's orbits—or the one by Newton, who unveiled the laws of physics behind gravitation that could finally explain why the computations done by Kepler were right.

The other approach, closer to the one of Newton, is to discover governing equations from data [2]. These methods need for some assumptions on the form of the particular sought physical laws, but determines a precise form of governing laws even in the presence of noised data.

The main limitation that can be envisaged about these two approaches is their ability to cope with large amounts of data. Furthermore, in an ICME approach we want to create new materials, still inexistent, by extrapolating the conclusions obtained by experimental and computational data. This is not possible without employing some form of *machine learning*, able to extract trends from data and to foresight the properties of materials yet to come.

2 A journey in data-driven approaches

2.1 Early times of data-driven approaches

Of course, data-driven approaches in computational mechanics trace back to early parameter identification methods, that had an important popularity after the mid-nineties. Essentially, this approach consisted of an inverse problem solving by finite elements so as to determine the value of the material parameter that best fits with the experimental results. However, this approach needs a pre-defined constitutive model and is therefore very intrusive in the process of material characterization.

By data-driven approaches, however, one tends to think of an approach that does no presuppose any form of constitutive equation. In fact, the work that is often considered as the first in the field, the one by Kirchdoerfer and Ortiz [10], does not employ any constitutive equation, and arose in an attempt to employ data directly in the computations.

Recent works by W. K. Liu and coworkers share important similarities with this rationale. For instance, in [1] a method is developed that works by designing a sort of *response database* for material RVEs, such that it very much eases the task of designing new materials by simply interpolating among selected microstructures. To circumvent this curse, Liu and coworkers developed a technique coined as *self-consistent clustering analysis* (SCA). Basically, it relies on k-means clustering techniques to characterize the macroscopic response of similar material microstructures.

2.2 The constitutive manifold

Recently, the authors introduced the concept of *constitutive manifold*. By applying manifold learning to pairs of experimental or numerical stress-strain values, the manifold structure of these data can be unveiled so as to ascertain the constitutive behavior of the material or structure [6, 7]. Assume that a set of $\mathtt{n}_{\text{exp}}$ experimental stress-strain couples are stored in our database. These couples are in fact points $\boldsymbol{X}_m \in \mathbb{R}^D$, $m = 1, \ldots, \mathtt{n}_{\text{exp}}$, in a space of dimension $D = 12$ (six stresses and six strains in Voigt notation). If some coherence exists between strains and stresses (and this is no more than a constitutive equation), then, these points could be projected without loss of information onto a manifold of dimension $d \ll D$. Consider, for instance, a set of randomly generated points according to a generalized Hooke's law. By employing Locally Linear Embedding (LLE) techniques [13], for instance, it is easy to find out that they pertain actually to a flat manifold. The result of embedding coordinates $\boldsymbol{X}_m$ onto the two-dimensional manifold gives the reduced coordinates ξ_m.

The concept of constitutive manifold not only provides with a very intuitive and visual concept (if the resulting manifold lives a small enough dimension). It allows to compute in a very efficient way by iterating between the equilibrium equation (which is always linear and global) and the non-linear and local constitutive manifold. The intersection between both manifolds will provide precisely with the sought state of the system in the phase space. A very simple iterating algorithm can thus be established that closely resembles the Large Time Increment technique by P. Ladeveze [9].

2.2.1 Hyperelasticity

Hyperelasticity deserves maybe a special comment, since it is characterized by the presence of a stored energy (potential) function so as to guarantee energy conservation in closed cycles. In this framework, data-driven approaches are directed towards the precise determination of the *shape* of this energy functional. While the general procedure is to try to reproduce existing, well-known constitutive laws by means of parameter fitting of experimental data, Montans and coworkers propose to avoid the use of existing laws and to simply interpolate experimental results with the help of splines. This approach is based upon an old technique developed by Sussman and Bathe [14] and is now known as *what you prescribe is what you get* (WYPIWYG) hyperelastcity. It has been applied to transversely isotropic as well as orthotropic materials, plasticity and compressible elasticity [11, 12].

2.2.2 Thermodynamic consistency

One of the recurrent questions when studying data-driven procedures in the framework of integrated computational materials engineering (ICME) is that of noise in the data. Eventually, this could led to inaccuracies that may have as a consequence the violation of some first principles. For instance, how

do we guarantee energy conservation and strict positive entropy generation in the presence of noise in the data ?

Recently, the authors have presented a method able to incorporate noisy data and still guarantee the thermodynamic consistency of the resulting simulations [3]. The method is developed by resorting to the GENERIC formalism [5]. In a nutshell, the GENERIC ("General Equation for Non-Equilibrium Reversible-Irreversible Coupling") formalism seeks for an expression of the time evolution of the necessary variables to describe the material at hand, $\dot{\boldsymbol{z}}_t$.

Basically, the GENERIC formalism assumes an evolution of the variables of the form

$$\dot{\boldsymbol{z}}_t = \boldsymbol{L}(\boldsymbol{z}_t)\nabla E(\boldsymbol{z}_t) + \boldsymbol{M}(\boldsymbol{z}_t)\nabla S(\boldsymbol{z}_t), \;\; \boldsymbol{z}(0) = \boldsymbol{z}_0, \tag{1}$$

where $\boldsymbol{L}$ is the so-called Poisson matrix, which is responsible for the reversible (Hamiltonian) part of the evolution of the system. E represents the energy of the system and $\boldsymbol{M}$ represents the friction matrix, responsible for the irreversible part of the evolution of the system. S represents the entropy of the system for the particular choice of variables $\boldsymbol{z}$. The choice of these variables is not particularly relevant, since even if they result to be finally related, this will be detected by the method.

Matrices $\boldsymbol{L}$ and $\boldsymbol{M}$ need to satisfy the following relationship :

$$\boldsymbol{L}(\boldsymbol{z}) \cdot \nabla S(\boldsymbol{z}) = \boldsymbol{0}, \tag{2a}$$

$$\boldsymbol{M}(\boldsymbol{z}) \cdot \nabla E(\boldsymbol{z}) = \boldsymbol{0}, \tag{2b}$$

often referred to as degeneracy conditions. This is fulfilled by simply choosing $\boldsymbol{L}$ skew-symmetric and $\boldsymbol{M}$ symmetric, positive semi-definite. Then it is straightforward to verify that

$$\dot{E}(\boldsymbol{z}) = \nabla E(\boldsymbol{z}) \cdot \dot{\boldsymbol{z}} = \nabla E(\boldsymbol{z}) \cdot \boldsymbol{L}(\boldsymbol{z})\nabla E(\boldsymbol{z}) + \nabla E(\boldsymbol{z}) \cdot \boldsymbol{M}(\boldsymbol{z})\nabla S(\boldsymbol{z}) = 0, \tag{3}$$

which is equivalent to the very basic principle of conservation of energy in closed systems. In turn,

$$\dot{S}(\boldsymbol{z}) = \nabla s(\boldsymbol{z}) \cdot \dot{\boldsymbol{z}} = \nabla S(\boldsymbol{z}) \cdot \boldsymbol{L}(\boldsymbol{z})\nabla E(\boldsymbol{z}) + \nabla S(\boldsymbol{z}) \cdot \boldsymbol{M}(\boldsymbol{z})\nabla S(\boldsymbol{z}) \geq 0, \tag{4}$$

guarantees the satisfaction of the second principle of thermodynamics.

The method consists, then, in the identification of matrices $\boldsymbol{L}$ and $\boldsymbol{M}$—something straightforward in the vast majority of the cases—and the particular structure of the gradients of energy and entropy (Hamiltonian and dissipative parts of the constitutive equations, respectively).

3 Hybrid methodologies

As just emphasized, a growing interest has arose on the development of data-driven techniques to avoid the employ of phenomenological constitutive models. While it is true that, in general, data do not fit perfectly to existing models, and present deviations from the most popular ones, we believe that this does not justify (or, at least, not always) to abandon completely all the acquired knowledge on the constitutive characterization of materials. Instead, what we recently proposed [8], by means of machine learning techniques, to develop correction to those popular models so as to minimize the errors in constitutive modeling.

Plenty of effort has been dedicated throughout history to create very accurate models, however, we also know that no model is perfect : it is always subjected to certain limiting hypotheses. In [8], we provided an alternative route by enhancing or correcting existing, well-known, models with information coming from data, thus performing a sort of *data-driven correction*. In that first work a special effort was put on the correction of plastic yield functions, while work in progress adresses more complex scenarios involving hardening and damage.

The proposed data driven correction technique is conceptually simple. Imagine that our departure point is a given, well-known parametric model $\mathscr{M}(\boldsymbol{p})$. It is important to keep in mind that we are looking for an enhancement or correction of the previous model based on the available experimental results. Therefore, a *discrepancy* model $\mathscr{D}(\boldsymbol{c})$, which applies to the first model, needs to be defined. So to speak, *reality*, $\mathscr{R}$, is approximated as

$$\mathscr{R} = \mathscr{M}(\boldsymbol{p}) + \mathscr{D}(\boldsymbol{c})\big|_{\boldsymbol{p}}, \tag{5}$$

where $\boldsymbol{p}$ represents the set of parameters governing the model and $\boldsymbol{c}$ represents the set of parameters needed to define the necessary correction.

Since our measurement capabilities will in general be constrained to some experimentally observable quantities, both our objective *reality* and the correction to the model will be restricted to these experimental settings. In other words,

$$\mathscr{R}\big|_{\boldsymbol{s}} \approx \mathscr{M}(\boldsymbol{p}) + \mathscr{D}(\boldsymbol{c})\big|_{\boldsymbol{p},\boldsymbol{s}}. \tag{6}$$

It is worth to mention that the way we define the observables $\boldsymbol{s}$ could have an important impact over the calibration of the set of correction parameters, $\boldsymbol{c}$ and remains a research field very active as discussed later.

In [4] a similar route was employed for enriching hyper-elastic models within the thermodynamic (GENERIC) rationale.

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