Available online at www.sciencedirect.com

ScienceDirect

Procedia Manufacturing 47 (2020) 693–695

Procedia MANUFACTURING

www.elsevier.com/locate/procedia

23rd International Conference on Material Forming (ESAFORM 2020)

Scientific Machine Learning for Coarse-Grained Constitutive Models

David González[a], Francisco Chinesta[b], Elías Cueto[a,*]

[a]*Aragón Institute of Engineering Research. Universidad de Zaragoza. Maria de Luna, s.n. 50018 Zaragoza, Spain.*
[b]*ESI Group Chair. Arts et Metiers Institute of Technology. 151 Bvd. De l'Hôpital. 75015 Paris, France.*

* Corresponding author. *E-mail address:* ecueto@unizar.es.

Abstract

We present here a review on some of our latest works concerning the development of thermodynamics-aware machine learning strategies for the data-driven construction of constitutive models. We suggest a methodology constructed upon three main ingredients. (i) the employ of manifold learning strategies to unveil the true dimensionality of data, thus pointing out the need for the definition of "internal" variables, different of the experimental ones. (ii) the process will be described by the so-called General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC). (iii) the precise form of the GENERIC terms will be unveiled by regression of data.

Keywords: Machine Learning; Scientific Machine Learning; GENERIC; Data-driven computational mechanics.

1. Introduction

We review in this contribution some of our latest results in the application of machine learning to the data-driven characterization of constitutive laws for complex multiscale materials. Particular attention is paid to the development of thermodynamics-aware methods, in which laws such as the first and second law of thermodynamics are fulfilled.

2. A dynamical systems approach to machine learning

Assume that the variables governing the behavior of the system at a particular level of description are stored in a vector

$$\dot{\boldsymbol{\xi}} = f(t, \boldsymbol{\xi}), \quad \boldsymbol{\xi}(0) = \boldsymbol{\xi}_0. \tag{1}$$

Under this prism, machine learning would be equivalent to finding f by regression, provided that sufficient data is available. How this regression is accomplished is of little importance: neural networks or classical (piecewise) regression are thus equivalent, if both work well.

To guarantee the thermodynamic admissibility of the resulting approximation, we impose Eq. (1) to have a GENERIC form [1]:

$$\dot{\boldsymbol{\xi}}_t = \boldsymbol{L}(\boldsymbol{\xi}_t)\nabla E(\boldsymbol{\xi}_t) + \boldsymbol{M}(\boldsymbol{\xi}_t)\nabla S(\boldsymbol{\xi}_t), \tag{2}$$

Where $\boldsymbol{L}$ represents the classical Poisson matrix of Hamiltonian mechanics (and is, therefore, skew-symmetric) and $\boldsymbol{M}$ represents the so-called friction matrix, that must be symmetric, semi-positive definite in order to guarantee thermodynamic consistency.

In our previous works, see [2] [3], we perform regression analysis from data so as to unveil the particular form of the expression for the energy, E, and entropy, S, potentials. The resulting formulation guarantees by construction thermodynamic admissibility and provides excellent results in the data-driven identification of complex behaviors.

3. Unveiling the need for internal variables

However, one particularly important question remains in this (and other) approaches to data-driven mechanics of materials.

2351-9789
10.1016/j.promfg.2020.04.211

Scientists have traditionally resorted to the employ of internal variables so as to take into account the influence on the model of unresolved degrees of freedom. This choice has been often phenomenological and motivated by intuition, something difficult to transmit to the world of machine learning. In Fig. 1 a sketch of this type of so-called Mori-Zwanzig projection is depicted.

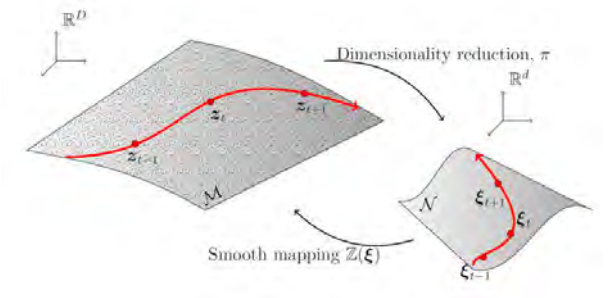

Fig. 1. Sketch of the Mori-Zwanzig projection to a less-detailed manifold, where the system is sampled experimentally. The influence of this sampling scale on the number of non-resolved degrees of freedom is analyzed.

In essence, the scale of molecular dynamics is Hamiltonian (Newton laws apply) and therefore only the Energy potential is needed. If subsequent coarse-graining is applied to the description of the system, the need for a second potential (entropy) is obvious. This arises from the well-known fluctuation-dissipation theorem (see [4] and references therein).

Moreover, it is well-known [5] that such a Mori-Zwanzig projection leads to the appearance of noise (fluctuation due to the unresolved degrees of freedom), which is equivalent to dissipation (and hence entropy), and also history dependence of the resulting description.

So the only possibility to unveil the need for internal variables is to be able to project back the experimental results from the coarse-grained manifold $\mathcal{N}$ to the fully-resolved one, $\mathcal{M}$, or at least one of a similar dimension. This can be accomplished by employing kernel-PCA (k-PCA) techniques [4]. These non-linear manifold learning techniques operate by projecting data to a higher (eventually, infinite) dimensional space, where everything can be separated by a hyperplane. Thus, projecting to a number of dimensions R, with $d \leq R \leq D$, could provide with insight on the true dimensionality of data, and hence the number of internal variables needed.

4. An example: polymeric flows

We consider, as a proof-of-concept, the case of Couette flow of a polymeric material, described by an Oldroyd-B-type constitutive law.

The Oldroyd-B model arises from the consideration of the stretching elasticity of polymer chains, and is well known to provide a description of the stress tensor in the fluid dependent on the conformation tensor, i.e.,

$$\boldsymbol{\tau} = -\frac{n}{2\zeta_{12}}\boldsymbol{c}^{\nabla},$$

where $\boldsymbol{c}^{\nabla}$ represents the Oldroyd derivative of the conformation tensor,

$$\boldsymbol{c} = \langle \boldsymbol{Q}\boldsymbol{Q} \rangle,$$

and $\boldsymbol{Q}$ represents the end-to-end vector of the polymeric chains. It is thus obvious that the model fully depends on small-scale degrees of freedom (end-to-end distances $\boldsymbol{Q}$) that cannot be obtained by experimental measurements.

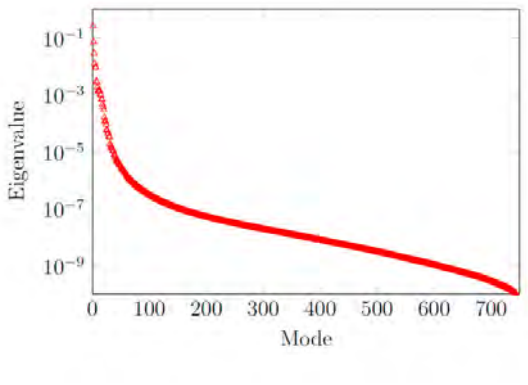

Fig. 2. K-PCA eigenvalues for 700 different experiments of the polymer flow.

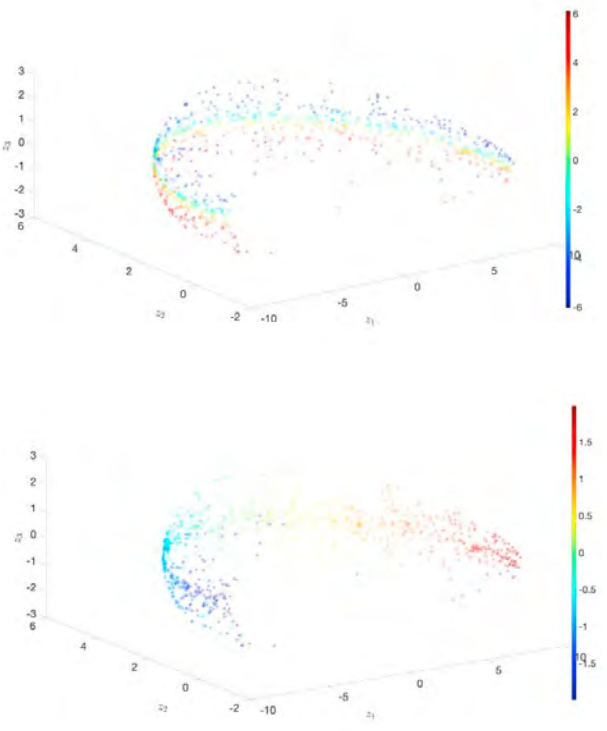

Fig. 3. K-PCA embedding of the 750 experimental results. (top) color plot represents the embedding according to the initial polymer chain orientation. (bottom) embedding according to the shear rate or, in other words, according to the history variable of the problem.

Experiments performed successively will depend on the initial state of the conformation tensor, giving apparently noise as a result. A careful analysis by k-PCAof 750 different experiments gave the eigenvalue plot shown in Fig. 2, that

reveals that some 4-5 degrees of freedom should be enough to describe the system.

If we plot the embedding of these experimental results on a space of three dimensions, we obtain the plots in Fig. 3.

In Fig. 3 it can readily be noticed how the proposed technique is able to clusterize the experimental results according to hidden variables in the model such as the initial polymer chains orientation or the shear rate in the flow.

5. Conclusions

We have presented a method for the machine learning of the presence of hidden, internal variables in the description of a material. In this case, a polymeric fluid has been chosen to this end. The presented method is able to unveil the dependence of the problem on details that are not available at the scale of experimental measurements, or that depend on the history of the fluid.

We refer the reader to the references below for a detailed description of these and other examples, as well as for a sound theoretical description of the developed method.

Acknowledgements

We acknowledge the help and comments provided by M. Grmela, V. Klika and M. Pavelka during the development of this work.

References

[1] Grmela M. and Öttinger, H. Ch. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. Phys. Rev. E, 1997: 56, 6620.
[2] González D., Chinesta F., Cueto E. Thermodynamically consistent data-driven computational mechanics. Continuum Mechanics and Thermodynamics, 2019;31:239–253.
[3] Gonzalez D., Chinesta F., Cueto E. Learning corrections for hyperelastic models from data. Frontiers in Materials, 2019;6:14.
[4] González D, Chinesta F, Cueto E. Learning non-Markovian physics from data. Submitted, 2019.
[5] E W. A proposal on machine learning via dynamical systems. Communications in Mathematics and Statistics, 2017;5:1-11.