LEARNED SIMULATORS THAT SATISFY THE LAWS OF THERMODYNAMICS

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ABSTRACT

When the physical phenomenon under scrutiny possesses conserved quantities (typically, energy), it is relatively easy to employ inductive biases to enforce these symmetries in the learned description. However, when the system presents dissipation, the right structure to impose is far from obvious. In this work we enforce a metriplectic structure to guarantee the fulfillment of the principles of thermodynamics, namely, the conservation of energy in closed systems and the positive production of entropy. The result is a learned energy-entropy-momentum integration scheme [*Energy-entropy-momentum integration schemes for general discrete non-smooth dissipative problems in thermomechanics. D. Portillo et al., Int. J. Numer. Meth. Engng 2017; 112:776–802*]. Examples are shown that demonstrate that the proposed technique needs fewer data and attains higher accuracy on training as well as tests data than standard black-box approaches.

1 INTRODUCTION

Traditional, engineered simulators have shown a tremendous success in many branches of engineering and applied sciences. Today, their main limitation is not their ability to reproduce faithfully complex physical phenomena, but their CPU consumption in daily practice. Thus, in situations such as many-query problems, inverse problems, high-dimensional parametric problems or real-time decision making, to name but a few, engineered simulators continue to show important limitations in terms of hardware requirement and time to response.

This opened the interest in the development of *learned* simulators. These are based on the employ, in general, of machine learning techniques (particularly, deep learning) that, fed with abundant data, could make predictions on a priori unseen scenarios. Despite the well-known advantages of deep learning, neural networks are well known to be prone to a black-box character.

Halfway between the two approaches, physics-based neural networks have appeared as an appealing possibility to satisfy both requirements: credibility of the predictions and short time to response. Among the first approaches of this type, one can cite, for instance, the works by Raissi et al. (2017a) or Raissi et al. (2017b).

2 PREVIOUS WORKS IN THE FIELD

One can think of the process of learning physical phenomena from data as a sort of dynamical system (E, 2017). Thus, we assume the system as governed by a set of variables $\boldsymbol{z} \in \mathcal{M} \subseteq \mathbb{R}^n$, with $\mathcal{M}$ the state space of these variables, which is assumed, thanks to the manifold hypothesis, to have the structure of a differentiable manifold in $\mathbb{R}^n$ (Fefferman et al., 2016).

Learning a simulator, therefore, would be equivalent to determine the time evolution of the system, as given by an ordinary differential equation (ODE) of the type

$$\dot{\boldsymbol{z}} = \frac{d\boldsymbol{z}}{dt} = F(\boldsymbol{x}, \boldsymbol{z}, t),\ \boldsymbol{x} \in \Omega \in \mathbb{R}^D,\ t \in \mathcal{I} = (0, T],\ \boldsymbol{z}(0) = \boldsymbol{z}_0, \tag{1}$$

where $\boldsymbol{x}$ and t refer to the space and time coordinates within a domain with $D = 2, 3$ dimensions. Following this rationale, $F(\boldsymbol{x}, \boldsymbol{z}, t)$ would be the function that gives, after some time T, the flow

map $\boldsymbol{z}_0 \rightarrow \boldsymbol{z}(\boldsymbol{z}_0, T)$. Discretizing in time Eq. (1) would provide the sought simulator that, once the state of the system at time t is known, is able to provide the state of the system at time $t + \Delta t$.

This rationale soon paved the way for the imposition of inductive biases, i.e., for the imposition of known characteristics in the function F. For instance, if certain symmetries apply to the system—conservation of energy is the most obvious one—it is straightforward to impose them in the loss function of the network. Different works have followed this route (Bertalan et al., 2019b; Greydanus et al., 2019; Toth et al., 2019; Zhong et al., 2019; Bertalan et al., 2019a; Jin et al., 2020b; Tong et al., 2020). More recently, the Poisson structure of such systems has also been exploited by Jin et al. (2020a).

However, no solution has been proposed, to the best of our knowledge, to the problem of learning simulators that preserve the general structure of the problem if dissipation is included, for instance.

3 Learned simulators that preserve the structure of the problem

3.1 The general setting

As mentioned before, to increase the credibility of learned simulators it is of utmost importance to develop techniques able to satisfy known properties of the system. If the system is conservative, it possesses a Hamiltonian structure, and can therefore be written in the form

$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}}, \tag{2}$$

where

$$\boldsymbol{L} : T^*\mathcal{M} \rightarrow T\mathcal{M},$$

with $T^*\mathcal{M}$ and $T\mathcal{M}$ represent, respectively, the cotangent and tangent bundles of $\mathcal{M}$, and E represents the Hamiltonian (the energy) of the system, which is precisely the magnitude that is conserved. $\boldsymbol{L}$ is the so-called Poisson matrix (since it defines a Poisson bracket $\{\boldsymbol{z}, E\}$).

If the phenomenon under scrutiny is dissipative, however, a second potential must be introduced into the formulation, the so-called Massieu potential (actually, entropy). Dissipation will be introduced by a dissipative or friction bracket $[\boldsymbol{z}, S]$, where S represents entropy. For clarity, we express the resulting formulation in matrix form:

$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}} + \boldsymbol{M}\frac{\partial S}{\partial \boldsymbol{z}}. \tag{3}$$

Here, $\boldsymbol{M} : T^*\mathcal{M} \rightarrow T\mathcal{M}$ represents the friction matrix. For $\boldsymbol{L}$ to construct a valid Poisson bracket, it is known that it must be skew symmetric, while $\boldsymbol{M}$ must be symmetric, positive semi-definite. For this to be valid, still one more requirement is needed: the so-called degeneracy conditions. These impose that the gradient $\frac{\partial S}{\partial \boldsymbol{z}}$ is in the null space (is a Casimir) of the $\boldsymbol{L}$ operator, while the gradient $\frac{\partial E}{\partial \boldsymbol{z}}$ is in the null space of $\boldsymbol{M}$,

$$\boldsymbol{L}\frac{\partial S}{\partial \boldsymbol{z}} = \boldsymbol{M}\frac{\partial E}{\partial \boldsymbol{z}} = \boldsymbol{0}. \tag{4}$$

These conditions guarantee the conservation of energy by the contribution of $\boldsymbol{M}$ to the dynamics or, equivalently, that entropy is not affected by the reversible dynamics. This mutual degeneracy requirements ensure that:

$$\frac{\partial E}{\partial t} = \frac{\partial E}{\partial \boldsymbol{z}} \cdot \frac{\partial \boldsymbol{z}}{\partial t} = \frac{\partial E}{\partial \boldsymbol{z}} \left(\boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}} + \boldsymbol{M}\frac{\partial S}{\partial \boldsymbol{z}} \right) = 0,$$

which expresses the conservation of energy in an isolated system. In other words, the first law of thermodynamics. Entropy S, in turn, satisfies:

$$\frac{\partial S}{\partial t} = \frac{\partial S}{\partial \boldsymbol{z}} \cdot \frac{\partial \boldsymbol{z}}{\partial t} = \frac{\partial S}{\partial \boldsymbol{z}} \left(\boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}} + \boldsymbol{M}\frac{\partial S}{\partial \boldsymbol{z}} \right) = \frac{\partial S}{\partial \boldsymbol{z}} \boldsymbol{M} \frac{\partial S}{\partial \boldsymbol{z}} \geq 0,$$

which guarantees the entropy inequality, this is, the second law of thermodynamics.

Eq. (3) is known as the General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) and is due to Grmela & Öttinger (1997). Such a formulation is called *metriplectic* for being a combination of metric and symplectic structures (Morrison, 1986).

3.2 THE PROPOSED METHODOLOGY

Our approach, therefore, is built on the assumption of a metriplectic structure for the system, and the data-based identification of such a structure, subject to the degeneracy conditions given by Eq. (4). For that purpose, we first discretize Eq. (eq:generic3) in time, by a standard forward Euler method, thus leading to

$$\frac{\boldsymbol{z}_{n+1}-\boldsymbol{z}_n}{\Delta t} = \mathsf{L}_n \cdot \frac{\mathsf{D}E_n}{\mathsf{D}\boldsymbol{z}_n} + \mathsf{M}_n \cdot \frac{\mathsf{D}S_n}{\mathsf{D}\boldsymbol{z}_n}, \tag{5}$$

such that $\boldsymbol{z}_{n+1} = \boldsymbol{z}_{t+\Delta t}$. L_n and M_n are the discretized version of the Poisson and friction operators. $\frac{\mathsf{D}E_n}{\mathsf{D}\boldsymbol{z}_n}$ and $\frac{\mathsf{D}S_n}{\mathsf{D}\boldsymbol{z}_n}$ represent the discrete gradients of the energy and the entropy. Finally, the identified structure must be subject to:

$$\mathsf{L}_n \cdot \frac{\mathsf{D}S_n}{\mathsf{D}\boldsymbol{z}_n} = \mathbf{0}, \quad \mathsf{M}_n \cdot \frac{\mathsf{D}E_n}{\mathsf{D}\boldsymbol{z}_n} = \mathbf{0}, \tag{6}$$

thus ensuring the thermodynamical consistency of the resulting model.

4 STRUCTURE-PRESERVING NEURAL NETWORKS

To construct structure-preserving neural networks, we first train standard feedforward networks of fully-connected layers with no cyclic connections so as to identify the metriplectic structure of the system under scrutiny. However, to unveil the intrinsic dimensionality of the system, regardless of the dimensionality of the data, we employ a sparse autoencoder. A sketch of the proposed architecture is depicted in Fig. 1.

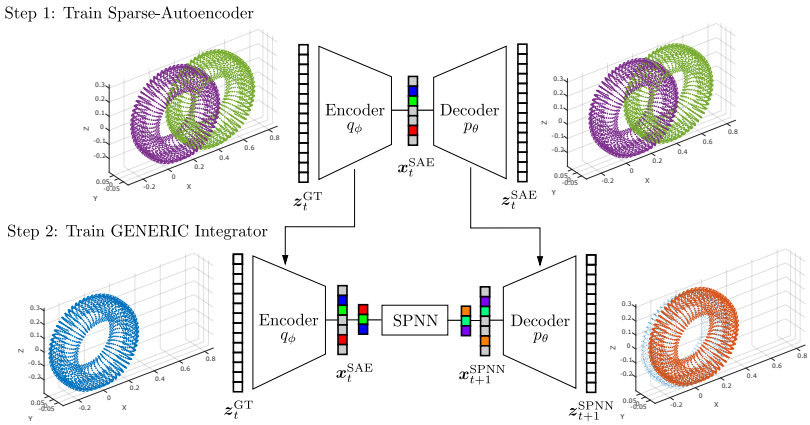

Figure 1: Sketch of the proposed algorithm for the rolling tyre problem, Section 5. Step 1: A sparse autoencoder (SAE) is trained with time snapshots of a ground truth physical simulation, in order to learn an encoded representation of the full-order space. Step 2: A structure-preserving neural network (SPNN) is trained to integrate the full time evolution of the latent variables, consistently with the GENERIC structure of the underlying physics of the problem.

The loss function for our neural network will therefore include three terms:

- **Data loss**: measuring the agreement between the network output and the real data,
$$\mathcal{L}_n^{\text{data}} = ||\boldsymbol{x}_{n+1}^{\text{SAE}} - \boldsymbol{x}_{n+1}^{\text{SPNN}}||_2^2. \tag{7}$$
- **Fulfillment of the degeneracy conditions**: This is the inductive bias that accounts for the degeneracy conditions, Eq. (6) in order to ensure the thermodynamic consistency of the solution,
$$\mathcal{L}_n^{\text{degen}} = ||\mathsf{L}_n \cdot \mathsf{D}\mathsf{S}_n||_2^2 + ||\mathsf{M}_n \cdot \mathsf{D}\mathsf{E}_n||_2^2. \tag{8}$$
- **Regularization**: In order to avoid overfitting, an extra L2 regularization term $\mathcal{L}^{\text{reg}}$ is added to the loss function,
$$\mathcal{L}^{\text{reg}} = \sum_{l}^{L} \sum_{i}^{n^{[l]}} \sum_{j}^{n^{[l+1]}} (w_{i,j}^{[l],\text{SPNN}})^2. \tag{9}$$

Data are split in a partition of train snapshots ($N_{\text{train}} = 80\%$ of the database snapshots) and test snapshots ($N_{\text{test}} = 20\%$ of the database snapshots) so that $N_T = N_{\text{train}} + N_{\text{test}}$.

5 PERFORMANCE TEST

We consider a simulation of the transient response of a rolling tire ($D_{\text{tire}} = 0.66$ m) impacting with a curb ($h_{\text{curb}} = 0.025$ m). The tire is inflated at 200 kPa, and is subjected to a load of 3300 N in the vertical axis. The free rolling conditions are determined in a separated analysis, corresponding to $\omega = 8.98$ rad/s for a translational horizontal velocity of $v_0 = 10$ km/h (see Fig. 2). More details can be found at Hernandez et al. (2020).

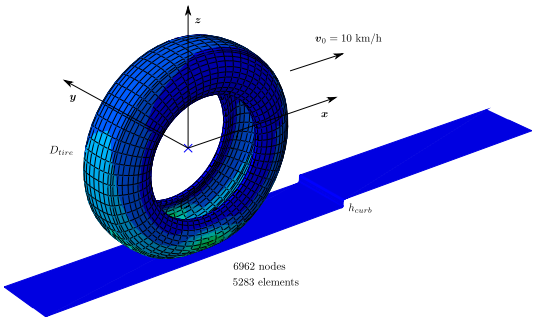

Figure 2: Hyperelastic tire rolling towards a curb. 3D position, 3D velocity and Cauchy stress tensor components are tracked for the total of 4140 selected nodes.

The number of hidden layers in both the encoder and decoder is $N_h^{\text{SAE}} = 2$ in the three variables with 40 neurons each in position and velocity, and 80 neurons in the stress tensor, with ReLU activation functions and linear in the first and last layers. The number of bottleneck variables is set to $N_{d,q} = 10$ for the position, $N_{d,v} = 10$ for velocity and $N_{d,\sigma} = 20$ for the stress tensor. Thus, the total dimensionality of the bottleneck latent vector is $N_d = N_{d,q} + N_{d,v} + N_{d,\sigma} = 40$. Results in the prediction of a simulation not seen before by the system arre shown in Fig. 3, where the time evolution of the state variables $\boldsymbol{z}$ is shown.

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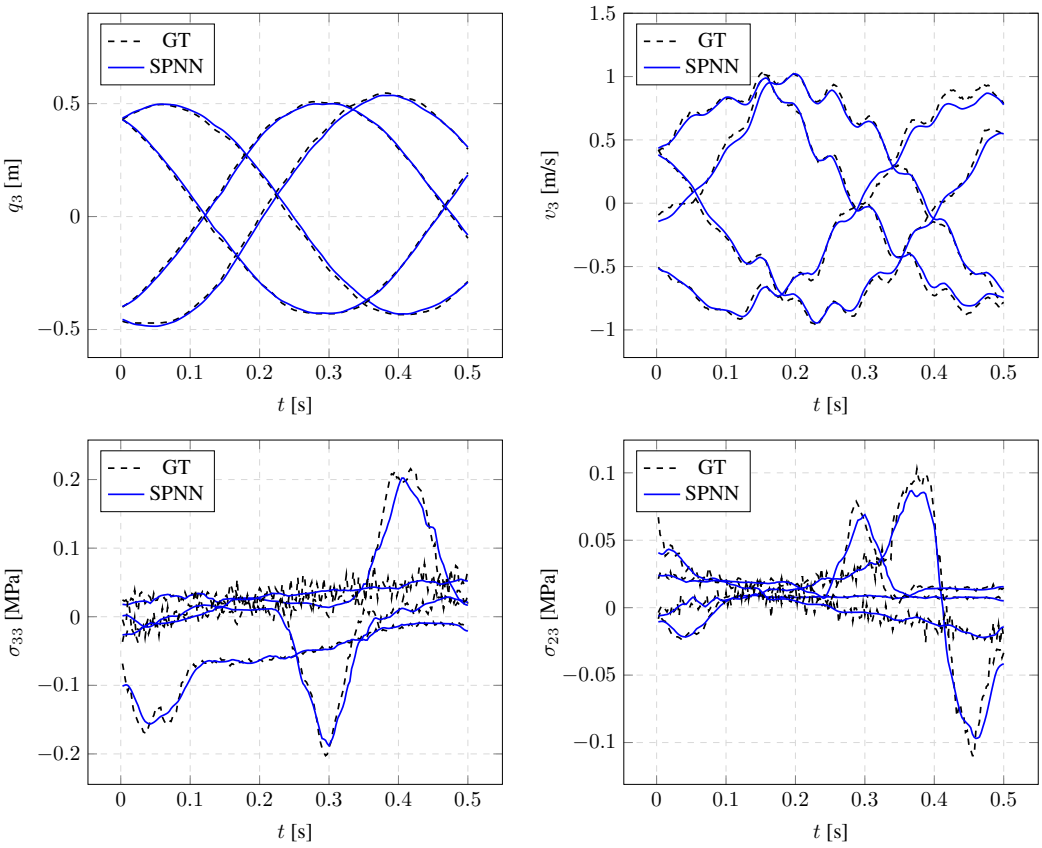

Figure 3: Results of the complete integration scheme (SPNN) with respect to the ground truth simulation (GT) for 4 different nodes and 4 different variables (q_3, v_3, σ_{33} and σ_{23}) of the hyperelastic rolling tire database.

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