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A data-driven method for dissipative thermomechanics

D. Ruiz * **D. Portillo** *,** **I. Romero** *,**

* *Universidad Politécnica de Madrid, Madrid, 28006 Madrid, Spain*
** *IMDEA Materials Institute, Getafe, 28906 Madrid, Spain*

Abstract: We present a method based on quadratic programming for learning dissipative models from data. For that, we take advantage of the metriplectic structure of the system to preserve the two laws of thermodynamcis, i.e. energy conservation and non-decreased entropy. This method can be used in conjunction with EEM integrators to generate structure preserving integrators for dissipative thermomechanics. We illustrate the results by an example.

Keywords: Dissipative systems, GENERIC, Metriplectic systems, Lagrangian and Hamiltonian systems, Convex optimization, Data-driven

1. INTRODUCTION

Structure preserving integrators have been employed with remarkably success in a broad class of dynamic systems. An important subclass of these systems are the Hamiltonian systems. The general formalism of Hamiltonian problems has enabled the development of general structural preserving method to different problems, such as molecular dynamics, Euler equations of fluid flow, nonlinear mechanics of solids, etc.

However, Hamiltonian systems fail when trying to model dissipative systems, such as thermomechanic problems. In this case, the only class of structure preserving methods, to the authors' knowledge, is the Energy-Entropy-Momentum (EEM) integrators presented in Romero (2009), Romero (2010a), Romero (2010b), Portillo et al. (2017) for general thermomechanical systems. These methods are based on two main ingredients: formulatting the problem as a metriplectic system and using discrete derivatives to approximate the driven forces (see Romero (2009) for a complete description). As a consequence the main difficulty of these methods is obtaining the metriplectic structure of the problem, which is not obvious in general, as we will see in section 2.

Methods such as machine learning and data driven have attracted much interest to obtain knowledge from data. In the case of Hamiltonian systems, studies in this area have been presented, e.g. Schmidt and Lipson (2009), Ahmadi et al. (2018). In Schmidt and Lipson (2009), a method to extract all the physics of the problem is presented, but it is computationally expensvie. On the other hand, the approach in Ahmadi et al. (2018) provides a method based on quadratic programming to approximate the Hamiltoninan from data. In the case of solid mechanics recent works Kirchdoerfer and Ortiz (2016) have taken advantage of some fundamental physics of the system to substitute material law modelling with experimental data. Also, in González et al. (2018) and Hernández et al. (2021) the metriplectic structure has been taken into consideration to develop a data-driven method and neural networks that preserve the two laws of thermodynamics for general dissipative systems. However, in these works a non convex optimization problem is used and some structure of the metriplectic operators might be used *a priori* to reduce computational cost.

We propose here a data driven method to extract the metriplectic structure of smooth thermomechanical problems in entropy variables. We extend the method in Ahmadi et al. (2018) to metriplectic systems in entropy variables to approximate the Hamiltonian and also the friction operator from data. The proposed method is based on quadratic programming and preserve the two laws of thermodynamics, i.e. energy conservation and non-decreased entropy. Also, other *a priori* known simmetries can be added.

The article is organized as follows. A brief summary of the GENERIC formalism for thermomecanical systems is presented in section 2. In section 3, we propose the data driven method based on quadratic programming for approximating both the Hamiltonian and the friciton operator. In section 4 we show an example to illustrate the proposed method. Finally, section 5 closes the article with the most relevant results and the future work.

2. THE GENERIC FORMALISM FOR THERMOMECHANICS

GENERIC was introduced by Grmela and Öttinger Grmela and Öttinger (1997); Öttinger and Grmela (1997) for describing thermodynamical systems away from equilibrum. It provides a complete framework for the mathematical description of metriplectic systems Morrison (1986), including very general thermomechanical models (see Öttinger (2005) for a complete account of the theory). Next, we summarize the main ingredients of GENERIC, defining the notation for the remainder of the article.

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2.1 Thermodynamic state and governing equations

The thermodynamic state of an isolated system is described by a variable $x \in \Sigma$, where Σ is the *state space*, a set which we assume has the structure of a differentiable manifold, and whose tangent and cotangent bundles are denoted, respectively, $T\Sigma$ and $T^*\Sigma$. The system must also possess energy and entropy densities, which are described by differentiable functions $E, S \in \mathcal{F}$, the space of differentiable functions defined on Σ. According to GENERIC, the thermodynamic description of an arbitrary system is completed with two algebraic or differential operators

$$L : T^*\Sigma \to T\Sigma \ , \qquad M : T^*\Sigma \to T\Sigma, \tag{2.1}$$

that determine the evolution in time of this system by a differential equation of the form:

$$\dot{x} = L(x)\, \boldsymbol{d}E(x) + M(x)\, \boldsymbol{d}S(x), \tag{2.2}$$

where $\boldsymbol{d} : \mathcal{F} \to T^*\Sigma$ denotes the exterior derivative and $\dot{x} : \Sigma \to T\Sigma$ is the vector field of time derivatives of the state variables.

The operators $L, M : T^*\Sigma \to T\Sigma$ cannot be arbitrary, since the system is constrained to verify the two laws of thermodynamics. First, for every $x \in \Sigma$, $L(x)$ must define a bilinear operation $\{\cdot,\cdot\} : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$, through the relation:

$$\{f, g\}(x) = \boldsymbol{d}f(x) \cdot L(x)\boldsymbol{d}g(x) \ , \tag{2.3}$$

where $f, g \in \mathcal{F}$, and this operation must be a *Poisson bracket*. On the other hand, the operator $M(x)$ defines another bilinear operation $[\cdot,\cdot] : \mathcal{F} \times \mathcal{F} \to \mathbb{R}$ through

$$[f, g](x) = \boldsymbol{d}f(x) \cdot M(x)\boldsymbol{d}g(x) \ , \tag{2.4}$$

for every f, g in $\mathcal{F}$. This second operation must be symmetric, positive semidefinite and is referred to as a *dissipative bracket*.

The evolution equations can be written as

$$\dot{f} = \{f, E\} + [f, S], \tag{2.5}$$

for every $f \in \mathcal{F}$. In addition to the previously stated properties, the Poisson and dissipative brackets must satisfy the *orthogonality conditions*:

$$0 = \{S, f\}, \qquad 0 \in [E, f], \tag{2.6}$$

for every $f \in \mathcal{F}$. In terms of the operator L, the Poisson orthogonality of the entropy can be reformulated as

$$L(x)\boldsymbol{d}S(x) = 0 \ . \tag{2.7}$$

The orthogonality of the energy is expressed by the relation

$$M(x)\boldsymbol{d}E(x) = 0 \ . \tag{2.8}$$

Since the part of the vector field $\dot{x}$ associated with L is orthogonal to the entropy, we call this the *reversible contribution* to the dynamics of the system; likewise, the part generated by M is the *irreversible part* of the vector field $\dot{x}$. Combining Eqs. (2.5) and (2.6), it is straightforward to show that energy E and the entropy S are, respectively, preserved and non-decreased by the flow.

2.2 GENERIC systems for thermomechanics solids in entropy variables

From now on we consider thermodynamic systems of a restricted class for which their state can be described by the variables $x = (q, p, s)$, where q denotes the position, p the momentum, and the entropy density s. We note here that all these variables are arrays, $z = \{z_i\}_{i=1}^{N_z} \quad z = q, p, s$. This class of systems encompasses, for example, standard models for thermoelastic solids (see, e.g., Maugin (1992)). With this description, the exterior derivative of an arbitrary function $f \in \mathcal{F}$ can be expressed as

$$\boldsymbol{d}f(x) = \frac{\partial f}{\partial q}(x)\boldsymbol{d}q + \frac{\partial f}{\partial p}(x)\boldsymbol{d}p + \frac{\partial f}{\partial s}(x)\boldsymbol{d}s, \tag{2.9}$$

where $\{\boldsymbol{d}q, \boldsymbol{d}p, \boldsymbol{d}s\}$ form a basis of the cotangent space $T_x^*\Sigma$. As a result of this choice of coordinates, the *linear* operators $L(x)$ and $M(x)$ must have a block structure and we can write the Poisson and friction operators as

$$\begin{aligned} L &= \begin{bmatrix} L_{qq} & L_{qp} & L_{qs} \\ L_{pq} & L_{pp} & L_{ps} \\ L_{sq} & L_{sp} & L_{ss} \end{bmatrix} \\ M &= \begin{bmatrix} M_{qq} & M_{qp} & M_{qs} \\ M_{pq} & M_{pp} & M_{ps} \\ M_{sq} & M_{sp} & M_{ss} \end{bmatrix} \end{aligned} \tag{2.10}$$

where the dependency on x has been omitted for simplicity. We omit it in the rest of the article.

For some particular systems and entropy variables, further simplifications in these block structures are possible. For the case of the Poisson operator, the symplectic stratification theorem Marsden and Ratiu (1994) assures that it can be written as the cosymplectic form for some local coordinate system. Assuming (q, p, s) form this local coordinate system, we can write L as

$$L = \begin{bmatrix} 0 & I & 0 \\ -I & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{2.11}$$

This form of the Poisson operator is physically justified by the fact that any dissipative effect is only related to the friction operator. This is the case for the entopies (by definition) and the internal variables, which are associated with dissipative effects.

On the other hand, since the dynamics of (q, p) are fully described by the reversible part, only the blocks of the friction operator M associated with irreversible processes are not zero. So, we can write M as

$$M = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & M_{ss} \end{bmatrix} \tag{2.12}$$

Finally, the exterior derivatives of the energy and the entropy take the following form

$$\boldsymbol{d}E = \left(\frac{\partial E}{\partial q}, \frac{\partial E}{\partial p}, \frac{\partial E}{\partial s}\right)^T \quad , \quad \boldsymbol{d}S = (0, 0, 1)^T \tag{2.13}$$

It is worth to note that with these simplifications, S trivially satisfies the orthogonality condition (2.8)

To sum up, the main goal of this work is finding approximated expressions of E, $\widehat{E}$, and M, $\widehat{M}$, for systems that can be written as explained in this section. These expressions should preserve some structural properties of a metriplectic system. In particular, we impose $\widehat{M}$ to be skewsymmetric and $\widehat{E}$ to satisfy the orthogonality condition $\widehat{M}\boldsymbol{d}\widehat{E} = 0$. These properties, as well as a relaxation

on $\widehat{M}$ to be positive semidefinite which will be explained in the next section, are the necessary conditions for preserving the two laws of thermodynamics.

3. OPTIMIZATION PROBLEM

In this section, we propose a method based on convex optimization for approximating the metriplectic structure of the class of dissipative systems explained in the previous section. That is, given $\{t_k, x(t_k), \dot{x}(t_k)\}_{k=1}^{N}$, find approximatios of the friction operator, $\widehat{M}$ and the Hamiltonian $\widehat{E}$.

For that purpose, we define $\mathcal{F}_{\widehat{e}}$, $\mathcal{F}_{\widehat{M}_{SS}}$ functional spaces with basis $\left\{\Phi^{E}(q,p,s)\right\}_{i=1}^{d_E}$, $\left\{\Phi^{M_{SS}}(q,p,s)\right\}_{i=1}^{d_{M_{SS}}}$. Then, the approximated Hamiltonian $\widehat{E}$ is defined to belong to $\mathcal{F}_{\widehat{E}}$ and every nonzero entry of M, $m_{ss}^{lm} \quad l,m \in \{S\}$ is approximated by a function in $\mathcal{F}_{\widehat{M}_{ss}}$, denoted $\widehat{m}_{ss}^{lm}$.

The requirements on the functional spaces depend on the nature of the dynamics, as well as on numerical reasons. For example, for the case of the Hamiltonian, the basis should be a set of differenciable functions because the driven force of the reversible part of the process is the derivative of the Hamiltonian. On the other hand, avoiding numerical oscilations can justify the choice of a polynomial basis with lower order.

Then, the approximated Hamiltonian has the form

$$\widehat{E}(q,p,s) = \sum_{i=1}^{d_E} \alpha_i^E \, \Phi_i^E(q,p,s) \tag{3.1}$$

where $\{\alpha_i\}_{i=1}^{d_E}$ is a set of constants. And the approximated entries of the friction operator can be written as

$$\widehat{m}_{ss}^{lm}(q,p,s) = \sum_{i=1}^{d_{M_{ss}}} \beta_i^{M_{ss}^{lm}} \, \Phi_i^{M_{ss}}(q,p,s) \tag{3.2}$$

where $\left\{\beta_i^{M_{ss}^{lm}}\right\}_{i=1}^{d_{M_{ss}}}$ is a set of constants. Therefore, obtaining the approximated functions is equivalent to obtaining the set of variables $\left\{\left\{\alpha_i^E\right\}_{i=1}^{d_E}, \left\{\beta_i^{M_{ss}^{lm}}\right\}_{i=1}^{d_{M_{ss}}}\right\}$

Taking into accout the metriplectic structure of the system we can now define an optimization problem for approximating the dynamics. First, the reversible part is driven by the derivative of the Hamiltonian and the Poisson operator, so substituting (3.1) into (2.2) we have

$$\begin{aligned} \dot{q} &= \sum_{i=1}^{d_E} \alpha_i^E \frac{\partial \Phi_i^E}{\partial p} \\ \dot{p} &= -\sum_{i=1}^{d_E} \alpha_i^E \frac{\partial \Phi_i^E}{\partial q} \end{aligned} \tag{3.3}$$

Using the given data, $\{(t_k, x_k, \dot{x}_k)\}_{k=1}^{N}$, we can define the following functions

$$\begin{aligned} \eta_{q_k} &= \dot{q}_k - \sum_{i=1}^{d_H} \alpha_i^E \frac{\partial \Phi_i^E(q,p,s)_k}{\partial p} \\ \eta_{p_k} &= \dot{p}_k + \sum_{i=1}^{d_H} \alpha_i^E \frac{\partial \Phi_i^E(q,p,s)_k}{\partial q} \end{aligned} \tag{3.4}$$

These functions allow us to define a cost function that measures the deviation of the approximated Hamiltonian from the reversible dynamics driven force

$$\eta_L = \frac{1}{N} \sum_{k=1}^{N} \left(\frac{\eta_q \cdot \eta_q}{\bar{\dot{q}}} + \frac{\eta_p \cdot \eta_p}{\bar{\dot{p}}} \right) \tag{3.5}$$

where $\bar{\dot{q}}$ and $\bar{\dot{p}}$ are some characteristic value of the position and the momentum velocities respectively. In this work we take the mean plus the standard deviation.

On the other hand, if we look at the irreversible part of the system and we substitute (3.2) into (2.2), we get the following evolution equations

$$\dot{S} = \textstyle\sum_{i=1}^{d_{M_{ss}}} \beta_i^{M_{ss}^{lm}} \, \Phi_i^{M_{ss}^{lm}}(q,p,s)_k \tag{3.6}$$

Similar to (3.4) we can define the function

$$\eta_{s_k} = \dot{s}_k - \sum_{i=1}^{d_{M_{ss}}} \beta_i^{M_{ss}^{lm}} \, \Phi_i^{M_{ss}^{lm}}(q,p,s)_k \tag{3.7}$$

And the corresponding cost function that measures the error on the approximated friction operator can be defined as

$$\eta_M = \frac{1}{N} \sum_{k=1}^{N} \left(\frac{\eta_s \cdot \eta_s}{\bar{\dot{s}}} \right) \tag{3.8}$$

where $\bar{\dot{s}}$ is defined analogously to $\bar{\dot{q}}$ and $\bar{\dot{p}}$.

Once we have defined (3.5) and (3.8), we need to minimize those functions subject to some constraints. In particular we want the Hamiltonian to be orthogonal to the friction operator and also to ensure non-decreasing entropy in the given data. We can define the following optimization problem

$$\begin{aligned} \min_{\alpha^E, \beta^{M_{ss}}} \quad & \eta_L + \eta_M \\ \text{s.t.} \quad & \boldsymbol{d}S\widehat{M}\boldsymbol{d}S \geq 0 \\ & \widehat{M}\boldsymbol{d}\widehat{E} = 0 \end{aligned} \tag{3.9}$$

The above optimization problem presents the following propperties:

- The objective function $\eta = \eta_L + \eta_M$ is a convex function because $\{\eta\}_{i \in \{x\}}$ are affine functions of α and β, the square of an affine function is convex and the sum of convex functions is convex.
- It is not a convex problem because the orthogonality constraint is not linear and we cannot ensure that the solution set is convex.
- $\widehat{M}$ is not forced to be positive semidefinite, but the constraint $dS\widehat{M}dS = (0,0,1)^T\widehat{M}(0,0,1)^T$ guarantees the second law of thermodynamics

In order to obtain a convex optimization problem, we split problem (3.9) into two separate convex problems. First, we solve friction operator subject to entropy production constraint

$$\begin{aligned} \min_{\beta^{M_{ss}}} \quad & \eta_M \\ \text{s.t.} \quad & \boldsymbol{d}S\widehat{M}\boldsymbol{d}S \geq 0 \end{aligned} \tag{3.10}$$

Once $\widehat{M}$ is known, we solve the Hamiltonian part subjecto to orthogonality condition

$$\begin{aligned} \min_{\alpha^E} \quad & \eta_L \\ \text{s.t.} \quad & \widehat{M}\boldsymbol{d}\widehat{E} = 0 \end{aligned} \tag{3.11}$$

Notation	Description	1/a	2/b
q_0	Initial position	$\left(\frac{5\sqrt{2}}{2}, \frac{5\sqrt{2}}{2}\right)$	$(0, 5)$
p_0	Initial momentum	$(0, 1)$	$(0, 0)$
θ_0	Initial temperature	380	360
m	Mass	1	1
λ^{ref}	Reference length	0.1	0.1
H	Stiffness	1	1
θ_{ref}	Reference temperature	320	320
k	Conductivity	$\frac{1}{2}$	
c	Heat capacity	10	10

Table 1. Data for numerical examples

The constraints in problems (3.10) and (3.11) are linear (note that $\widehat{M}$ is already known in problem (3.11)) so these two problems are convex optimization problems and optimality is then guaranteed. In fact, they are both quadratic programs and specific solvers for these type of problems can be used.

We note here that the order in the splitting is because of the nature of the constraints. The orthogonality constraint should be understood as a constraint on the Hamiltonian and not on the friction operator. If we know both the dynamics (the given data) and the irreversible driven force (derivative of entropy), the structure of M should be defined and problem (3.10) obtains the best entropy producer fit of M. Then, the best fit of the reversible dynamics is obtained subject to irreversible independency ($M\boldsymbol{d}\widehat{E} = 0$). If we would split it the other way around, i.e. solving first the Hamiltonian part with no restrictions and secondly the irreversible part with entropy production and orthogonality constraints, we would overconstrain the friction part and the irreversible part of the dynamics might not be accurate.

4. NUMERICAL RESULTS

We apply the previously developed ideas to a symple problem. The system under consideration is an isolated, plane, thermoelastic double pendulum. The model problem is depicted in figure (4.1) and the problem conditions are summarized in table (1). The metriplectic structure of this problem is well known (see Romero (2009) for details). We briefly summarize the main concepts.

The entropy variables for the problem are

$$x = (q, p, s) = (q_1, q_2, p_1, p_2, s_a, s_b) \tag{4.1}$$

The total energy of the system is

$$E = \frac{|p_1|^2}{2m_1} + \frac{|p_2|^2}{2m_2} + e_a(x) + e_b(x) \tag{4.2}$$

where $e_a(x)$ and $e_b(x)$ are the internal energies of the springs, which can be defined as

$$e_i(x) = H_i \frac{(\lambda_i - \lambda_i^{ref})^2}{2} + c_i(\theta_i - \theta_i^{ref}) \quad i = a, b \tag{4.3}$$

where $\lambda_a = |q_1|$, $\lambda_b = |q_2 - q_1|$ and the temperatures are functions of the entropy

$$\theta_i = \theta_i^{ref} \exp \frac{s_i}{c_i} \quad i = a, b \tag{4.4}$$

We solve the optimization problems (3.10) and (3.11) to obtain the dynamics of the system. The given data is a set of 160 points equally spaced in time with $\Delta t = \frac{1}{20}\frac{2\pi}{\sqrt{\frac{H}{m}}}$. We use polynomial basis for both problems and we take the minimum order within acceptable errors: in this case $n_{M_{ss}} = 1$ and $n_E = 2$.

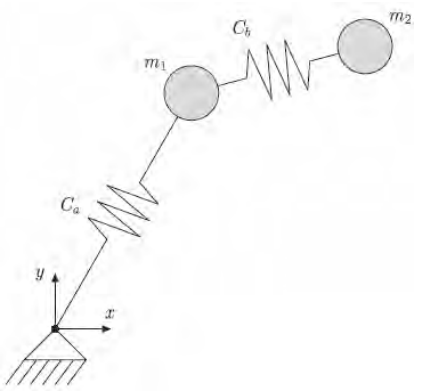

Fig. 4.1. Themoelastic double pendulum problem

Figures (4.2), (4.3), (4.4) illustrate the results for the state evolution of the system for the given data (in dashed line) and for future times (solid line). Figure (4.5) shows the maximum error with sign, defined as the maximum of $\frac{|\dot{x}_k - \widehat{\dot{x}}_k|}{\bar{\dot{x}}_k}$ $x = q, p, s$ with the corresponding sign of the difference, in each time step. The error remains small even for times greater than twice the maximum of the given data. The energy orthogonality constraint is satisfied up to numerical error (10^{-16}) and the non-decreased entropy constraint remains within acceptable margins, obtaining small fluctuations for almost stationary entropy.

However it should be noted that this excellent global agreement is because of the problem conditions. In this case, the Hamiltonian is almost quadratic due to the large initial springs elongation and the entropy changes are small. For other problems or conditions, the order of the polynomial basis might be higher and it might generate spurious oscillations and/or less accurate global results.

5. CONCLUDING REMARKS

We have presented a novel approach for aproximating a limited class of dissipative systems from data. This class of systems encompasses, for example, standard models for thermoelastic solids. The method we introduced takes advantage of the metriplectic structure of the system to generate convex optimization problems that guarantees optimality of the solution, in contrast to González et al. (2018). In addition, these convex problems are quadratic programs that can be solved in an efficient manner and there is no need of neural networks as in Hernández et al. (2021).

The presented approach can be used in conjunction with the preserving numerical methods described in Romero (2009) to obtain thermodynamically consistent numerical schemes directly from data, avoiding the modeling step.

Future work will focus on extending this method to other dissipative systems with smooth or non-smooth dissipative mechanisms. Moreover, experimental data is always

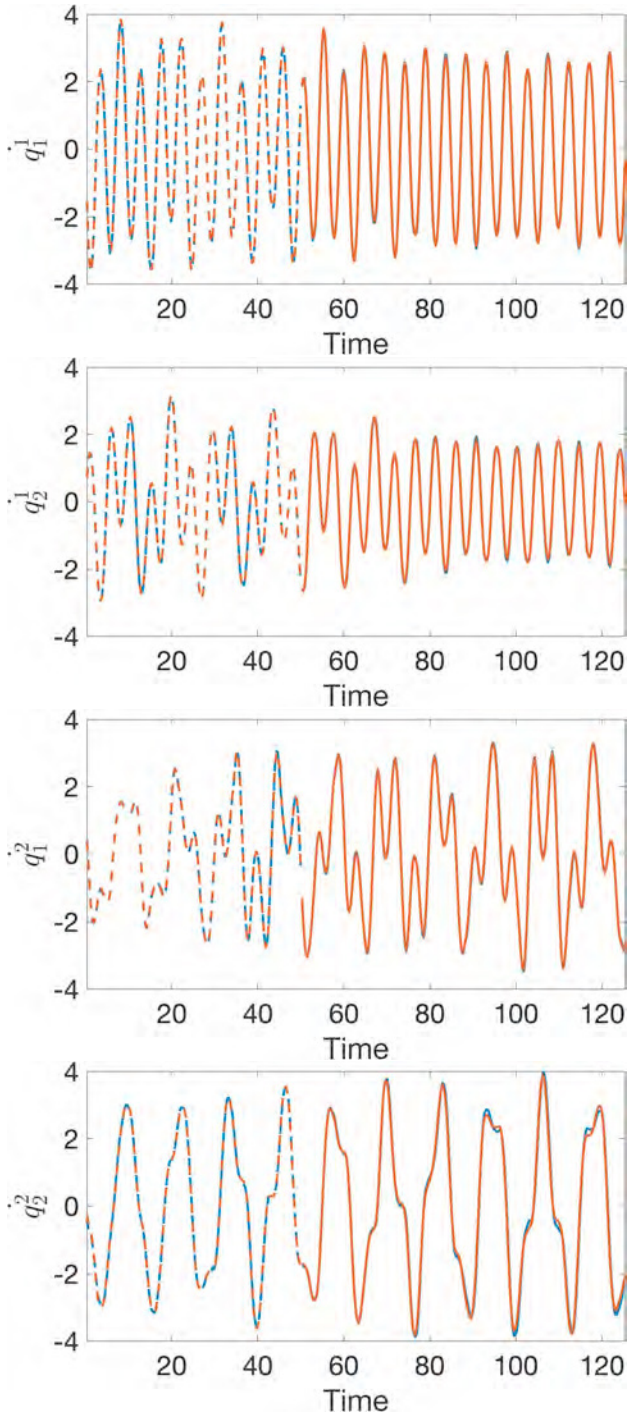

Fig. 4.2. Position velocities (orange) and their approximations (blue). In dashed line, the given data and its approximation. In solid line, the evolution and its approximation in future times

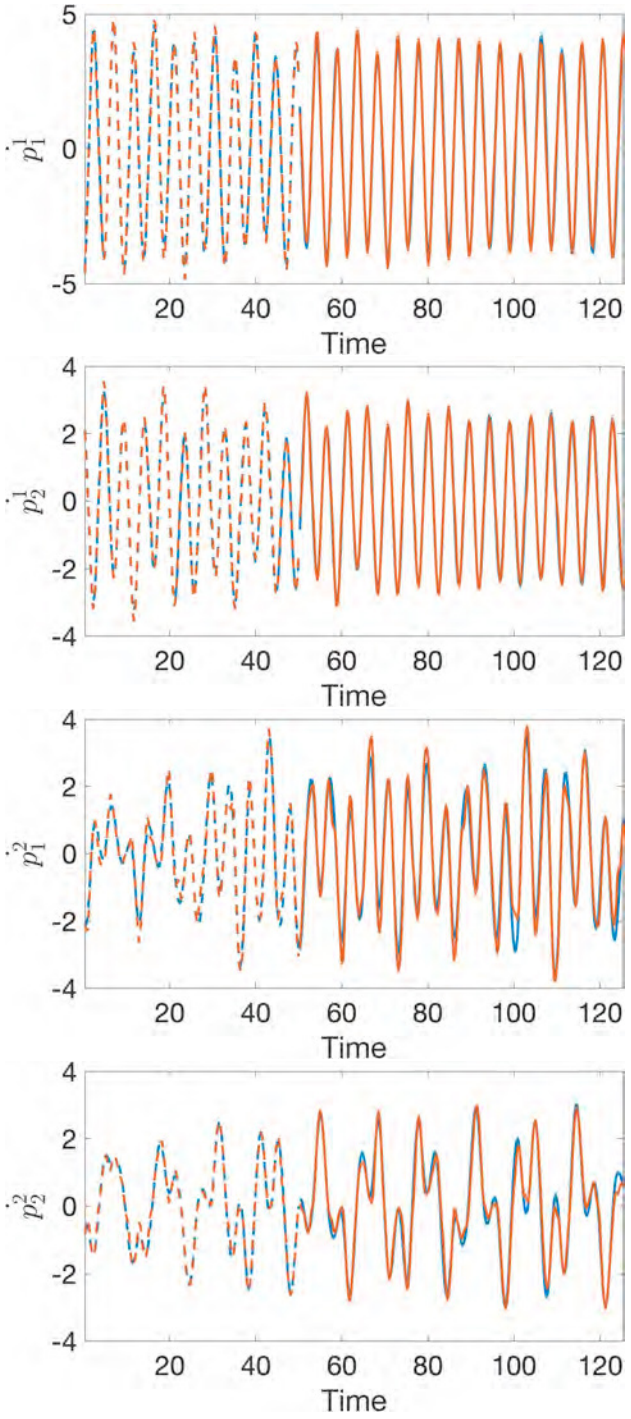

Fig. 4.3. Momentum velocities (orange) and their approximations (blue). In dashed line, the given data and its approximation. In solid line, the evolution and its approximation in future times

corrupted by noise and it should be taken into account in future research.

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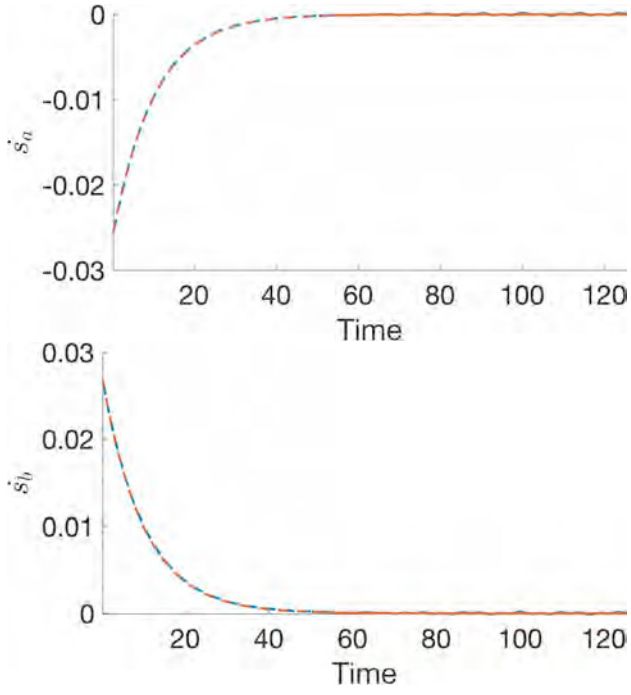

Fig. 4.4. Entropy velocities (orange) and their approximations (blue). In dashed line, the given data and its approximation. In solid line, the evolution and its approximation in future times

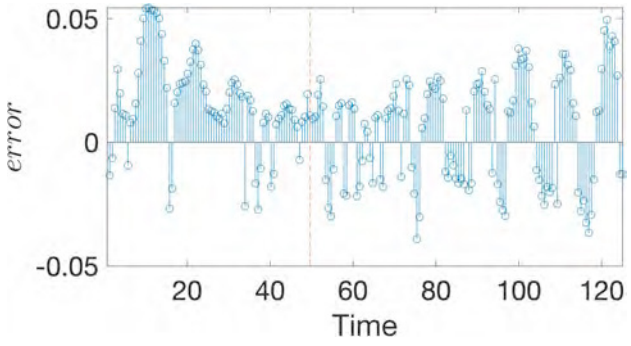

Fig. 4.5. Maximum error with sign, defined as the maximum of $\frac{|\dot{x}_k - \widehat{\dot{x}}_k|}{\dot{x}_k}$ $x = q, p, s$ with the corresponding sign of the difference, in each time step

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